Langevin's Dynamics

$$m\frac{d^2}{dt^2}\mathbf{r} = -\nabla V(\mathbf{r}) - m\gamma\frac{d}{dt}\mathbf{r} + \mathbf{R}(t)$$

- Other numerical solutions (assume interpart. interactions nearly constant within Δt [i.e. Δt is small]) by Ermak and Buckholtz (1980):

$$\mathbf{r}(t+\delta t) = \mathbf{r}(t) + c_1\left(\frac{d\mathbf{r}}{dt}\right)_t \Delta t + c_2\left(\frac{d^2\mathbf{r}}{dt^2}\right)_t \Delta t^2 + \Delta\mathbf{r}^G$$

$$\mathbf{v}(t+\delta t) = c_0\left(\frac{d\mathbf{r}}{dt}\right)_t + c_1\left(\frac{d^2\mathbf{r}}{dt^2}\right)_t \Delta t + \Delta\mathbf{v}^G$$

Langevin's Dynamics

- Where the vector gaussian random noise:

$$\Delta\mathbf{r}^G \qquad \Delta\mathbf{v}^G$$

- Have variance

$$\sigma_r^2 = \Delta t^2\left(\frac{k_BT}{m}\right)\frac{1}{\gamma\Delta t}\left(2 - \frac{1}{\gamma\Delta t}(3 - 4exp(-\gamma\Delta t) + exp(-2\gamma\Delta t))\right)$$

$$\sigma_v^2 = \left(\frac{k_BT}{m}\right)(1 - exp(-\gamma\Delta t))$$

Langevin's Dynamics

- And numerical coefficients:

$$c_0 = exp(-\gamma\Delta t)$$
$$c_1 = \frac{1-c_0}{\gamma\Delta t}$$
$$c_2 = \frac{1-c_1}{\gamma\Delta t}$$

Langevin's Dynamics

$$m\frac{d^2}{dt^2}\mathbf{r} = -\nabla V(\mathbf{r}) - m\gamma\frac{d}{dt}\mathbf{r} + \mathbf{R}(t)$$

- More “accurate” solutions for low γ (and interparticle forces linearly dependent on time):

$$\mathbf{r}(t+\delta t) = \mathbf{r}(t) + c_1\left(\frac{d\mathbf{r}}{dt}\right)_t \Delta t + c_2\left(\frac{d^2\mathbf{r}}{dt^2}\right)_t \Delta t^2 + \Delta\mathbf{r}^G$$

$$\begin{aligned}\mathbf{v}(t+\delta t) = c_0\left(\frac{d\mathbf{r}}{dt}\right)_t + (c_1 - c_2)\left(\frac{d^2\mathbf{r}}{dt^2}\right)_t \Delta t \\ + c_2\left(\frac{d^2\mathbf{r}}{dt^2}\right)_{t+\Delta t} \Delta t + \Delta\mathbf{v}^G\end{aligned}$$

As γ→ 0, recover velocity Verlet

Monte Carlo Simulations

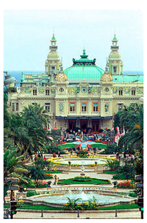
- An experiment?
  - It “samples” by generating large numbers of random numbers
- Usually two types:
  - “Simple” Monte Carlo: estimates values of integrals by generating uniform sampling of the integrand and adding it up
  - Metropolis Monte Carlo: generates a trajectory in phase space. Good for thermodynamics.

Early Sampling Methods

- Some deterministic mathematical problems can be treated by finding a probabilistic analogue
- Then solve this analogue by a stochastic sampling experiment
- Early developments:
  - eighteenth-century French “naturalist.” Buffon's Needle problem and geometric probability, 2l/πd
  - Italian mathematician Lazzerini (1901): needle exp. 3408 times, estimated π to accuracy of 10^{-7}

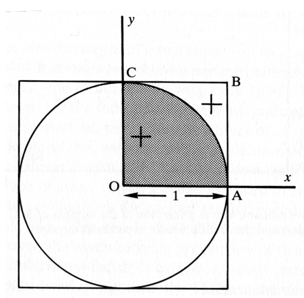
Simple Monte Carlo

- Estimate value of π by determining the area of one cuadrant of the circle using random numbers

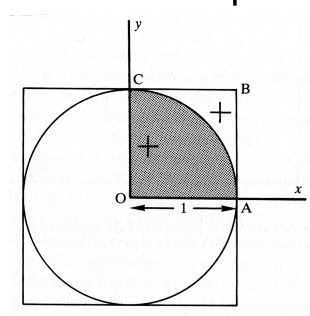


Neumann, Ulam, and Metropolis (1947)

Named for the Monte Carlo Casino



Simple Monte Carlo

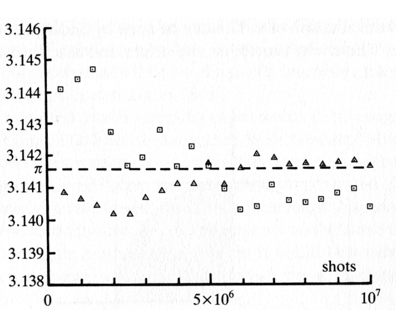


- Generate 2 random numbers and create (x,y)
- If $x^2+y^2 \leq 1$ count it inside as a “hit”

$$\pi \approx \frac{4 \times area\ under\ the\ curve\ AC}{area\ of\ the\ square\ OABC} = \frac{4\tau_{hit}}{\tau_{shots}}$$

demo

Simple Monte Carlo



- After 107 trials, the value is still 3.14173
- Another decimal will require an order of magnitude more random numbers