Monte-Carlo and Langevin dynamics

Arkadiy Simonov

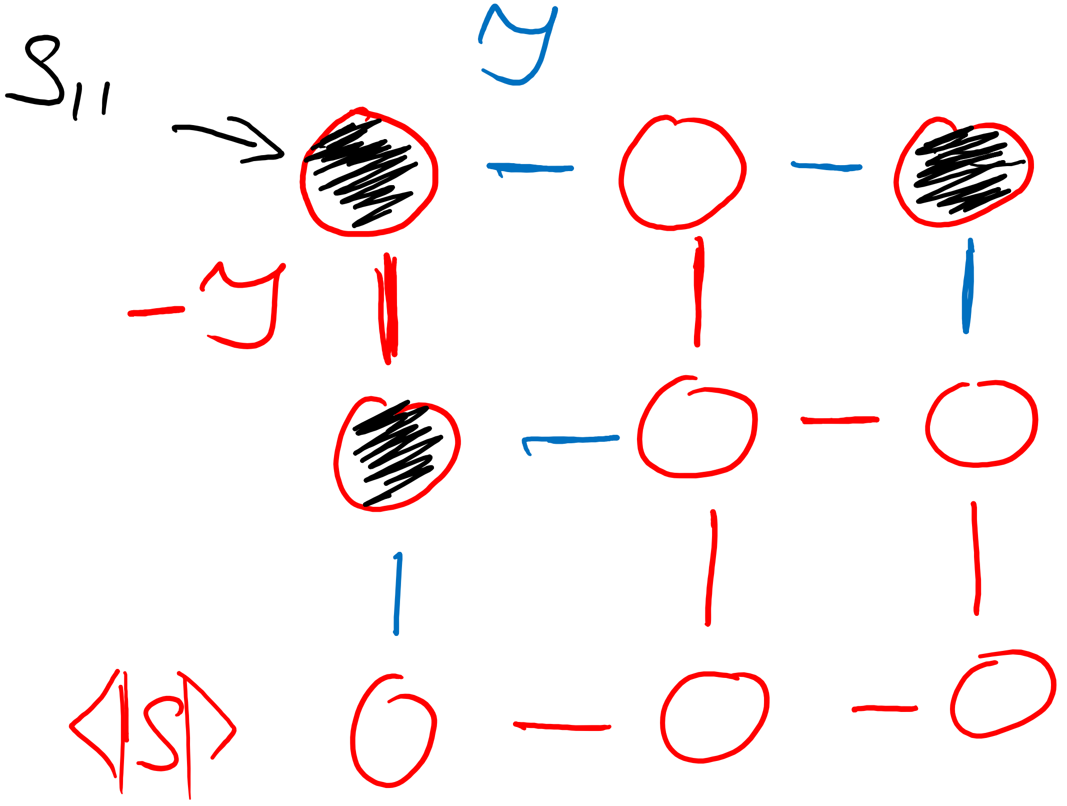
$$U(x) = \sum_{i,j,i',j'}^{neigs.} -J s_{i,j} s_{i',j'}$$

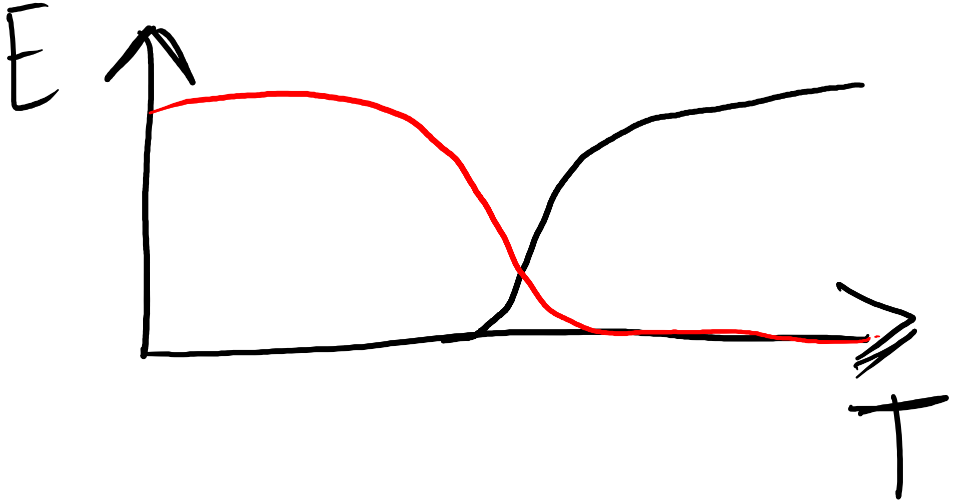
$$X = \{ S_{11}, S_{12} \dots \}$$

$$S = \{ -1 ; 1 \}$$

$$U(x) = 5y - 7y = -2y$$

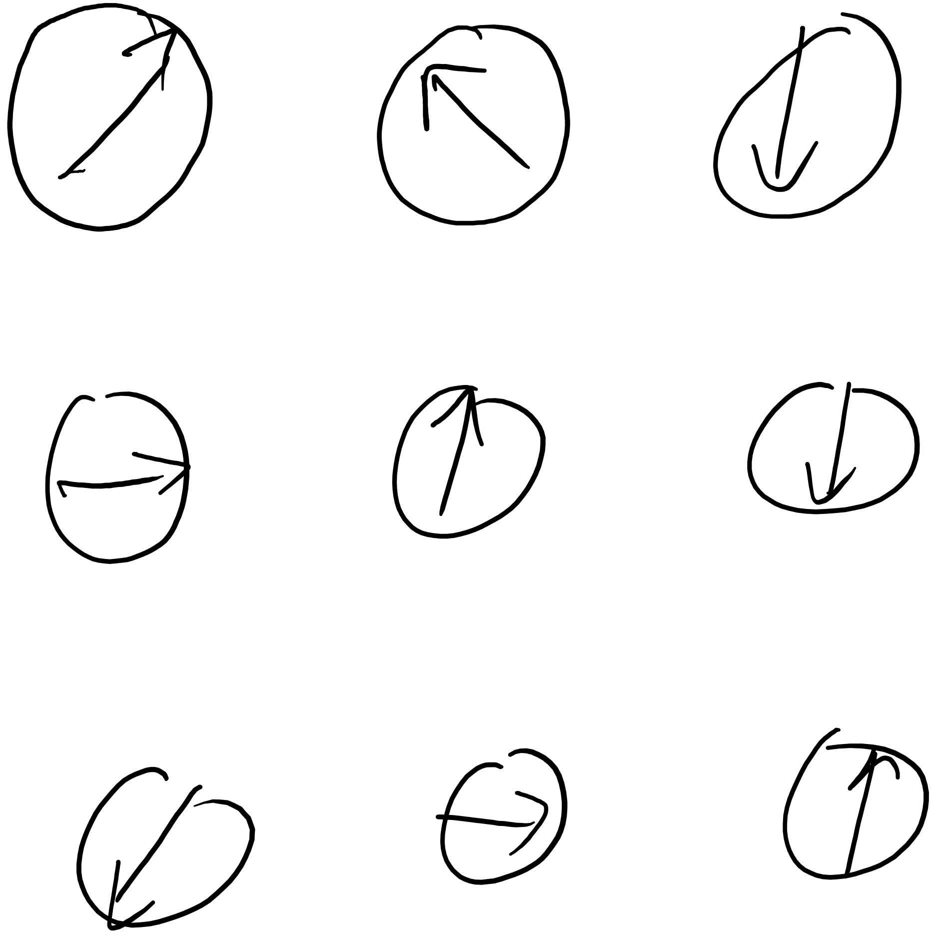
$$S = +3$$





$$U(x) = \sum_{i,j,i',j'}^{neigs.} -J\boldsymbol{s}_{i,j} \cdot \boldsymbol{s}_{i',j'}$$

$$\bar{S} = \{ \nearrow \}$$



Problem:

$$\underbrace{\langle O \rangle} = \sum_{x} \underbrace{P(x)}\underbrace{O(x)}$$

$$P(x) = \frac{1}{Z} \underbrace{e^{-\frac{U(x)}{kT}}}$$

$$\underbrace{Z = \sum_{x} e^{-\frac{U(x)}{kT}}}$$

x	state of the system
$U(x)$	(potential) energy of the system
$P(x)$	probability of state x
Z	partition function
O	observable property, *e.g.* energy

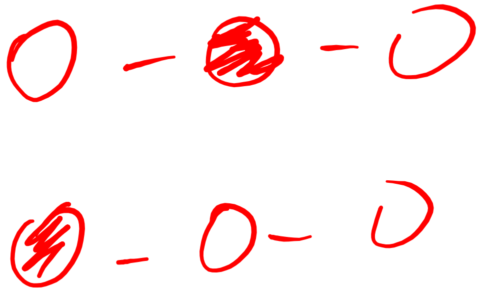
9 spins   2 states

$2^9 = 512$

How can we approximate observables?

$$\underbrace{\langle O \rangle}_{} = \frac{1}{\underbrace{N_s}_{}} \sum_{x_i} \underbrace{O(x_i)}_{}$$

X



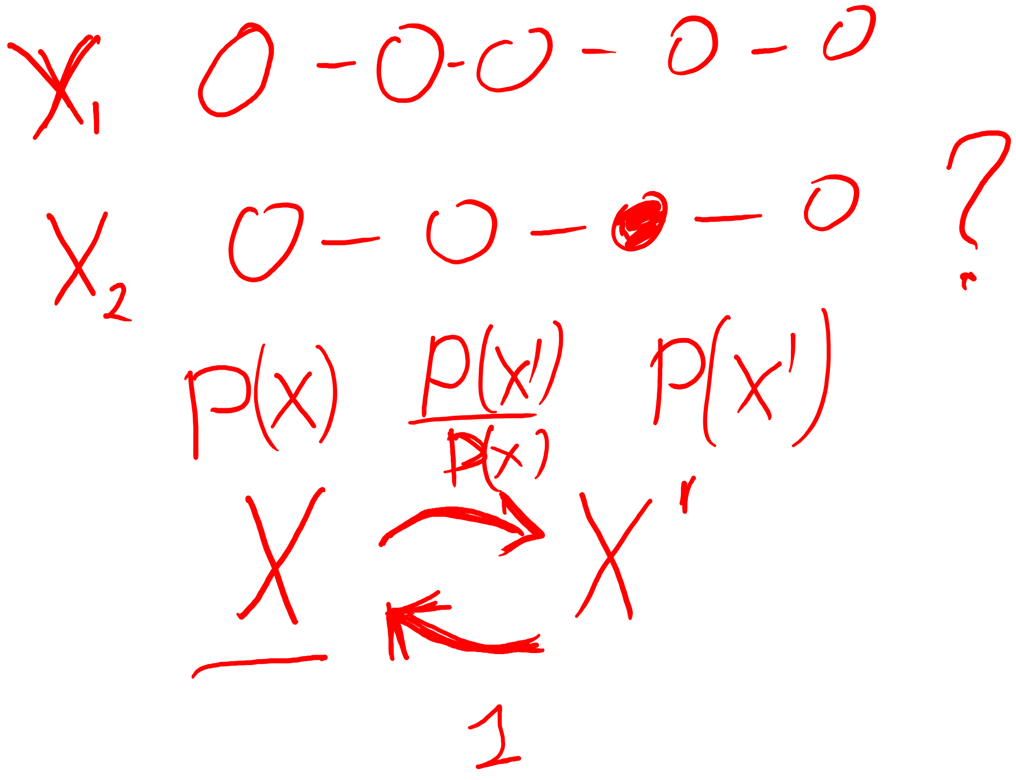
x_i is from $\underbrace{P(x) = \frac{1}{Z} e^{-\frac{U(x)}{kT}}}_{}$

How do we sample?
One bit at a time, using Metropolis rejection

$$x_1 \to x_2 \to x_3 \to \cdots \to x_N$$

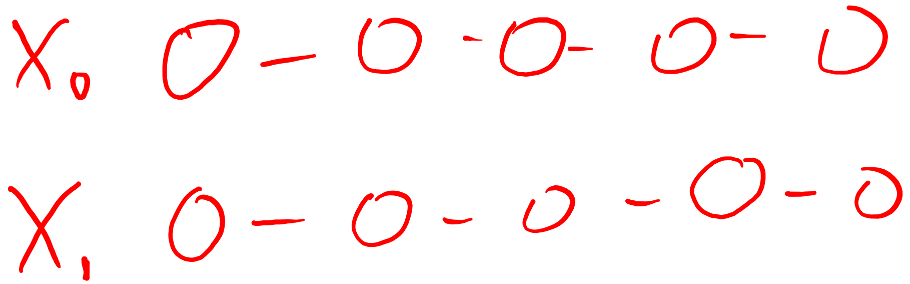
x_i is from $P(x) = \frac{1}{Z} e^{-\frac{U(x)}{kT}}$ if

$$A(x \to x') = \min\left[1, \frac{P(x')\mathcal{T}(x' \to x)}{P(x)\mathcal{T}(x \to x')}\right]$$



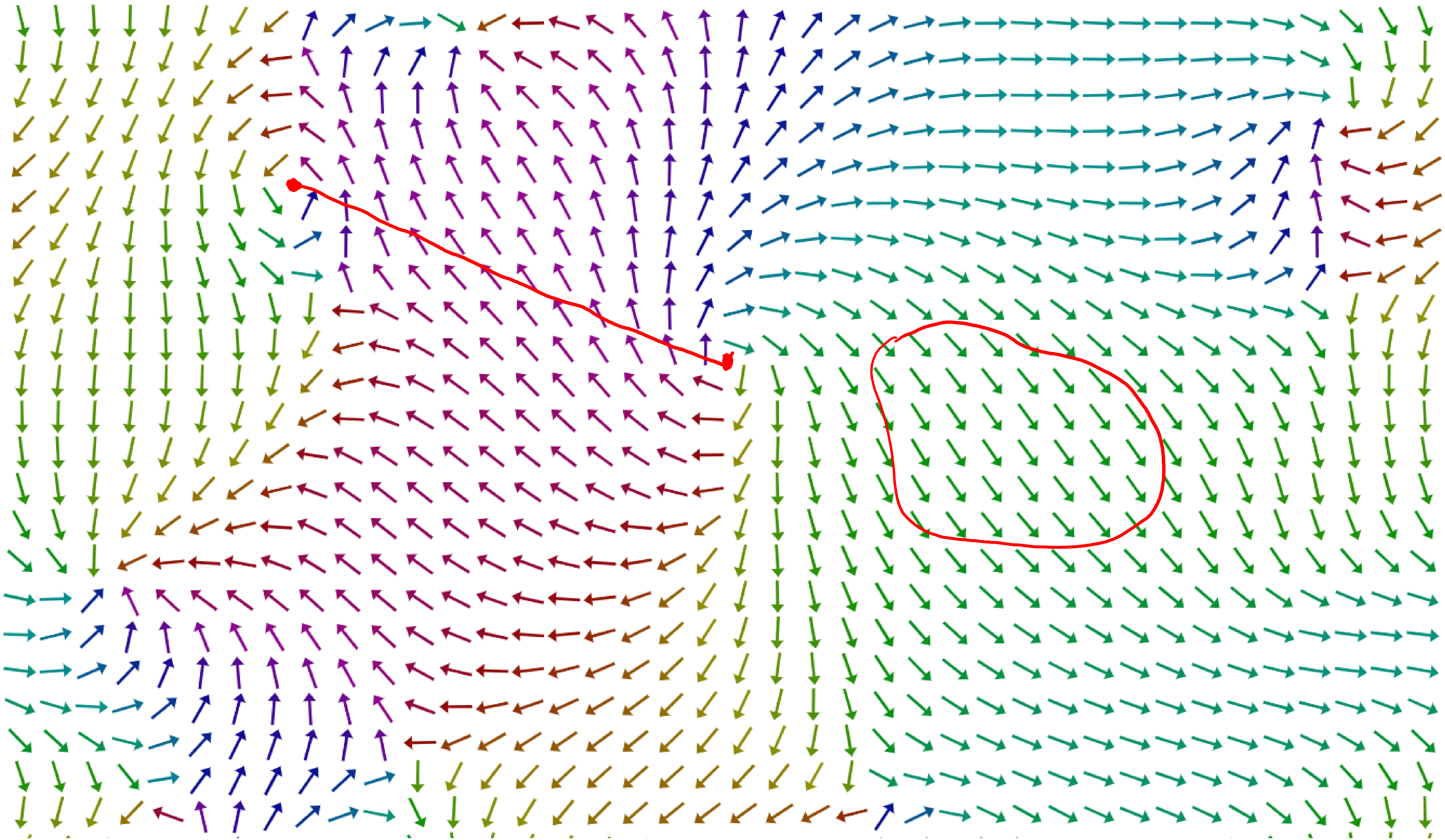
* $A(x \to x')$ above ensures detailed balance

Monte Carlo with Metropolis rejection

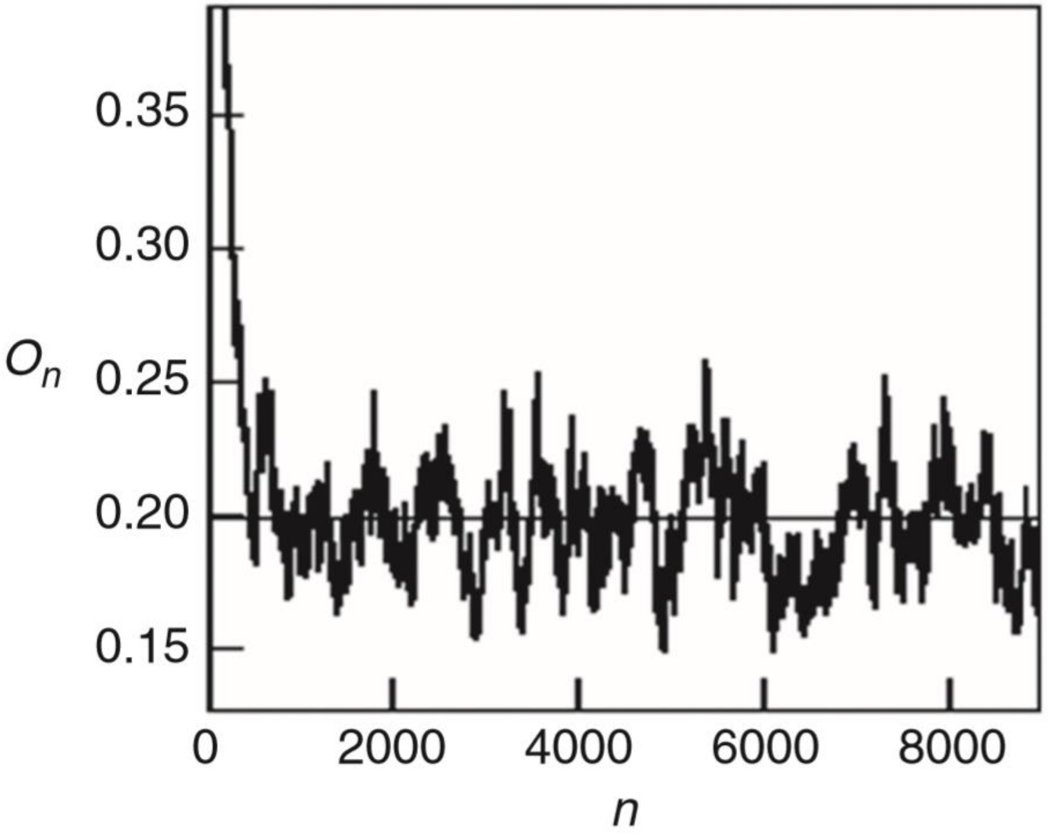


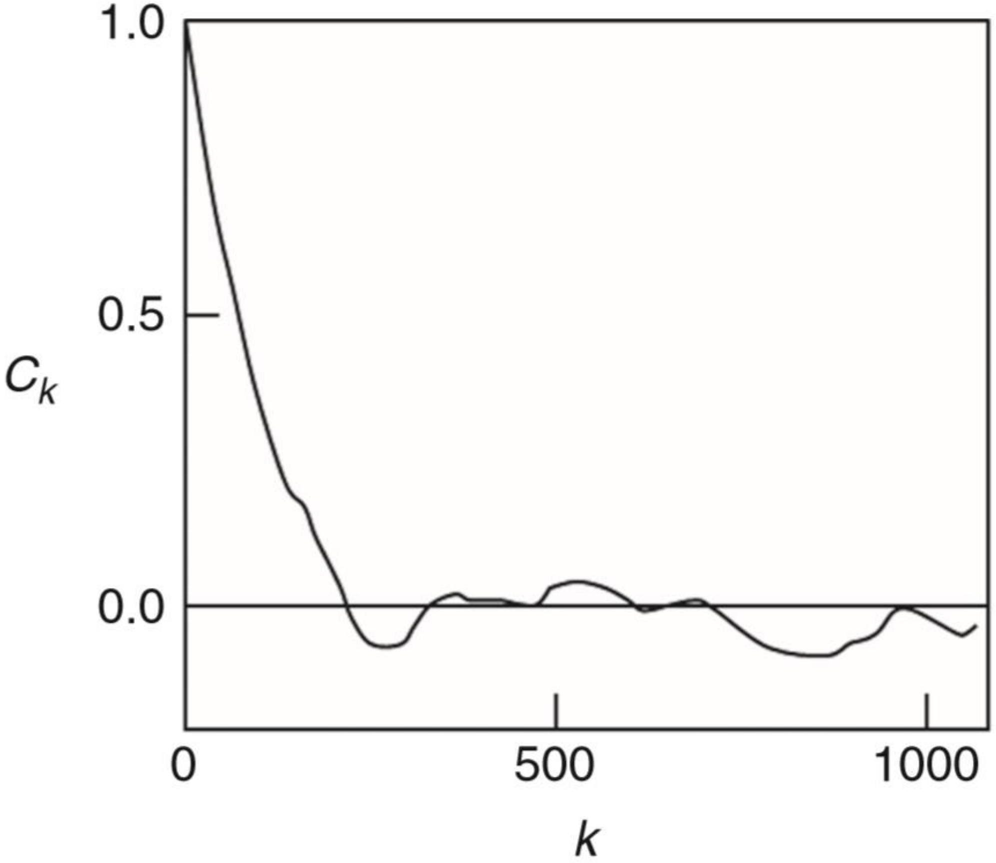
1. Start from a state x_0
2. Iterate the following N times
   - Propose a move $x_i \rightarrow x_{i+1}$
   - If $U(x_{i+1}) < U(x_i)$ accept the move
     else accept the move with probability $p = \exp(-\frac{U(x_{i+1}) - U(x_i)}{kT})$
   - Compute and output observables regardless of whether the move is accepted

Demo



Calculation of the observables





From [Martin *et al* Interacting Electrons ch. 22]

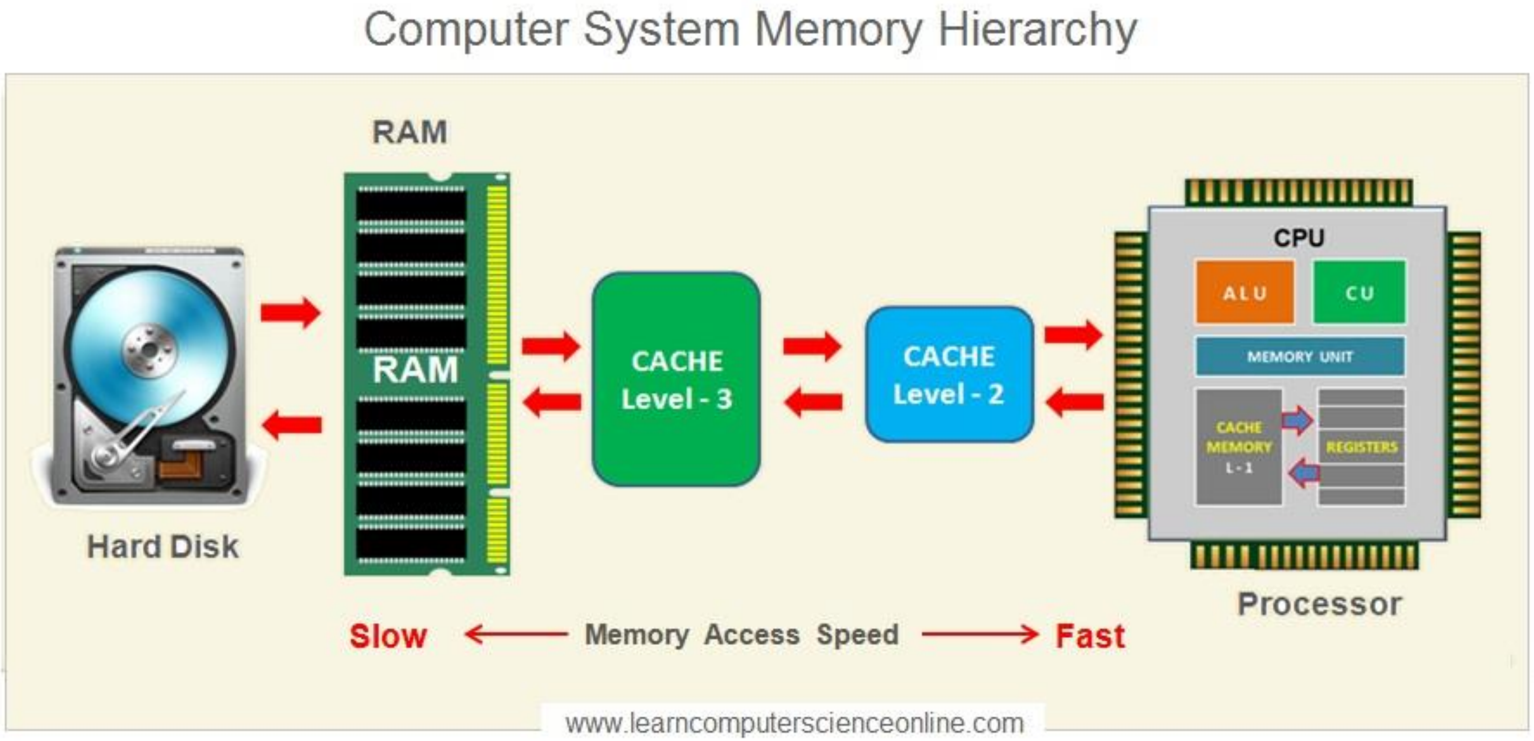
Computer performance I

- Select random spin – 2
- Propose change – 1
- Calculate Energy – 4
- Accept or reject – 30

<100

Computer performance I

- Select random spin
- Propose change
- Calculate Energy
- Accept or reject



Computer performance II (oversimplification)

```
// The worst you can do
i = randi(N);
j = randi(M);
if(s[i,j]==...)
  ...
```

```
// The best you can do
for(i=0; i<N; i++)
  for(j=0; j<M; j++)
    s[i,j] += ...
```

Other sampling methods: Molecular dynamics

$$H(p, x) = U(x) + T(p)$$

$$\mathrm{d}x = M^{-1} p \mathrm{d}t$$

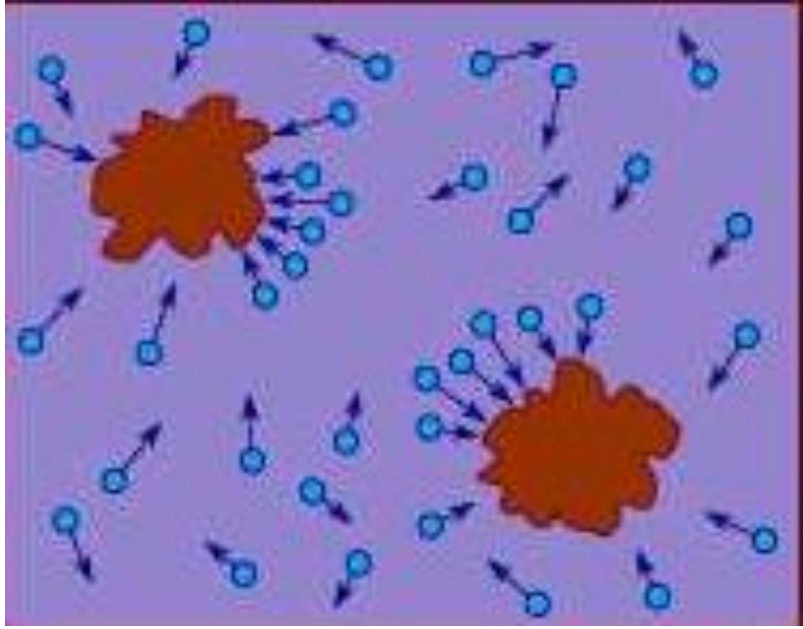
+ thermostat

$$\mathrm{d}p = -F(x)\mathrm{d}t \ = -\frac{\partial U(x)}{\partial x}\mathrm{d}t$$

$$P(p, x) = \ \frac{1}{Z} e^{-\frac{U(x)+T(p)}{kT}}$$

$$P(x) = \sum_{p} P(p, x) = \ \frac{1}{Z} e^{-\frac{U(x)}{kT}}$$

Other sampling methods



- Brownian dynamics

$$\mathrm{d}x = M^{-1}F(x)\mathrm{d}t + \sqrt{2kT}M^{-1/2}dW$$

- Langevin dynamics*

$$\mathrm{d}x = M^{-1}p\mathrm{d}t \qquad \mathrm{d}p = [F(x) - \gamma p]\mathrm{d}t + \sigma M^{\frac{1}{2}}dW$$

*See [Leimkuhler, Matthews AMRX (2013) v 1 p 34] for implementation details

Brownian dynamics: Implementation

$$\mathrm{d}x = M^{-1}F(x)\mathrm{d}t + \sqrt{2kT}M^{-1/2}dW$$

Implement as

$$x_{n+1} = x_n + M^{-1}F(x_n)h + \sqrt{2kTh}M^{-1/2}R_n$$

$R_n = \mathcal{N}(0,1)$

M- free parameter

h- time step

Brownian dynamics: Implementation

$$\mathrm{d}x = M^{-1}F(x)\mathrm{d}t + \sqrt{2kT}M^{-1/2}dW$$

Implement as

$$x_{n+1} = x_n + M^{-1}F(x_n)h + \sqrt{2kTh}M^{-1/2}R_n$$

or better as*

$$x_{n+1} = x_n + M^{-1}F(x_n)h + \sqrt{2kTh}M^{-1/2}\frac{R_n + R_{n+1}}{2}$$

$R_n = \mathcal{N}(0,1)$

M- free parameter

h- time step

*[Leimkuhler, Matthews AMRX (2013) v 1 p 34]

Brownian dynamics: Implementation

```
// Calculate forces first, then update is simply
for(i=0; i<N; ++i)
  for(j=0; j<M; ++j)
    x[i,j] += F[i,j]*h + sqrt(2*T*h)*nrand();
```

Demonstration

Erratum

Equation

$$\mathrm{d}x = M^{-1}F(x)\mathrm{d}t + \sqrt{2kT}M^{-1/2}dW$$

does has unit of time missing, correct equation is

$$\begin{aligned} x_{n+1} &= x_n + \frac{\delta t^2}{2} M^{-1} F(x_n) + \frac{\delta t}{2} M^{-1}(p_n + p_{n+1}) \\ &= x_n + \frac{\delta t^2}{2} M^{-1} F(x_n) + \frac{\delta t}{2} \sqrt{k_B T} M^{-1/2}(R_n + R_{n+1}), \end{aligned}$$