PHY604 Lecture 20

November 14, 2023

Review: More accurate approximations: Crank-Nicholson

- As we saw before, numerically stable does not mean accurate
- More accurate scheme: Crank-Nicholson
  - Average of implicit and explicit FTCS:

$$i\hbar \frac{\psi_j^{n+1} - \psi_j^n}{\tau} = \frac{1}{2} \sum_{k=0}^{N-1} H_{jk} (\psi_k^n + \psi_k^{n+1})$$

  - Where:

$$H_{jk} = -\frac{\hbar^2}{2m} \frac{\delta_{j+1,k} + \delta_{j-1,k} - 2\delta_{jk}}{h^2} + V_j \delta_{jk}$$

- Isolating the *n*+1 term:

$$\Psi^{n+1} = \left(\mathbf{I} + \frac{i\tau}{2\hbar} \mathbf{H} \right)^{-1} \left(\mathbf{I} - \frac{i\tau}{2\hbar} \mathbf{H} \right) \Psi^n$$

Review: Crank-Nicolson for tridiagonal matrices

$$\Psi^{n+1} = \mathbf{Q}^{-1}\Psi^n - \Psi^n, \quad \mathbf{Q} = \frac{1}{2}\left[\mathbf{I} + \frac{i\tau}{2\hbar}\mathbf{H}\right]$$

- Now we can solve for the next timestep by solving the linear system:

$$\mathbf{Q}\chi = \Psi^n$$

- And then:

$$\Psi^{n+1} = \chi - \Psi^n$$

- Recall that for banded matrices, solving linear systems via, e.g., Gaussian elimination, is particularly efficient

Example: Numerical solution of the Schrödinger equation

- Initial conditions: Gaussian wave packet
  - Localized around x_0
  - Width of σ_0
  - Average momentum of: $p_0 = \hbar k_0$

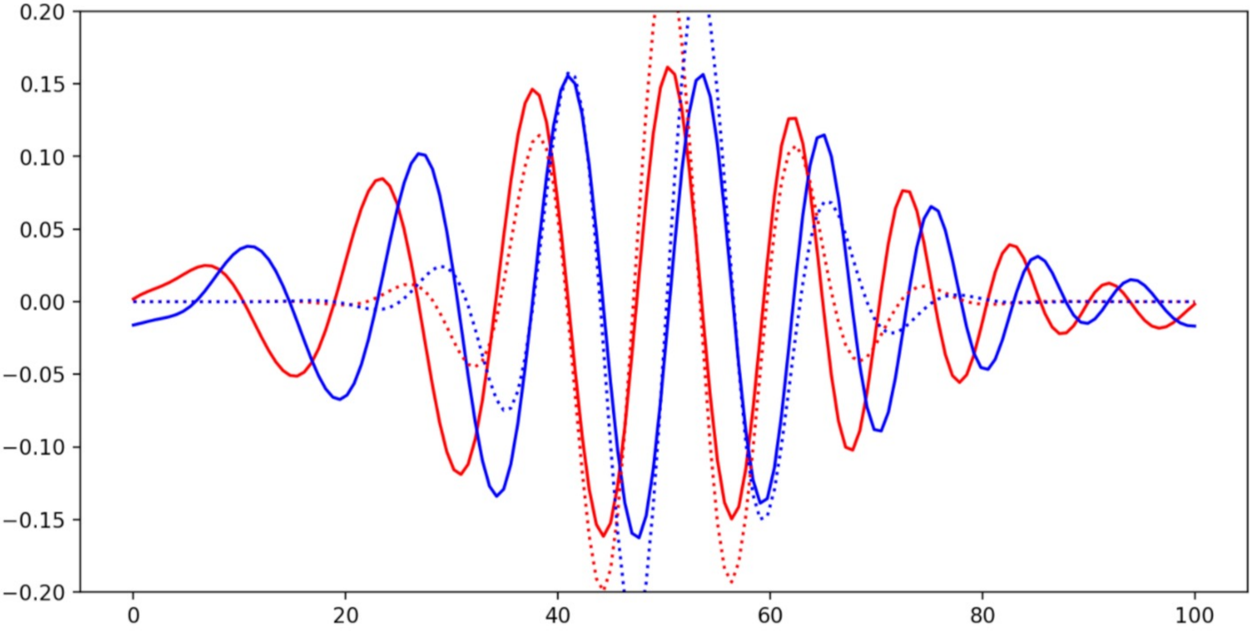
$$\psi(x, t = 0) = \frac{1}{\sqrt{\sigma_0 \sqrt{\pi}}} \exp\left(ik_0 x\right) \exp\left[-\frac{(x - x_0)^2}{2\sigma_0^2}\right]$$

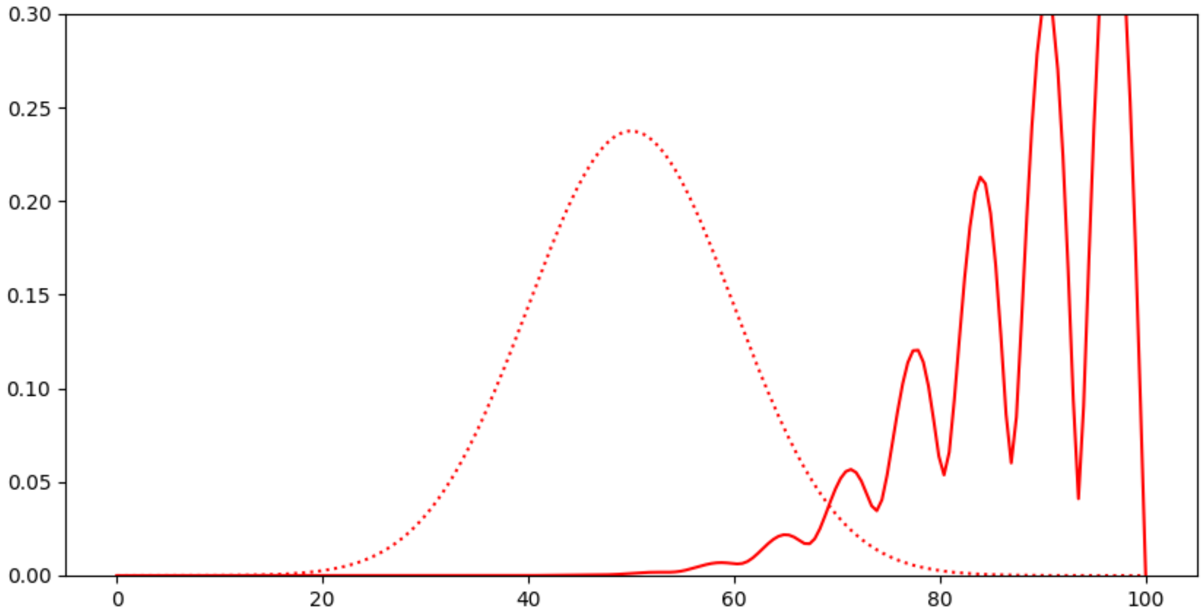
- Which is normalized so that:

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

- Also, has the special property that uncertainty produce $\Delta x \Delta t$ is minimized $(\hbar/2)$

Review: 1D Schrödinger equation



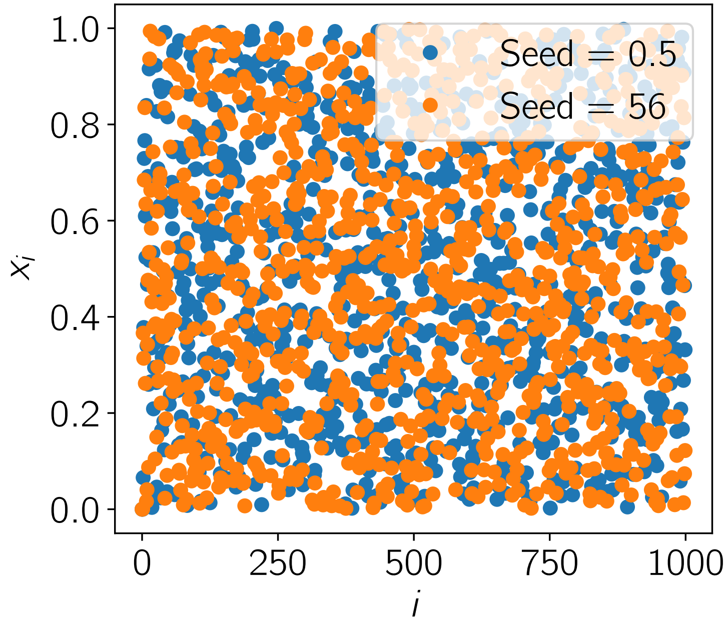


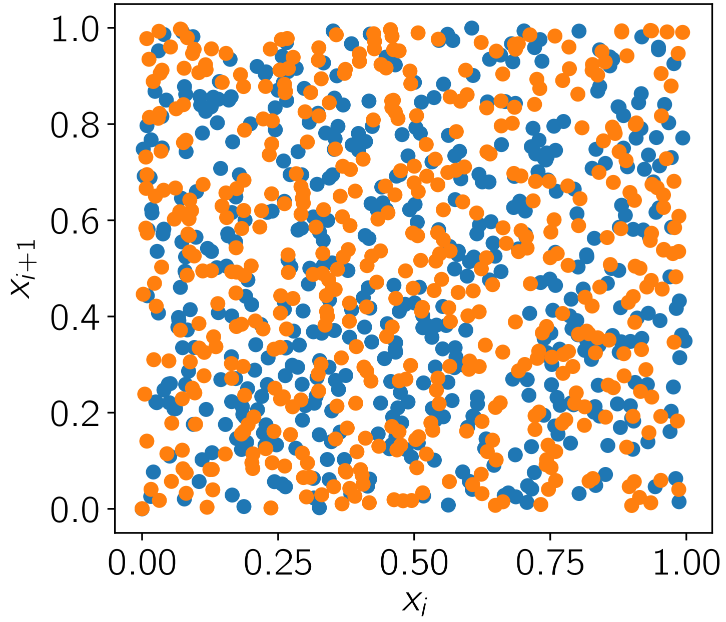
Review: Example of a simple random number generator

- Simplest generator made using the linear congruent scheme
- Random numbers are generated in sequence from the linear relation:

$$x_{i+1} = (ax_i + b) \mod c$$

- *a*, *b*, and *c* are "magic numbers" which determine the quality of the generator
  - Typical choices: $a = 7^5$, $b = 0$, $c = 2^{31} - 1$
  - x_0 is the seed, allows for reproducibility





Today's lecture:
Random numbers and Monte Carlo integration

- Random numbers
- Monte Carlo integration

Random versus pseudo random

- The numbers generated on the previous slide are actually pseudorandom
  - Wikipedia: Appears to be statistically random despite having been produced by a completely deterministic and repeatable process
  - Usually, good enough for most applications (except if you are doing cryptography)
  - Good for testing code, since you get the same values every time
  - Can randomize the seed (e.g., clock time)
- "True" random numbers can be generated by physically random processes
  - Some noise or random process of the computer hardware (e.g., clock time)
  - Thermal noise from a resistor
  - Quantum shot noise
  - Atmospheric noise: https://www.random.org/
  - Lava lamps: https://patents.google.com/patent/US5732138

Random numbers from the RAND corporation

- If you want your random numbers in analog format, you can download a book of them: https://www.rand.org/pubs/monograph_reports/MR1418.html

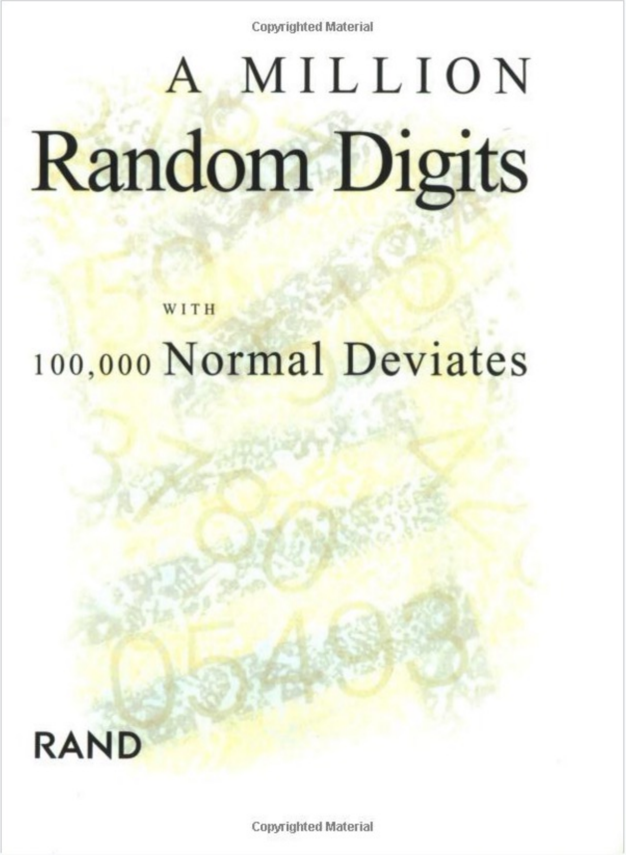


TABLE OF RANDOM DIGITS 3

00100	03991	10461	93716	16894	66083	24653	84609	58232	88618	19161
00101	38555	95554	32886	59780	08355	60860	29735	47762	71299	23853
00102	17546	73704	92052	46215	55121	29281	59076	07936	27954	58909
00103	32643	52861	95819	06831	00911	98936	76355	93779	80863	00514
00104	69572	68777	39510	35905	14060	40619	29549	69616	33564	60780
00105	24122	66591	27699	06494	14845	46672	61958	77100	90899	75754
00106	61196	30231	92962	61773	41839	55382	17267	70943	78038	70267
00107	30532	21704	10274	12202	39685	23309	10061	68829	55986	66485
00108	03788	97599	75867	20717	74416	53166	35208	33374	87539	08823
00109	48228	63379	85783	47619	53152	67433	35663	52972	16818	60311
00110	60365	94653	35075	33949	42614	29297	01918	28316	98953	73231
00111	83799	42402	56623	34442	34994	41374	70071	14736	09958	18065
00112	32960	07405	36409	83232	99385	41600	11133	07586	15917	06253
00113	19322	53845	57620	52606	66497	68646	78138	66559	19640	99413
00114	11220	94747	07399	37408	48509	23929	27482	45476	85244	35159

The 100,000 "normal deviates" cited in the title of this volume constitute a subset of random numbers whose occurrence can be plotted on a bell-shaped curve. RAND legend has it that this seemingly self-contradictory mathematical expression caused the New York Public Library to misshelve the volume in the Psychology section.

Best bet is to use previous implementations for random number generators

- Correlations between random samples can be difficult to detect and cause errors in computations

- See: https://docs.python.org/3/library/random.html or https://numpy.org/doc/stable/reference/random/index.html for details on how python does it

Radioactive decay (see Newman Sec. 10.1)

- One of the quintessential random processes in physics
- Parent atoms decay with characteristic half-life τ
- We will consider ^{208}Tl, which decays to ^{208}Pb with τ = 183.18 sec.

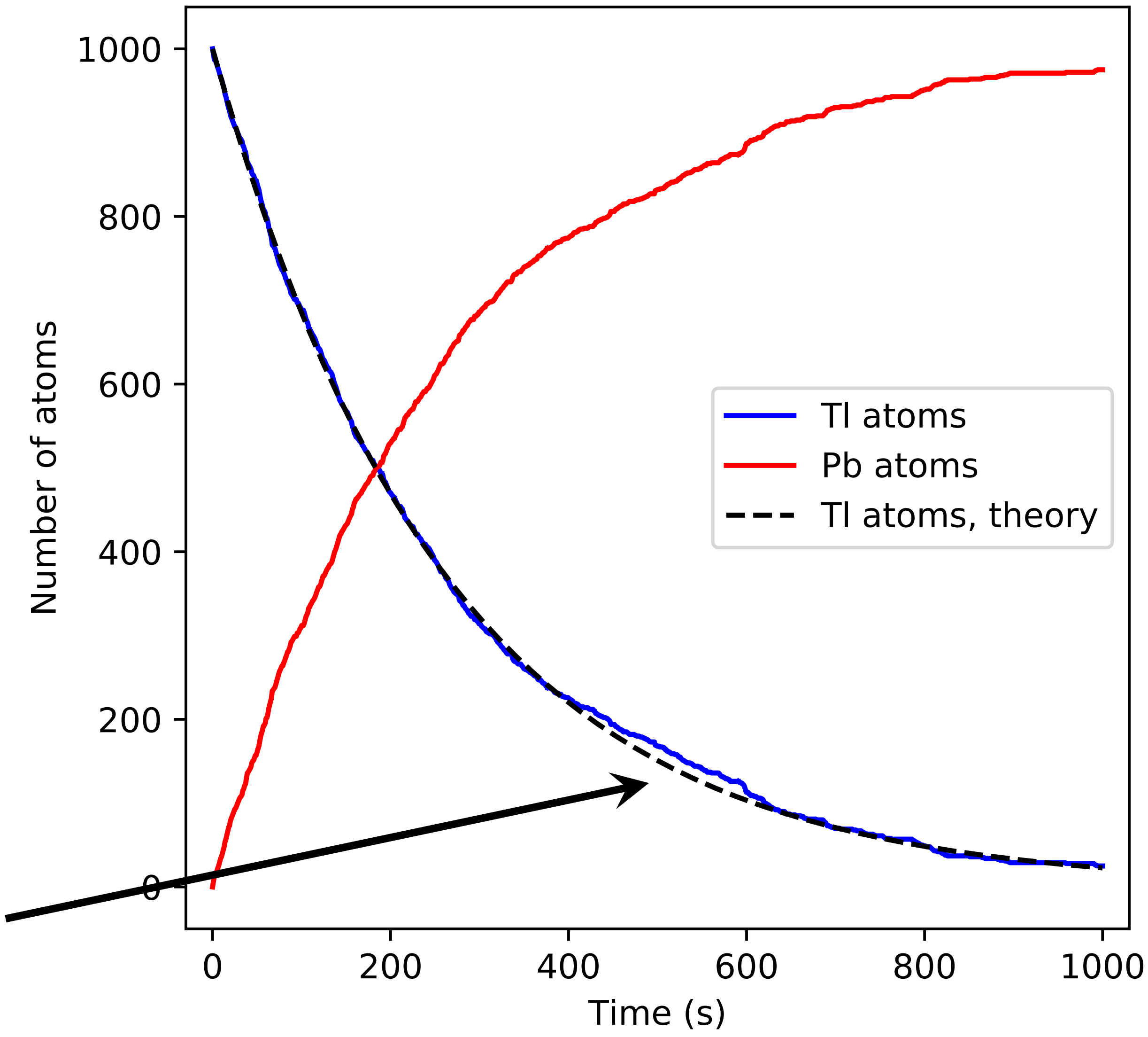
- Number of parent atoms falls off exponentially:

$$N(t) = N(0)2^{-t/\tau}$$

- Probability that a particular atom has decayed in a time interval *t*:

$$p(t) = 1 - 2^{-t/\tau}$$

Radioactive decay



$$N(t) = N(0)2^{-t/\tau}$$

Nonuniform distributions

- We can also select random numbers from a distribution that is not constant over the range
  - I.e., all numbers are not selected with equal probability
- Consider the radioactive decay example:
  - Probability of decay in time interval *dt* is:

$$p(t) = 1 - 2^{-dt/\tau} = 1 - \exp\left(-\frac{dt}{\tau}\ln 2\right) \simeq \frac{\ln 2}{\tau} dt$$

- What is the probability to decay in time window $t + dt$?
  - Needs to survive without decay until t (probability $2^{-t/\tau}$)
  - Then must decay in *dt*
  - Total probability is:

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

Nonuniform distribution for decay example

- Nonuniform probability distribution:

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

- Decay times t are distributed in proportion to $2^{-t/\tau}$
- We could calculate the decay of N atoms by drawing N random samples from this distribution
  - More efficient than previous method
  - Need to generate nonuniform distribution of random numbers
- Can generate nonuniform random numbers from a uniform distribution

Transformation method for changing distributions

- We have a source of random numbers *z* drawn from distribution *q*(*z*)
  - Probability of generating a number between *z* and *z*+d*z* is *q*(*z*)d*z*
- Now we choose a function *x* = *x*(*z*) whose distribution *p*(*x*) is the one we want
- We know that: $p(x)dx = q(z)dz$
- If our random numbers are drawn from a uniform distribution [0,1), *q*(*z*)=1 from 0 to 1, zero elsewhere
- Then:

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

- We need to do the integral on the left and then solve for *x*(*z*)
  - Not always possible

Transformation method to exponential distribution

- Say we want to generate random real numbers that are > 0 with the distribution:

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

- μ is for normalization
- Then:

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

- So:

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

Nonuniform distribution for decay example

- We can write the probability distribution for the decay example as

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

- So:

$$x = -\frac{\tau}{\ln 2} \ln(1 - z)$$

Nonuniform distribution for decay example

- We can write the probability distribution for the decay example as

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

- So:

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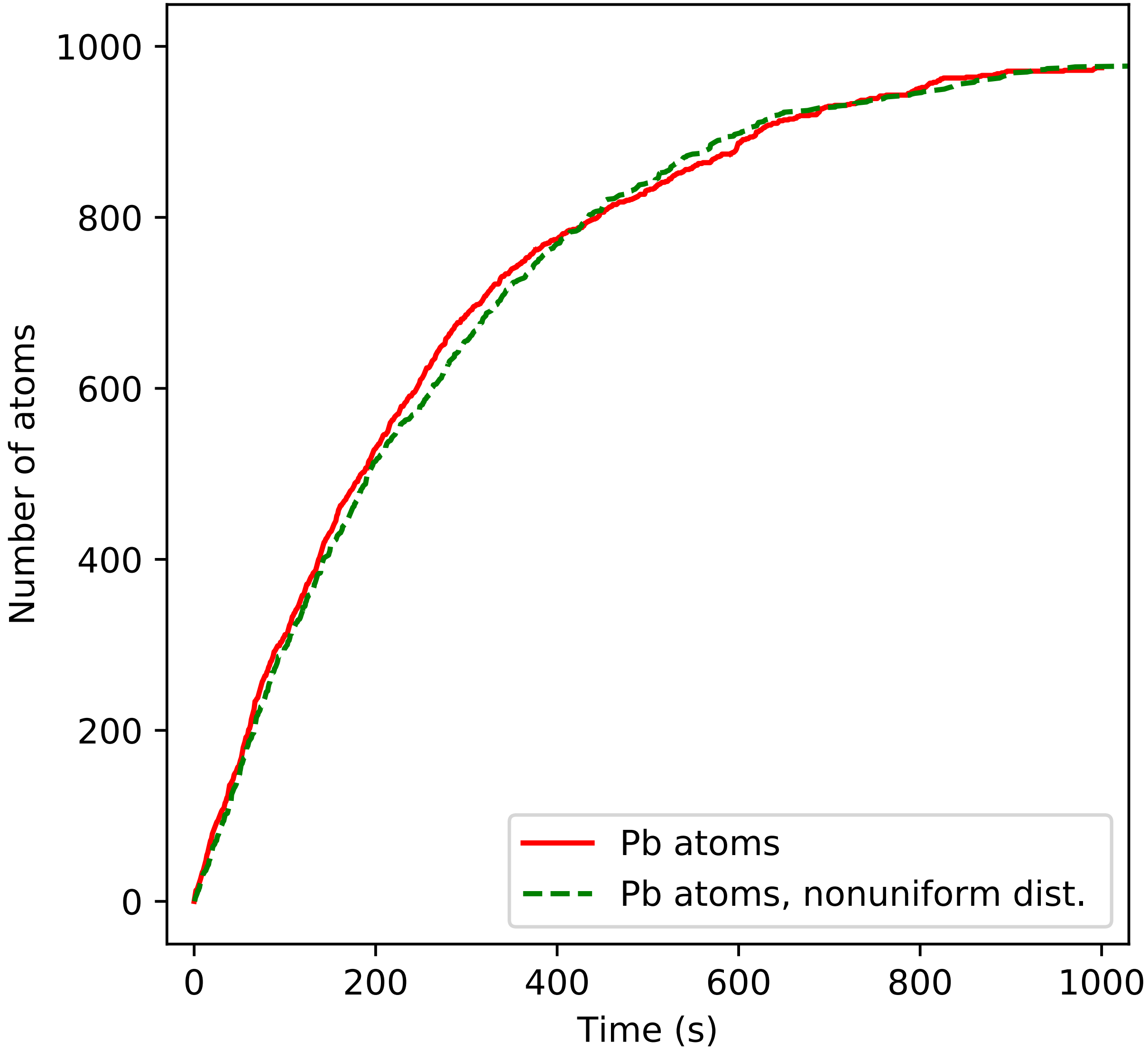


Gaussian random numbers

- In many cases we would like to draw numbers from a Gaussian (i.e., normal) distribution:

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

- Let's try the transformation method:

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

- The solution to this integral and the resulting equation is complicated

Gaussian random numbers

- Trick: consider two random numbers *x* and *y*, both drawn from Gaussian distribution with the same standard deviation
- Probability that point with position (*x*,*y*) falls in some element d*x*d*y* on *xy* plane is:

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

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

- Now convert to polar coordinates:

$$p(r,\theta)drd\theta = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right) rdrd\theta = \frac{r}{\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right) dr\frac{d\theta}{2\pi}$$

2D transformation method

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

- The point in polar coordinates will have the same distribution as the original point in cartesian (*x*,*y*)
  - Solving in polar coordinates and transforming back to Cartesian gives us two random points from a Gaussian distribution
- θ part is just a uniform distribution: $p(\theta) = 1/2\pi$
- Radial part can be treated with transformation method:

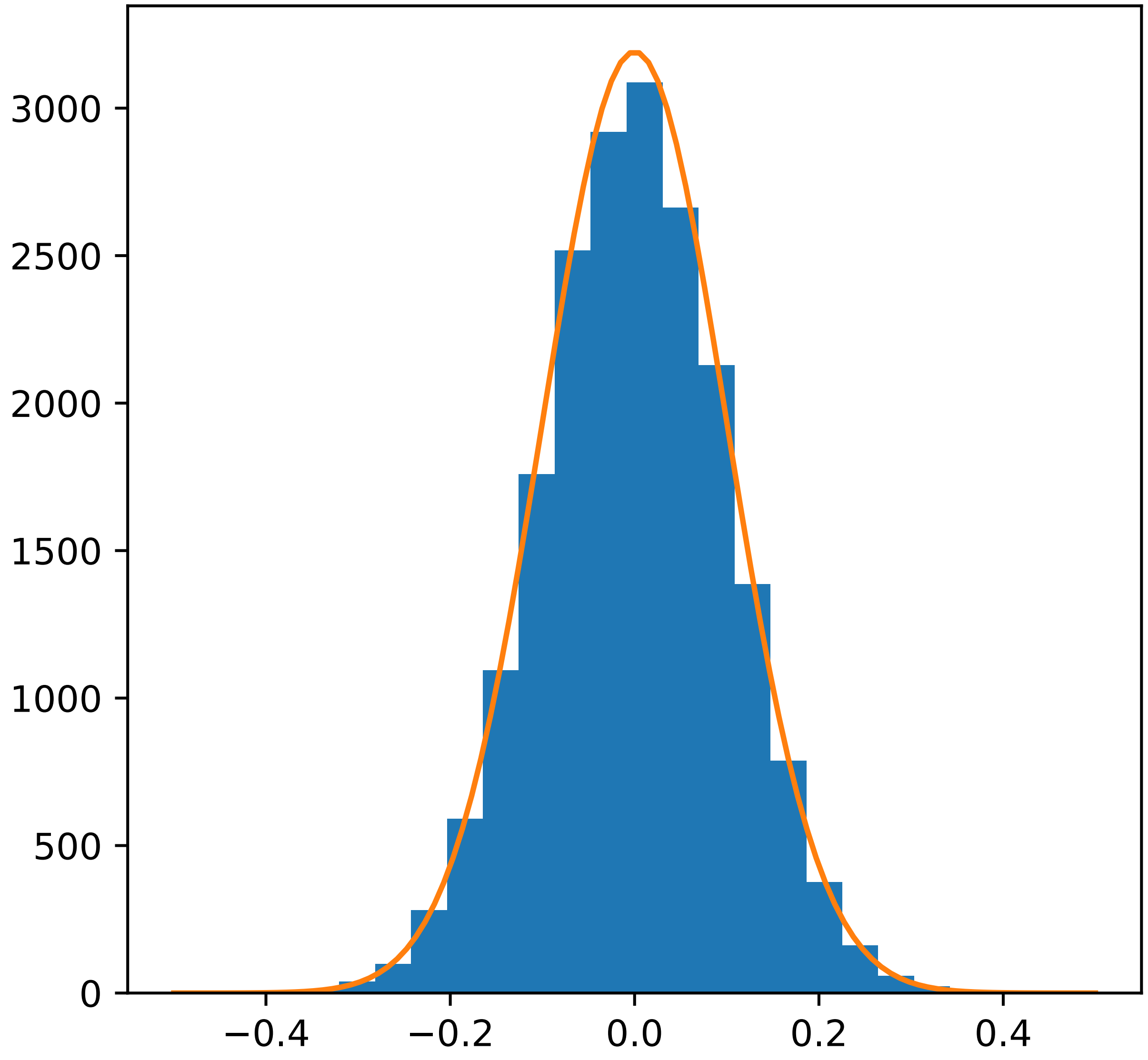
$$\frac{1}{\sigma^2}\int_0^r \exp\left(-\frac{r'^2}{2\sigma^2}\right)r'dr' = 1 - \exp\left(-\frac{r^2}{2\sigma^2}\right) = z$$

- So:

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

- And random numbers are: $x = r\cos\theta, \quad y = r\sin\theta$

Random numbers from Gaussian distribution



Example: Rutherford scattering

- α particles (helium nuclei) scatter when they pass close to an atom with angle:

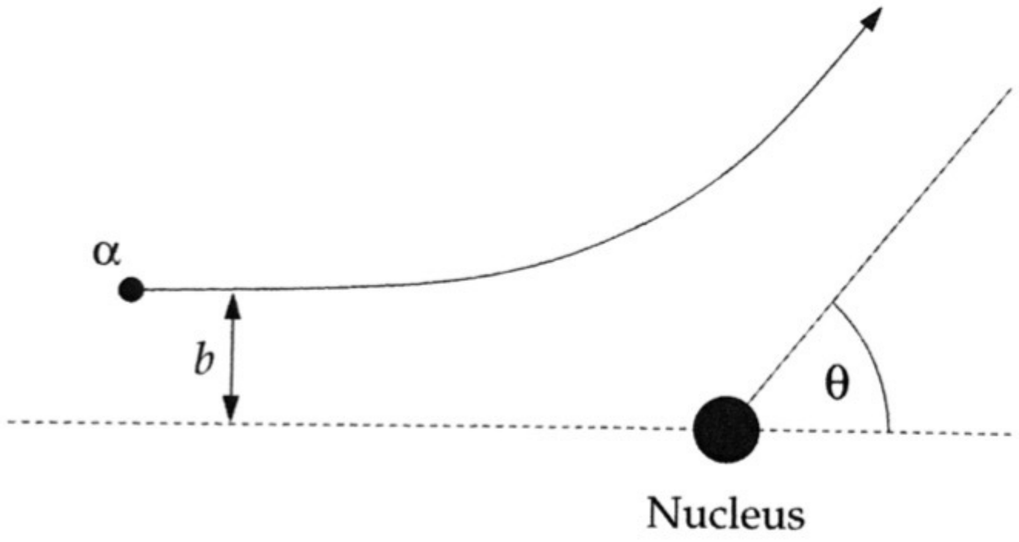
$$\tan\left(\frac{\theta}{2}\right) = \frac{Ze^2}{2\pi\epsilon_0 Eb}$$

- *E* is the kinetic energy of the α particle, *b* is the impact parameter

- Consider Gaussian beam of particles with σ=a_0/100 and *E*=7.7MeV fired at a gold atom

- How many "bounce back" (scattering angle > 90 degrees)?

$$b \leq \frac{Ze^2}{2\pi\epsilon_0 E}$$



Analytic solution to Rutherford scattering

- The impact parameter (distance from gold atom) are radially distributed:

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

- Thus, the probability of scattering by more that 90 degrees is:

$$\frac{1}{\sigma^2}\int_0^b \exp\left(-\frac{r'^2}{2\sigma^2}\right) r'dr' = 1 - \exp\left(-\frac{b^2}{2\sigma^2}\right) = 1 - \exp\left(-\frac{Z^2 e^4}{8\pi^2\epsilon_0^2\sigma^2 E^2}\right)$$

- Exact solution: 1557 particles backscattered out of 1,000,000
  - In good agreement with our stochastic calculation

Today's lecture:
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- Monte Carlo integration

Monte Carlo integration

- Let's come back to the Rutherford scattering example

- One way to look at: Our stochastic solution was in good agreement with the exact one

- Another way to look at it: Using a random process, we obtained an approximate solution to the integral:

$$\frac{1}{\sigma^2}\int_0^b \exp\left(-\frac{r'^2}{2\sigma^2}\right) r' dr'$$

- **Monte Carlo integration**: Approximate the value of an integral (which has an exact solution) with random calculations

After class tasks

- Homework 4 due today
- Final project ideas due Nov. 20

- Readings:
  - Newman Sec. 10.2