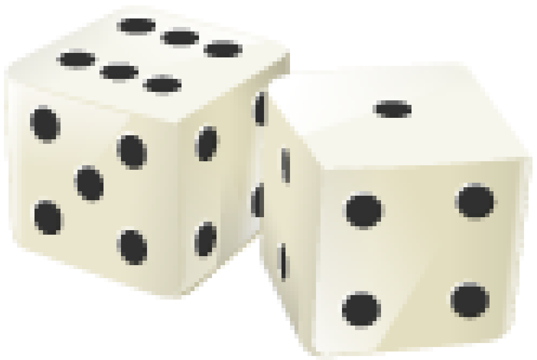
Classical Monte Carlo Simulations



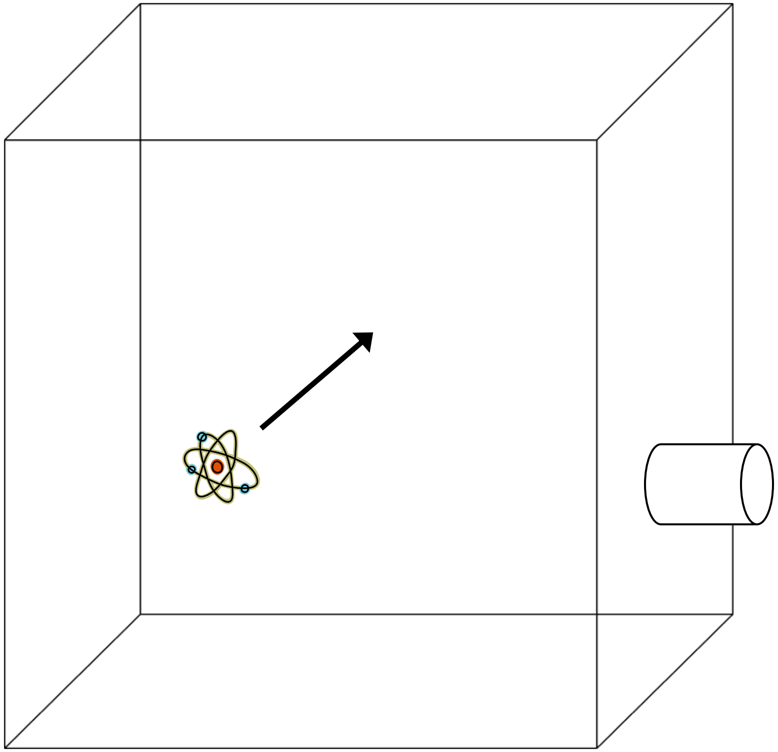
… you can calculate anything with dice.

Introduction

Calculate …

- the number of **bounces** (mean and variance)
- and **time** (mean and variance)

for a gas molecule at temperature T to leave this box:



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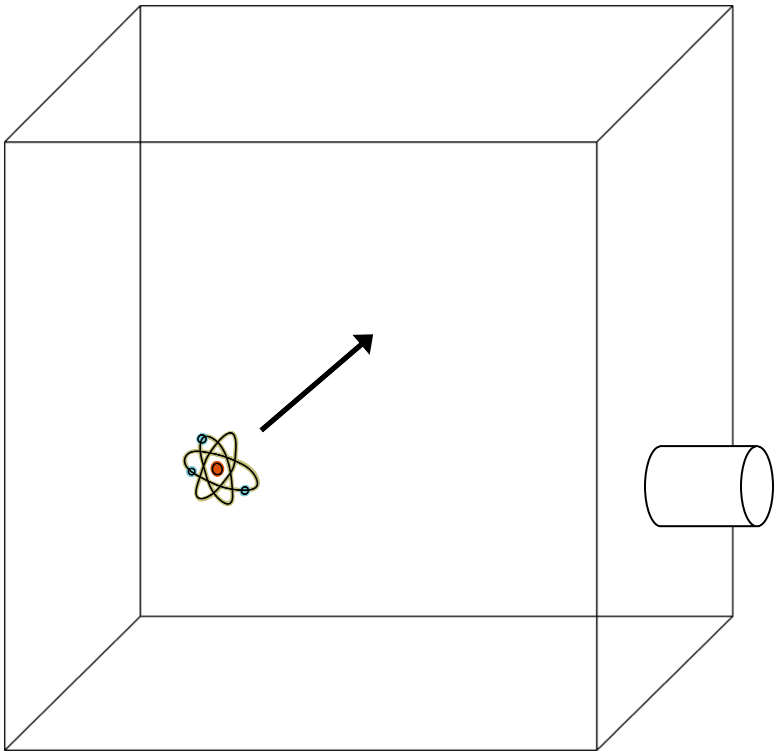

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- molecule re-thermalize on each wall bounce.
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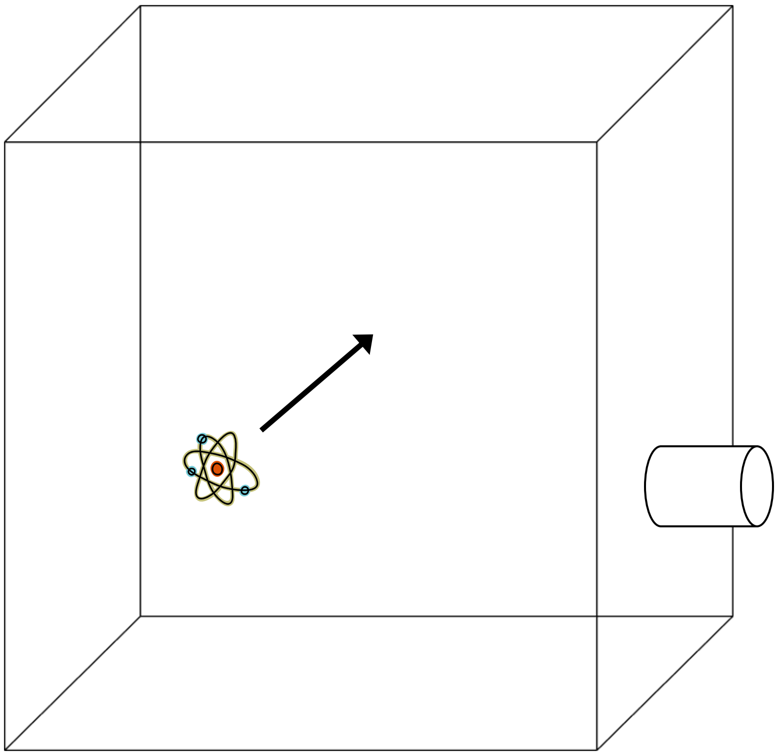

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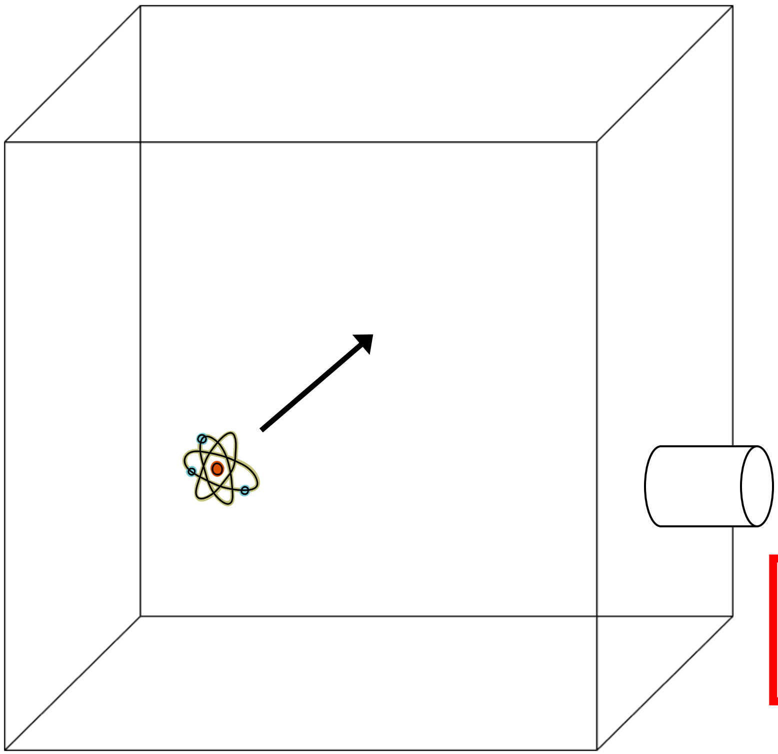

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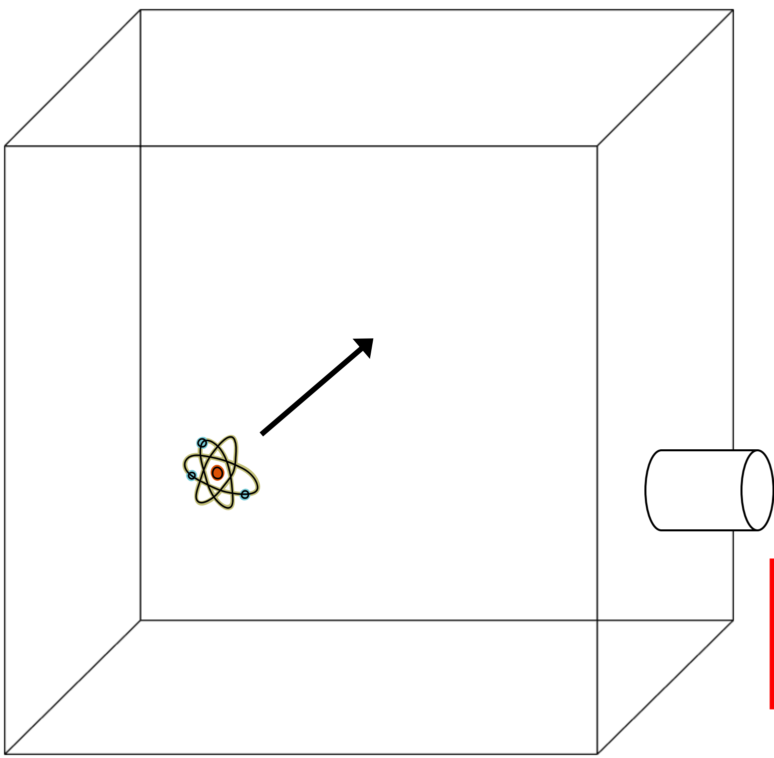

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… fairly simple and quick on a computer.

Definition

The Monte Carlo method is any numerical method in which the solution is obtained by ***averaging over many probabilistic simulation instances***.

Example: Numerical Integration

The Monte Carlo method is frequently used to evaluate difficult integrals (in many dimensions):

$$\text{“calculus” average:} \quad \left\langle f(x) \right\rangle_{[a,b];\,calculus} = \frac{1}{b-a}\int_a^b f(x)\,dx$$

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x_i=probabilistic variable

i.e. choose x_i's randomly on [a,b] with a uniform probability distribution.

Theorem

If f(x) is well behaved on [a,b] (i.e. does not diverge), then in the limit of N→∞, the following is true (in the probabilistic sense)

$$\boxed{\left\langle f(x) \right\rangle_{[a,b];\,calculus} = \left\langle f(x) \right\rangle_{[a,b];\,statistical,N} \pm \frac{\sigma_{f(x),N}}{\sqrt{N}}}$$

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where $$\sigma^2_{f(x),N} = \frac{1}{N-1}\left(\sum_{i=1}^{N} f(x_i)^2 - N\langle f(x)\rangle^2_{[a,b],N}\right) = \frac{1}{N-1}\sum_{i=1}^{N}\left(f(x_i)-\langle f(x)\rangle\right)^2$$

$$= \text{standard deviation of simulations}$$

Advantages

- Monte Carlo simulations are generally easy to formulate and set-up.

- Monte Carlo simulations are generally faster than other numerical methods, especially for problems in a large number of dimensions.