Monte Carlo Simulations

-80A.

First, Some (New) Logistics

- Homework #2 is due Thursday. Then HW #3 comes on the current topic
 - General advice (& applies this week) DON'T spend time on EC if you're struggling with basics. Focus on main HW question; keep reports short.
- DANGER: avoid upgrading your OS while taking this class ;-)
 - Mac examples from past: 64 bit versus 32 bit, and new processor (M1) which came with new laptop which I bought that made Kaleidagraph not work :-(
 - Windows even more notorious for breaking with upgrades, although Mac has become pretty bad about this too in recent years, especially with Xcode and C++
- Secondly: you don't need to submit all versions of your code, nor the extra credit as separate *.cpp
 - Use if statements including hash-if's (pre-processor directives), user input (cin and/or scanf and/or input files and/or argv, argc), switch blocks, comments. Plots not separate but embedded in reports

History of the Monte Carlo

MCs often easier to implement than other methods and easier to get uncertainties from. Use them!

The first thoughts and attempts I made to practice [the Monte Carlo Method] were suggested by a question which occurred to me in 1946 as I was convalescing from an illness and playing solitaires. The question was what are the chances that a Canfield solitaire laid out with 52 cards will come out successfully? After spending a lot of time trying to estimate them by pure combinatorial calculations, I wondered whether a more practical method than "abstract thinking" might not be to lay it out say one hundred times and simply observe and count the number of successful plays. This was already possible to envisage with the beginning of the new era of fast computers, and I immediately thought of problems of neutron diffusion and other questions of mathematical physics, and more generally how to change processes described by certain differential equations into an equivalent form interpretable as a succession of random operations. Later [in 1946], I described the idea to John von Neumann, and we began to plan actual calculations.



[Stanisław Ulam, co-inventer of the hydrogen bomb]

"Stanisław Ulam is probably best known for realising that electronic computers made it practical to apply statistical methods to functions without known solutions, and as computers have developed, the <u>Monte Carlo method</u> has become a ubiquitous and standard approach to many problems." [Wikipedia on Stanislaw Ulam]

19-5 Mean Free Path

In considering the motion of molecules, a question often arises: If molecules move so fast (hundreds of meters per second), why does it take as long as a minute or so before you can smell perfume when someone opens a bottle across a room (only a few meters away)? To answer this question, we continue to examine the motion of molecules in an ideal gas. Figure 19-5 shows the path of a typical molecule as it moves through the gas, changing both speed and direction abruptly as it collides elastically with other molecules. Between collisions, our typical molecule moves in a straight line at constant speed. Although the figure shows all the other molecules as stationary, they too are moving similarly.

One useful parameter to describe this random motion is the **mean free path** λ of the molecules. As its name implies, λ is the average distance traversed by a molecule between collisions. We expect λ to vary inversely with *N/V*, the number of molecules per unit volume (or "number density" of molecules). The larger *N/V* is, the more collisions there should be and the smaller the mean free path. We also expect λ to vary inversely with the size of the molecules, say, with their diameter *d*. (If the molecules were points, as we have assumed them to be, they would never collide and the mean free path. We can even predict that λ should vary (inversely) as the *square* of the molecular diameter because the cross section of a molecule—not its diameter—determines its effective target area.



From Prof. Bill Lanford

Chapter 19 of textbook: The Kinetic Theory of Gases

FIGURE 19-5 A molecule traveling through a gas, colliding with other gas molecules in its path. Although the other molecules are shown as stationary, we believe they are also moving in a similar fashion.

The expression for the mean free path does, in fact, turn out to be

$$\lambda = \frac{1}{\sqrt{2\pi}d^2 N/V} \quad \text{(ideal gas mean free path).} \tag{20-24}$$

To justify Eq. 19-24, we focus attention on a single molecule and assume—as Fig. 19-5 suggests—that our molecule is traveling with a constant speed v and that all the other molecules are at rest. Later, we shall relax this assumption.

We assume further that the molecules are spheres of diameter d. A collision will then take place if the centers of the molecules come within a distance d of each other, as in Fig. 19-6a. Another, more helpful way to look at the situation is to consider our single molecule to have a *radius* of d and all the other molecules to be *points*, as in Fig. 19-6b. This does not change our criterion for a collision.

As our single molecule zigzags through the gas, it sweeps out a short cylinder of cross-sectional area πd^2 between successive collisions. If we watch this molecule for a time interval Δt , it moves a distance $v\Delta t$, where v is its assumed speed. Thus, if we align all the short cylinders swept out in Δt , we form a composite cylinder (Fig. 19-7) of length $v\Delta t$ and volume $(\pi d^2)(v\Delta t)$. The number of collisions that occur in time Δt is then equal to the number of (point) molecules that lie within this cylinder.



FIGURE 19-6 (a) A collision occurs when the centers of two molecules come within a distance d of each other, d being the molecular diameter. (b) An equivalent but more convenient representation is to think of

the moving molecule of interest as having a *radius* d and all other molecules as being points. The condition for a collision is unchanged.

Since *N/V* is the number of molecules per unit volume, the number of molecules in the cylinder is *N/V* times the volume of the cylinder, or $(N/V)(\pi d^2 v \Delta t)$. This is also the number of collisions in time Δt . The mean free path is the length of the path (and of the cylinder) divided by this number:



This equation is only approximate because it is based on the assumption that all the molecules except one are at rest. Ir fact, *all* the molecules are moving; when this is taken properly into account, Eq. 19-24 results. Note that it differs from the (approximate) Eq. 19-25 only by a factor of $1/\sqrt{2}$.



REST fine assumption for us

FIGURE 19-7 In time Δt the moving molecule effectively sweeps out a cylinder of length $v \Delta t$ and radius d.

We can even get a glimpse of what is "approximate" about Eq. 19-25. The v in the numerator and that in the denominator are—strictly—not the same. The v in the numerator is $\langle v \rangle$, the mean speed of the molecule *relative to the container*. The v in the denominator is $\langle v^{rel} \rangle$, the mean speed of our single molecule *relative to the other molecules*, which are moving. It is this latter average speed that determines the number of collisions. A detailed calculation, taking into account the actual speed distribution of the molecules, gives $\langle v^{rel} \rangle = \sqrt{2} \langle v \rangle$ and thus the factor $\sqrt{2}$.

The mean free path of air molecules at sea level is about $0.1 \ \mu\text{m}$. At an altitude of 100 km, the density of air has dropped to such an extent that the mean free path rises to about 16 cm. At 300 km, the mean free path is about 20 km. A problem faced by those who would study the physics and chemistry of the upper atmosphere in the laboratory is the unavailability of containers large enough to hold gas samples that simulate upper

Can replace with > cross section, which is not literally geometric anymore, in most cases, in highenergy particle and nuclear physics atmospheric conditions. Yet studies of the concentrations of freon, carbon dioxide, and ozone in the upper atmosphere are of vital public concern.

Recall the question that began this section: If molecules move so fast, why does it take as long as a minute or so before you can smell perfume when someone opens a bottle across a room? We now know part of the answer. In still air, each perfume molecule moves away from the bottle only very slowly because its repeated collisions with other molecules prevent it from moving directly across the room to you.

TOUCHSTONE EXAMPLE 19-3: Mean Free Path

(a) What is the mean free path λ for oxygen molecules at temperature T = 300 K and pressure P = 1.00 atm? Assume that the molecular diameter is d = 290 pm and the gas is ideal.

SOLUTION The **Key Idea** here is that each oxygen molecule moves among other *moving* oxygen molecules in a zigzag path due to the resulting collisions. Thus, we use Eq. 19-24 for the mean free path, for which we need the number of molecules per unit volume, N/V. Because we assume the gas is ideal, we can use the ideal gas law of Eq. 19-1 ($PV = Nk_BT$) to write $N/V = P/k_BT$. Substituting this into Eq. 19-24, we find

$$\lambda = \frac{1}{\sqrt{2\pi}d^2 N/V} = \frac{k_B T}{\sqrt{2\pi}d^2 P}$$

= $\frac{(1.38 \times 10^{-23} \text{ J/K})(300 \text{ K})}{\sqrt{2\pi}(2.9 \times 10^{-10} \text{ m})^2 (1.01 \times 10^5 \text{ Pa})}$ (Answer
= $1.1 \times 10^{-7} \text{ m}.$

This is about 380 molecular diameters.

(b) Assume the average speed of the oxygen molecules is $\langle v \rangle = 450$ m/s. What is the average time interval Δt between successive collisions for any given molecule? At what rate does the molecule collide; that is, what is the frequency *f* of its collisions?

SOLUTION To find the time interval Δt between collisions, we use this **Key Idea**: Between collisions, the molecule travels, on average, the mean free path λ at average speed $\langle v \rangle$. Thus, the average time between collisions is

$$\langle vt \rangle = \frac{\text{(distance)}}{(\text{average speed})} = \frac{\lambda}{\langle v \rangle} = \frac{1.1 \times 10^{-7} \text{ m}}{450 \text{ m/s}}$$
 (Answer
= 2.44×10⁻¹⁰ s ≈ 0.24 ns.

This tells us that, on average, any given oxygen molecule has less than a nanosecond between collisions.

To find the frequency *f* of the collisions, we use this **Key Idea**: The average rate or frequency at which the collisions occur is the inverse of the average time $\langle \Delta t \rangle$ between collisions. Thus,

$$f = \frac{1}{2.44 \times 10^{-10} \text{ s}} = 4.1 \times 10^9 \text{ s}^{-1}.$$
 (Answer)

This tells us that, on average, any given oxygen molecule makes about 4 billion collisions per second.

What is Cross Section?

<u>https://www.symmetrymagazine.org/article/speak-physics-what-is-a-cross-section</u>



Not to be confused with standard deviation or error!





Plot Digitization

- For the current assignment: Java-based Plot Digitizer for Windows, Apple Mac, and Linux \ Unix (at least some flavors) at <u>http://plotdigitizer.sourceforge.net/</u>
 - If for any reason this fails to work for your machine, Googling "digitizing plots" as an exact phrase should provide alt programs. (Beware of logs!)
- Often much easier, and much faster, than asking the original authors to provide you the raw data ③

Homework #3: A Simple MC Simulation due Thur. Feb 15



You should Create a MC sim for my Lithium Fluoride assume spherical symmetry • You only have to do 1 initial starting energy *E*, of 17 MeV Start with >= 100,000 neutrons from center • Use the standard method for converting a mass density into a number density by means of Avogadro's number

<u>FINAL RESULT</u>: 1 figure i.e. plot, the fraction of neutrons captured as a function of radius, in the report to Shane



Keep units of cm, cm^2, cm^3, cm^-3 everywhere for simplicity until final result • And energy in eV everywhere (thus, convert 17 above)

Assume the cross section is only one of two options: capture or scatter (sum the elastic and inelastic curves from slides) • 4 options: capture or scatter on Li-7, or one of those on F

Methodologies

- Kinetic (and potential) energy will be deposited by an energetic traveling particle in the lithium fluoride solid
 Kinetic = elastic, potential = inelastic. Real life has rich mixture of both
- Simulate MFP mean free path as a "live" function of neutron kinetic energy. For simplicity, assume the energy goes as x0.5 with each collision (of any type)
 So, if your energy variable is called E then E /= 2.0 is an acceptable code line
 The energy depends on the target masses and angle in real life, and E levels

• Also, assume new random angles in three dimensions

- Randomize phi between 0 and 2pi (RADIANS) but COSINE of theta from -1 to
 1. The cosine very critical there, otherwise you don't have direction uniformity.
 <u>http://corysimon.github.io/articles/uniformdistn-on-sphere/</u>
 <u>v = r * sin(theta) * cos(phi)</u>
 <u>y = r * sin(theta) * sin(phi)</u>
 <u>v = r * cos(theta)</u>
- Next: coding instructions in English haha, not in C++. To get good results (ignoring fission, secondary particles)
 In real-life research, you very often do not know what the "correct" answer is.



Step-by-Step Instructions

- Usual headers (will also need <random>) and namespace
- You'll need uniform real (double) random num gens
 One from 0 to 1 and one from -1 to 1 ideally (latter for cos of theta, as explained)
- Loop within loop: while for interactions within a for loop of the #of neutrons. (Unless debugging, don't cout or cerr!)
 - Initialize to random direction in 3D but position at origin (0,0,0). Energy = 17e6 eV
 - The while loop continues until the neutron is captured, leaves, or goes too low in E
 - Don't allow 0 or negative energy of course, and use for loop for multiple neutrons
- Set MFP (mean free path) with sigma(E), i.e. cross-section
 But this is only MEAN. Choose a random free path length based on exp ran num
 Otherwise, you wouldn't actually be randomizing enough, getting lot of sameness
- Update variables within your primary, type 'while' loop
 New position based on previous direction; new energy; new random direction
- After while loop ends, and after for loop ends, write out to screen or file the total FRACTION of neutrons within radius
 What radius? Infinite, or go in half-log steps (1, 2, 5, 10, 20, 50, 100, 200, 500 cm) 15

STILL only 17 MeV, not any other different *E*. Continue to ignore fission byproducts
Bonus

- Keep your code almost exactly the same, except include the contribution of Li-6 within natural Lithium, instead of simulating enriched Lithium (enriched in Lithium-7). Use 6's natural % Impress me with new plot
- In your report, explain why Lithium-7 enrichment is a good idea for nuclear reactors based on 7's fission



sum the miscellaneous "neutron producing interactions" into inelastic, just like before, and count Li-6+n->... in red as capture ("death" of n)

Trying is not enough for extra credit, as usual. You MUST succeed.

This is Nuclear Physics

Not just "modern," but CONTEMPORARY Physics. Not usually covered anywhere

Lithium-7-Powered Nuclear Fission Subcritical Reactor

A lithium-based fission reactor that generates safe, clean electricity while reducing the amount of discarded lithium batteries in landfill

Published: 6th July 2023



Source: Emanuel Corso, https://stock.adobe.com/uk/604772398, stock.adobe.com

Background

Renewable energy sources such as solar, wind, and geothermal, have still failed to replace coal, oil, natural gas, and other fossil fuels, despite decades of technology development and (in many cases) strong governmental support for these alternatives. As a result, energy production remains a major contributor to global environmental damage and climate change. Another potential environmental and safety issue is the current reliance on lithium batteries in a wide variety of devices. An effective infrastructure for recycling lithium batteries on a large scale has yet to be developed, As a result, lithium batteries generally end up in landfills, creating potential hazards due to their explosive flammability.

Technology Overview

This University at Albany technology is a nuclear reactor that uses lithium-7 as the fissionable fuel in place of uranium, plutonium, or other radioactive elements. The reactor is sub-critical, driven by a radioactive source that, when removed, does not allow for a runaway reaction. This is very different from "normal" nuclear fission which requires (epi-)thermal neutrons, such as in U235. The resulting reactor is safer while delivering a high yield. And lithium is already widely used in batteries, ensuring a ready supply of fuel. In addition, the use of spent lithium batteries as source fuel prevents them from ending up in landfills.

Stage of Development

Technology Readiness Level (TRL) 3 - Experimental proof of concept.

Benefits

- Provides clean (zero-carbon-footprint) energy
- Safer than other fission-based energy production methods
- Less expensive
- Relies on a readily available source of fuel (discarded lithium batteries)

Applications

This primary application for this technology is clean electricity generation.

Opportunity

This technology is available for licensing and would be of interest to anyone involved in electricity generation and/or research into this topic, including:

- Power utilities
- Military
- Government
- Research institutions

Patents

• Patent Pending (63/439,406)

IP Status

Seeking

- Patent application submitted
- Licensing

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