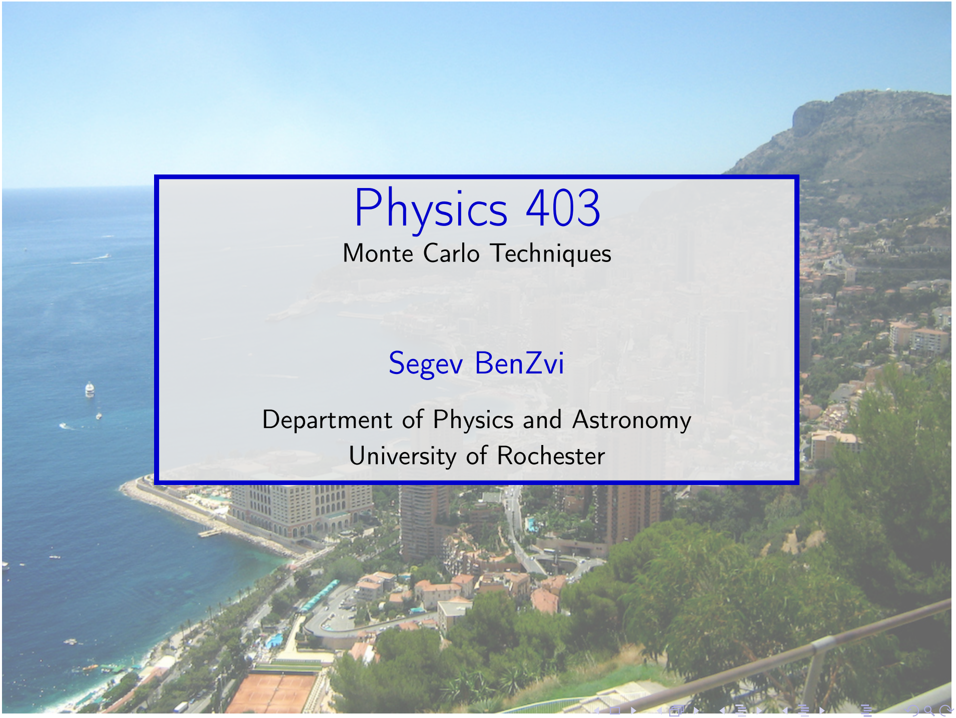

Physics 403

Monte Carlo Techniques

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Simulation and Random Number Generation in Physics

"Monte Carlo" methods are a broad set of techniques for calculating probabilities and related quantities using sequences of random numbers.

- Simulate physical systems with models of noise and uncertainty
- Simulate data with known inputs to stress-test your analysis ("data challenges"). Can be quite extensive...
- Perform calculations that cannot be done analytically or with a deterministic algorithm. E.g., function minimization, or many high-dimensional integrals
- Inverse Monte Carlo: estimate best-fit parameters with uncertainties using many simulated data sets – avoid explicit and difficult uncertainty propagation

All this depends upon the generation of (pseudo-)random numbers. This means you MUST understand how random number generators (RNGs) work!

Example Simulation from U of R Faculty

Physics of granular materials which become rigid with increasing density ("jamming" transition) [1]:

PRL **113,** 148002 (2014) PHYSICAL REVIEW LETTERS week ending 3 OCTOBER 2014

Universality of Jamming Criticality in Overdamped Shear-Driven Frictionless Disks

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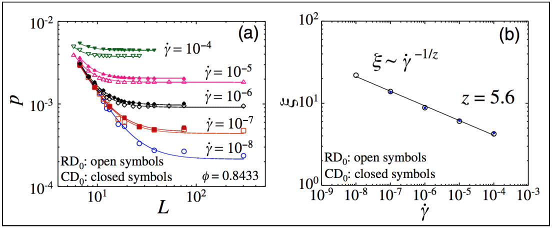
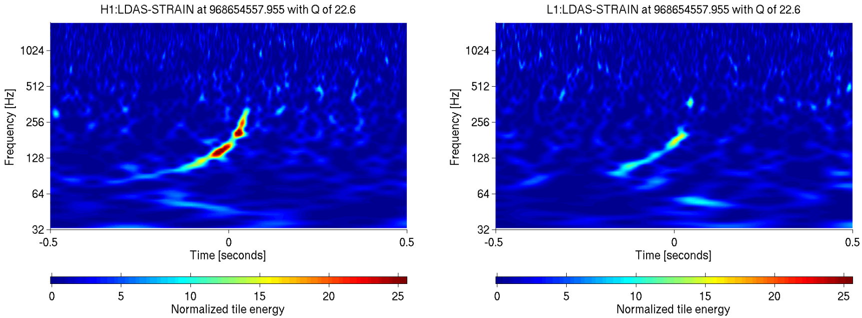
We investigate the criticality of the jamming transition for overdamped shear-driven frictionless disks in two dimensions for two different models of energy dissipation: (i) Durian's bubble model with dissipation proportional to the velocity difference of particles in contact, and (ii) Durian's "mean-field" approximation to (i), with dissipation due to the velocity difference between the particle and the average uniform shear flow velocity. By considering the finite-size behavior of pressure, the pressure analog of viscosity, and the macroscopic friction σ/p, we argue that these two models share the same critical behavior.



Example "Data Challenge"

The Laser Interferometer Gravitational Wave Observatory (LIGO) is (in)famous for carrying out extensive data challenges [2]



Very important to conduct end-to-end "stress tests" in background-dominated analyses. Above: fake binary merger injected into LIGO data stream, 2011

Example of Inverse Monte Carlo

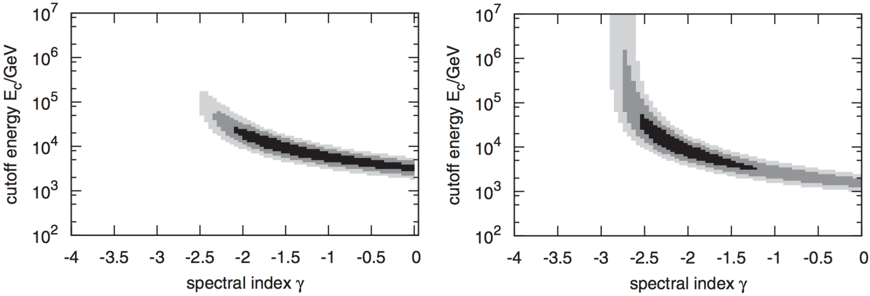
From paper on discovery of cosmic-ray "hot spots" [3]:

Selected for a Viewpoint in *Physics*
PRL **101,** 221101 (2008) PHYSICAL REVIEW LETTERS week ending 28 NOVEMBER 2008

Discovery of Localized Regions of Excess 10-TeV Cosmic Rays

A. A. Abdo,[1] B. Allen,[2] T. Aune,[3] D. Berley,[4] E. Blaufuss,[4] S. Casanova,[5] C. Chen,[6] B. L. Dingus,[7] R. W. Ellsworth,[8] L. Fleysher,[9] R. Fleysher,[9] M. M. Gonzalez,[10] J. A. Goodman,[4] C. M. Hoffman,[7] P. H. Hüntemeyer,[7] B. E. Kolterman,[9] C. P. Lansdell,[11] J. T. Linnemann,[12] J. E. McEnery,[13] A. I. Mincer,[9] P. Nemethy,[9] D. Noyes,[4] J. Pretz,[7] J. M. Ryan,[14] P. M. Saz Parkinson,[3] A. Shoup,[15] G. Sinnis,[7] A. J. Smith,[4] G. W. Sullivan,[4] V. Vasileiou,[4] G. P. Walker,[16] D. A. Williams,[3] and G. B. Yodh[6]

(Milagro Collaboration)



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Pseudo-Random Numbers

- We need to generate sequences of random numbers to model noise and uncertainty.

- Computers are not random, they are deterministic. So how do we get random sequences of numbers?
- Answer: we don't. We get *pseudo*-random sequences and try to use them in clever ways.

Pseudo-Random Number Generators (RNGs)

Linear Congruential Generator

- An old but popular technique of generating pseudo-random number sequences is the linear congruential generator (LCG)
- A sequence of values x_i is generated using the recurrence relation

$$x_{n+1} = (ax_n + c) \bmod m$$

- Generate integers in $[0, m-1]$. The longest sequence with no repeating values, called the **period** of the RNG, is at most m.
- Note: if m is an unsigned integer (`uint32_t` on most systems) then the period will be $2^{32} \approx 4 \times 10^9$. ($2^{64} \approx 10^{18}$.) Most real simulations need orders of magnitude more numbers than this!
- Hull-Dobell Theorem: the full period is achieved iff c and m are co-prime, $a-1$ is divisible by all prime factors of m, and $a-1$ is a multiple of 4 if m is a multiple of 4.

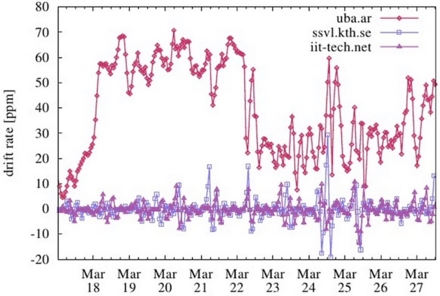
Choosing the Random Seed

- Note that the LCG is deterministic. If you start from the same x_0, a value known as the **seed**, you always get the same sequence.
- The choice of seed can affect the performance of the LCG; i.e., a poor choice could lead to a period $\ll m$.
- Determinism is great for debugging, but if you generate the same numbers over and over you aren't getting a pseudo-random sequence
- **Common mistake**: accidentally hardcoding the seed into your simulation code
- Solution 1: use system clock to choose x_0 via a call to `time(0)`; returns time in seconds since 00:00 UT, 1 Jan 1970 (Unix epoch).
  - Be careful to use the lowest-order bits of the time, including milliseconds. If you just use the seconds, what happens on a computing cluster if multiple jobs start simultaneously?

Good enough for physics simulations, but not cryptography

Choosing the Random Seed

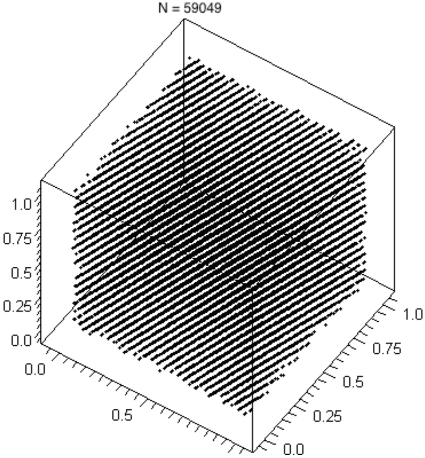
- Solution 2: use the reservoir of random bits in computer's entropy pool, accessible in `/dev/random`. Could be noise measured in a resistor, or clock drift [4], or a peripheral device connected to a source of quantum randomness



- However you generate the seed, make sure you always save the seed value so you can regenerate the sequence later for checks!

Known Issues to Watch For

- The LCG is fast but has some known problems
- Many RNGs can produce hidden long-range correlations between values in the sequence.
- **Ex.**: if you generate n-dimensional points with the LCG, the points will lie on $(n!m)^{1/n}$ hyperplanes [5].
- Clearly random numbers shouldn't do that.
- Could this affect your simulation? Maybe. Depends on your application.



Alternatives to the LCG

Mersenne Twister

- Most popular RNG currently in use is an algorithm called the Mersenne Twister [6], which uses the matrix linear recurrence relation

$$x_{k+n} = x_{k+m} \oplus (x_k^u \mid x_{k+1}^l)\boldsymbol{A}$$

  with $\mid$ = bitwise OR and $\oplus$ = bitwise XOR.

- For n = degree of recurrence, w = word size in bits, and $0 \leq r \leq w-1$ = bits in lower bitmask, the algorithm requires that the period length

$$2^{nw-r} - 1$$

  is a Mersenne prime – a prime number of the form $2^n - 1$.

- The MT implementation in Python and C++ (Boost, ROOT) has period $2^{19937} - 1 \approx 4 \times 10^{6001}$.

Alternatives to the LCG

Xorshift Algorithms

- Another class of RNG is called Xorshift ("XOR-shift"), which depends on a combination of XOR and bit shift operations [7].
- These are extremely fast because XOR and shifting are simple CPU instructions. Example: a $2^{128} - 1$ period algorithm

```
#include <cstdint>

// State variables; start s.t. not all = 0
uint32_t x, y, z, w;

uint32_t xorshift128() {
  uint32_t t = x ^ (x << 11);
  x = y; y = z; z = w;
  return w = w ^ (w >> 19) ^ t ^ (t >> 8);
}
```

Human-Generated Random Numbers

- How good are you at generating random numbers?

Example

Without over-thinking this, take a minute to write down as many random values between 1 and 100 as you can.

- What does the distribution of numbers look like?
- How would you tell if this is really a random sequence? Is it easy to predict parts of the sequence (auto-correlation)?
- Do we need to specify more information to answer this question?

Benford's Law

- If you are like most people, you didn't repeat numbers enough (remember the demon in the cartoon...)
- Also, your "random" sequence is probably uniform between 1 and 100
- However, in many sources of data the values follow a distribution known as Benford's Law: 1 is the leading digit 30% of the time, 2 is the leading digit 18% of the time, etc.
- If you pick a number randomly from the logarithmic number line, it will roughly follow Benford's Law

- This rule can be used to detect fraudulent numbers in elections, accounting (stock prices), and scientific papers.

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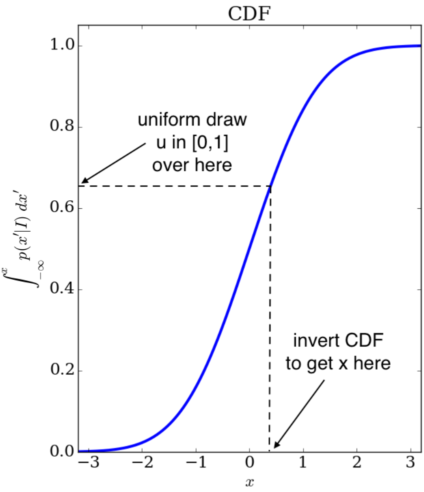
Generating Arbitrary Random Numbers

- All of the RNGs we have discussed will produce uniformly distributed random numbers:
  - LCG generates numbers between $[0, m]$
  - MT generates numbers between $[0, 1]$
- This is great for situations when you want a uniform distribution, but that does not correspond to most physical situations
- Luckily, there are several ways to convert a uniform distribution to an arbitrary distribution:
  1. Transformation or inversion method
  2. Acceptance/rejection method
- The transformation method is generally the most efficient technique, but it is only applicable in cases where the PDF you want is integrable and the CDF can be inverted
- Acceptance/rejection is less efficient but works for any PDF you will want to use for random draws

Transformation/Inversion Method



Given a PDF $p(x|I)$ and its CDF $F(x) = \int_{-\infty}^{x} p(x'|I)\,dx'$:

1. Generate a uniform random number u between $[0, 1]$
2. Compute the value x s.t. $F(x) = u$
3. Take x to be the random draw from $p(x|I)$

In other words, from u and the invertible CDF $F(x)$, the value $x = F^{-1}(u)$ is distributed according to $p(x|I)$.

Transformation/Inversion Method

Exponential Distribution

Example

The PDF of the exponential distribution is

$$p(x|\xi) = \frac{1}{\xi} e^{-x/\xi}$$

and the CDF is

$$F(x) = P(X \leq x|\xi) = \int_0^x \frac{1}{\xi} e^{-x'/\xi}\, dx' = 1 - e^{-x/\xi}$$

Therefore, given $u \in [0, 1]$ we can generate x according to $p(x|\xi)$ by inverting the CDF:

$$u = F(x) = 1 - e^{-x/\xi}$$
$$x = F^{-1}(u) = -\xi \ln(1-u) = -\xi \ln u$$

Limits of the Inversion Method

- Inversion is very efficient and great if you can invert your CDF
- Unfortunately this condition is not fulfilled even for many basic 1D cases

Example

The CDF of the Gaussian distribution is

$$F(x) = \int_{-\infty}^{x} p(x|\mu,\sigma) = \frac{1}{2}\left[1 + \text{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right)\right]$$

The error function cannot be expressed in closed form, though there are numerical approximations to erf and erf^{-1} in `scipy`.

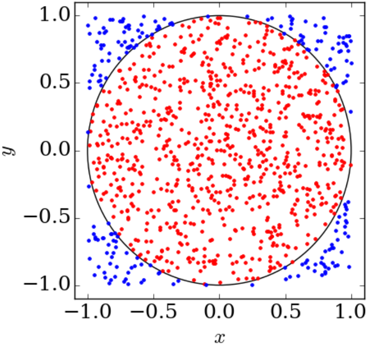
- A trick for complicated PDFs: express the CDF as a tabulated list of values $(u, F(x))$, "invert" it, and interpolate.

Acceptance/Rejection Method

Very old technique; modern form due to von Neumann. AKA "hit and miss," it generates x from an arbitrary $f(x)$ using a so-called instrumental distribution $g(x)$, where $f(x) < Mg(x)$ and $M > 1$ is a bound on $f(x)/g(x)$.

1. Sample x from $g(x)$ and $u \in [0, 1]$.
2. Check if $u < f(x)/Mg(x)$
   - Yes: accept x
   - No: reject x, sample again

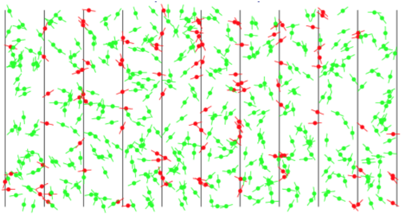
Very easy to implement, no limits on $f(x)$.

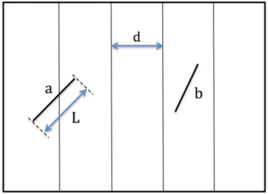


Calculation of π: uniformly generate (x, y) pairs in box, count up points inside the circle. $\pi \approx 4N_{\text{circle}}/N_{\text{box}}$.

Buffon's Calculation of π

- An early variant of the Monte Carlo approach can be seen in Buffon's Needle (1700s), a method of calculating π





Given a need of length L dropped on a plane with parallel lines d units apart, what is the probability the needle will cross a line if $L < d$?

- x is center distance to nearest line; $x \sim U(0, d/2)$
- θ is angle between needle center line: $\theta \sim U(0, \pi/2)$
- Needle crosses line if $x \leq L \sin\theta/2$. Joint PDF:

$$P = \int_0^{\pi/2} d\theta \int_0^{L\sin\theta/2} dx \frac{4}{\pi d} = \frac{2L}{\pi d}$$

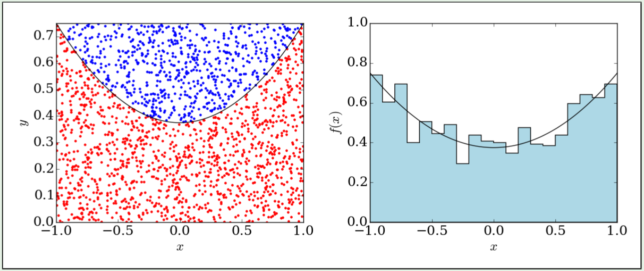
Acceptance/Rejection Method

Sampling from a 1D Distribution

Example

Suppose $f(x) = \frac{3}{8}(1 + x^2)$ for $-1 \leq x \leq 1$. (Aside: do you recognize this distribution?)

- Generate random $x \in [-1, 1]$ and $y \in [0, 0.75]$.
- If $y < f(x)$, populate the histogram with x.



Acceptance/Rejection Method

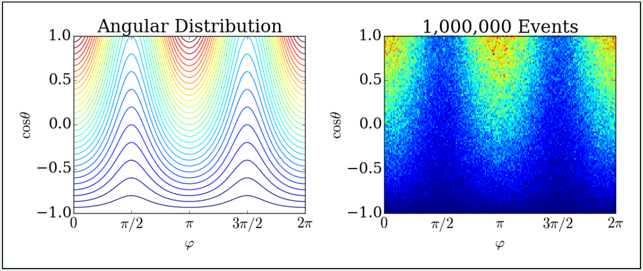
Sampling from a 2D Distribution

Example

Suppose we want to sample from the 2D angular distribution

$$\frac{1}{N}\frac{dN}{d\cos\theta d\varphi} = (1+\cos\theta)(1+\frac{1}{2}\cos 2\varphi)$$

Generate triplets (x, y, z), where $x = \varphi \in [0, 2\pi]$, $y = \cos\theta \in [-1, 1]$, and $z \in [0, 3]$, keeping (x, y) if $z < f(x, y)$:



Limitations of Acceptance/Rejection

Ideally you know f_{max} or normalize $f(x) = p(x|I)$ to have a maximum of 1.

- If not, you'll have to pre-scan the parameter space in advance.

If $f(x)$ ranges over many orders of magnitude, acceptance/rejection can be very inefficient as you'll waste lots of time in low-probability regions. Possible approaches:

- Subdivide x into ranges with different f_{max}.
- Use importance sampling, where you generate random numbers according to a function that evelopes the PDF you really want to sample

Example implementation: `vegas` package in Python, an implementation of the adaptive Monte Carlo VEGAS multi-dimensional integration algorithm [8]

Monte Carlo Integration

- We can also solve integrals (esp. in several dimensions) with Monte Carlo. Mathematically, we approximate the integral by the average of the function of the interval of integration:

$$I = \int_a^b f(x)\ dx \approx (b-a)\,\mathrm{E}\left(f(x)\right)$$

- We take discrete samples of f and let the MC estimate converge to the true integral as the number of samples gets large:

$$\mathrm{E}\left(f(x)\right) = \frac{1}{N}\sum_{i=1}^{N} f(u_i) \rightarrow \frac{1}{b-a}\int_a^b f(u)\ du$$

$$I = I_{\mathrm{MC}} = \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$$

- Error on the result given by the Central Limit Theorem:

$$\sigma = \frac{\sqrt{\mathrm{V}\left(f\right)}}{\sqrt{N}} \propto \frac{1}{\sqrt{N}}.$$

Generating a Gaussian Random Number

How would you generate a Gaussian random number?

1. You can use inversion if you can numerically estimate erf^{-1}.
2. You can use the acceptance/rejection method if you don't mind wasting some calculations.
3. You can exploit the Central Limit Theorem. Sum 12 uniform variables, which approximates a Gaussian of mean $12 \times 0.5 = 6$ and a variance of $12 \times (1/12) = 1$. Subtract 6 to get a mean of zero. This takes even more calculation and isn't exact.
4. Use the polar form of the binormal distribution

$$p(x, y|I) = \frac{1}{2\pi} \exp\left\{-\frac{1}{2}\left(x^2 + y^2\right)\right\}$$

to generate two Gaussian random numbers at once.

Box-Müller Algorithm

Re-express the 2D Gaussian PDF in polar coordinates:

$$\begin{aligned} p(x, y|I)\ dx\ dy &= \frac{1}{2\pi} \exp\left\{-\frac{1}{2}\left(x^2+y^2\right)\right\}\ dx\ dy \\ &= \frac{1}{2\pi} \exp -\frac{r^2}{2} r\ dr\ d\varphi \end{aligned}$$

Then generate an exponential variable $z = r^2/2$, change variables to r, and generate a uniform polar angle φ:

- $z = -\ln u_1$ for $u_1 \sim U(0, 1)$
- $r = \sqrt{2z}$
- $\varphi = 2\pi u_2$ for $u_2 \sim U(0, 1)$

Then $x = r\cos\varphi$ and $y = r\sin\varphi$ are two normally-distributed random numbers. Very elegant! But due to the calls to trascendental functions (`sqrt`, `log`, `cos`, etc.), numerical approaches could be faster in practice...

Generating a Poisson Random Variable

The best way to generate a Poisson random variable is to use inverse transform sampling of the cumulative distribution.

- Generate $u \sim U(0, 1)$
- Sum up the Poisson PDF $p(n|\lambda)$ with increasing values of n until the cumulative sum exceeds u:

$$s_n = \sum_{k=0}^{n} \frac{\lambda^k e^{-\lambda}}{k!}, \quad \text{while } s_n < u$$

- Return the largest n for which $s_n < u$.

This will work quite well until λ gets large, at which point you may start experiencing floating-point round-off errors due to the factor of $e^{-\lambda}$. But for large λ you an start to use the Gaussian approximation.

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