Take A Chance On Me

MCOM

Monte Carlo Condensed Matter

A very brief guide to Monte Carlo simulation.

An explanation of what I do.

A chance for far too many ABBA puns.

What's The Name Of The Game?

Simulation:
'I have a dream, a fantasy,
to help me through reality'

Given some model many-body system.

Simulate the evolution of the system.

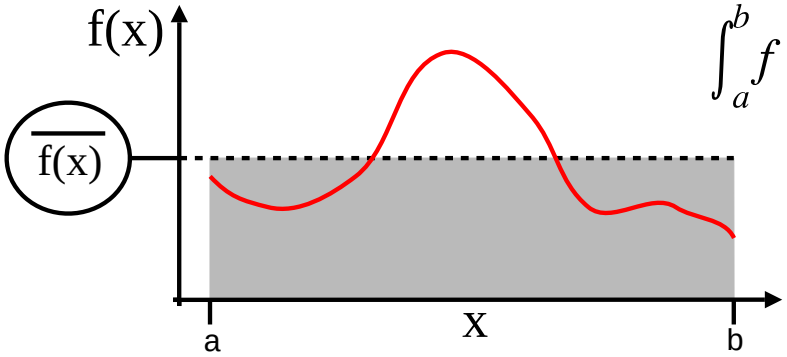
We can then measure various observables.

Attempt to predict properties of real systems.

Eg Equilibrium Properties
All about knowing free-energies,
phase behaviour, compressibility, specific heat,
knowing M(E), knowing μ.

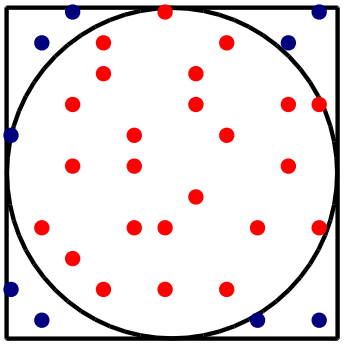
Monte Carlo Method

In 1 Dimension:



$$\int_a^b f(x)\,dx \equiv (b-a)\,\overline{f(x)} \approx \frac{1}{n}\sum_{i=1}^{N} f(\zeta_i)$$

In Two Dimensions:



$$\frac{A(circle)}{A(square)} = \frac{\pi r^2}{(2r)^2} = \frac{\pi}{4} \approx \frac{n_{inside}}{n_{total}}$$

$$\left[e.g.\ \frac{24}{33} = 2.9\right]$$

Can we do this for many-dimension integrations over phase space?

$$Z(N, V, T) = \prod_{i=1}^{3N}\left[\int_{-\infty}^{+\infty} d\dot{x}_i\right] \prod_{i=1}^{3N}\left[\int_{-\infty}^{+\infty} dx_i\right] \exp\left[-\frac{E(\{x\})}{k_B T}\right]$$

Can you hear the drums

FERNANDO

Monte Carlo In Statistical Mechanics:

Eg In the canonical ensemble (Constant N, V, T).

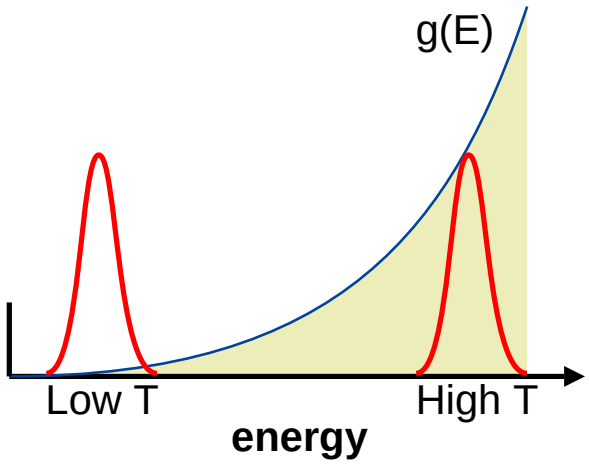
Generate microstates at random.

Estimate energy using...

$$\overline{E} \approx \frac{1}{n} \sum_{i=1}^{n} E_i \exp\left[-\beta E_i\right]$$

This doesn't work!

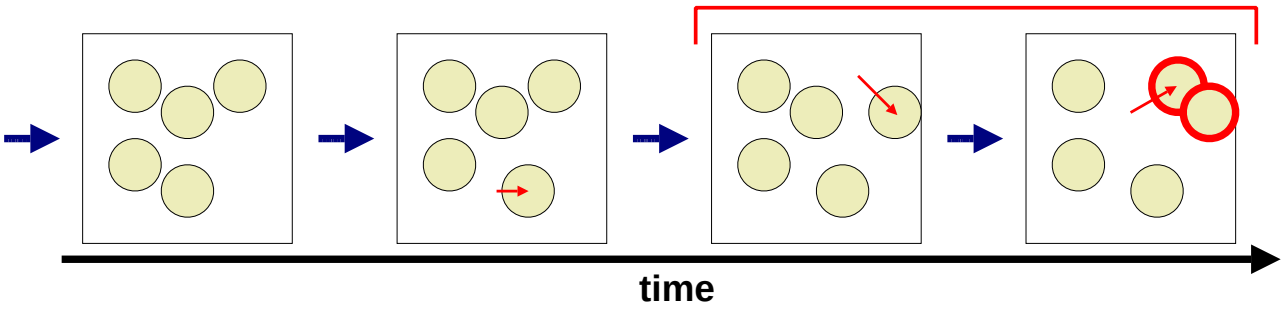
Eg Ising Model:
Tend to generate 'hot' configurations.



Can we generate the right (high Boltzmann weight) configurations all the time, instead of waiting for them?

Can we simulate, not just integrate?

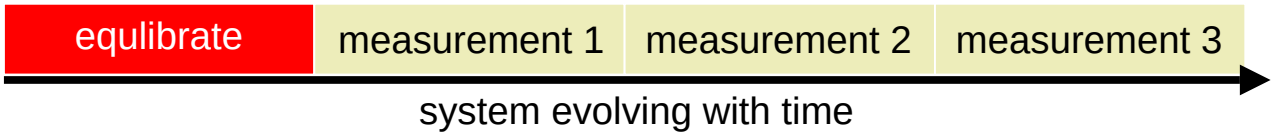
Markov Chains:



OK, but we can't accept all moves.

How do we decide whether to accept a trial move?

Convergence:



Can show that microscopic reversibility ('detailed balance') is a sufficient condition to ensure convergence.

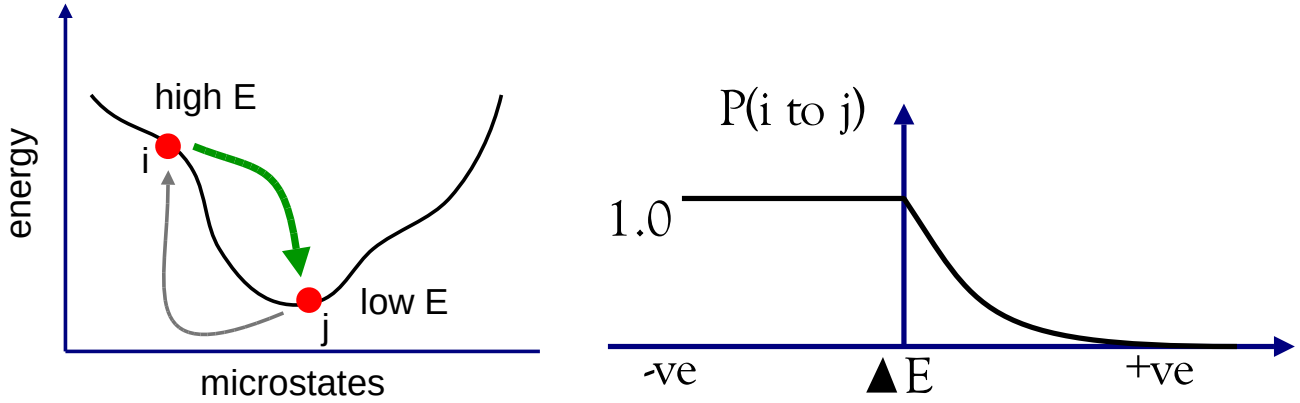
$$\frac{P(i)}{P(j)} = \frac{P_{tr}(j \rightarrow i)}{P_{tr}(i \rightarrow j)}$$

We need an algorithm that satisfies this condition and will sample with the Boltzmann distribution.

Importance Sampling:

Moves to lower energies are ALWAYS accepted.

Moves up are accepted sometimes...



$$P(i \rightarrow j) = \min[\,1.0,\ \exp(-\beta(E_j - E_i))\,]$$

$$P(i) = \frac{1}{Z}\exp(-\beta E_i)$$

Putting these into the detailed balance condition:

$$\exp(-\beta E_i) \times 1.0 = \exp(-\beta E_j) \times \exp(-\beta(E_i - E_j))$$

This generates a sequence of Boltzmann distributed microstates.

Estimate observables like this:

$$\overline{E} \approx \frac{1}{n}\sum_{i=1}^{n} E_i$$

Limitations:

Finite system size

Trying to predict the behaviour of an infinite system,
using only a few hundred/thousand particles.

One should always examine a range of system sizes.
Can then estimate the effects of finite size.

Finite Simulation Time

Trying to predict the equilibrium behaviour of real systems,
i.e. minutes or hours or even months of real time.

Simulation can only usually provide a few microseconds.

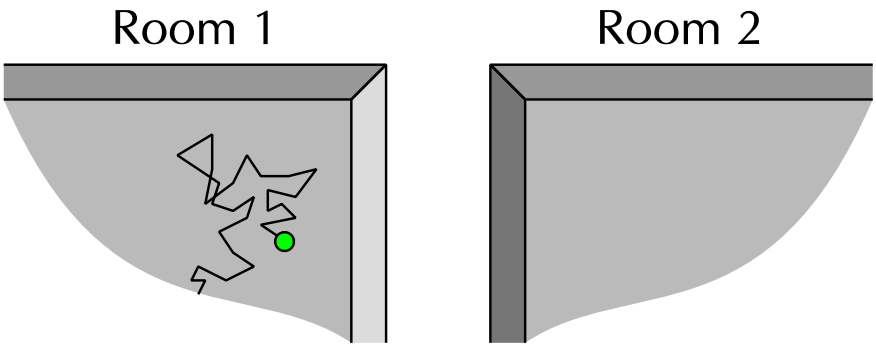
I'm interested in structural phase transitions,
using importance sampling I would have to wait
decades to observe an fcc to hcp transition.

Is Monte Carlo finally facing it's Waterloo.

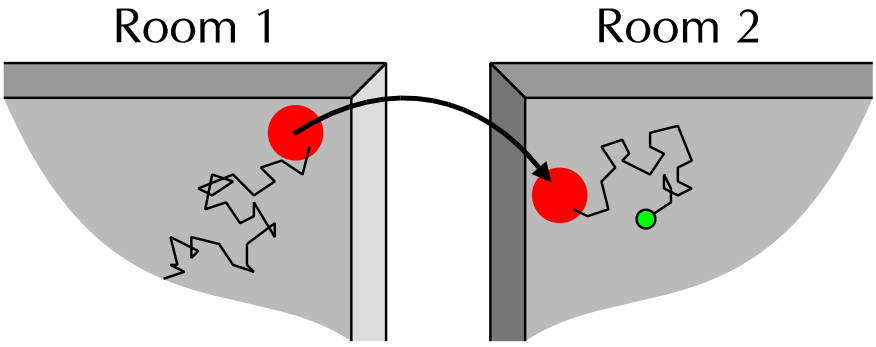
Beating The System

Eg The Double Disco Dancing Queen:

Normal Monte Carlo



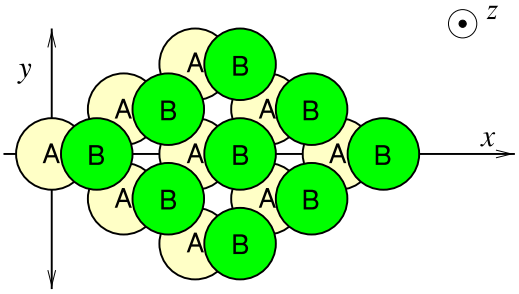
Ensemble Switching



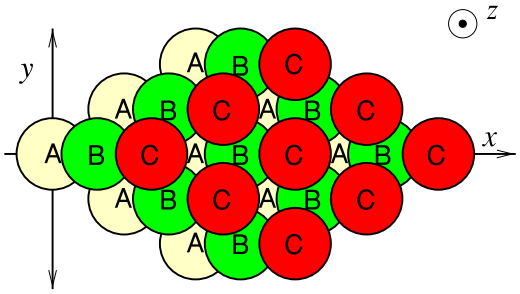
What I do:

Compare structures, Eg...

Hexagonal Close-Packed

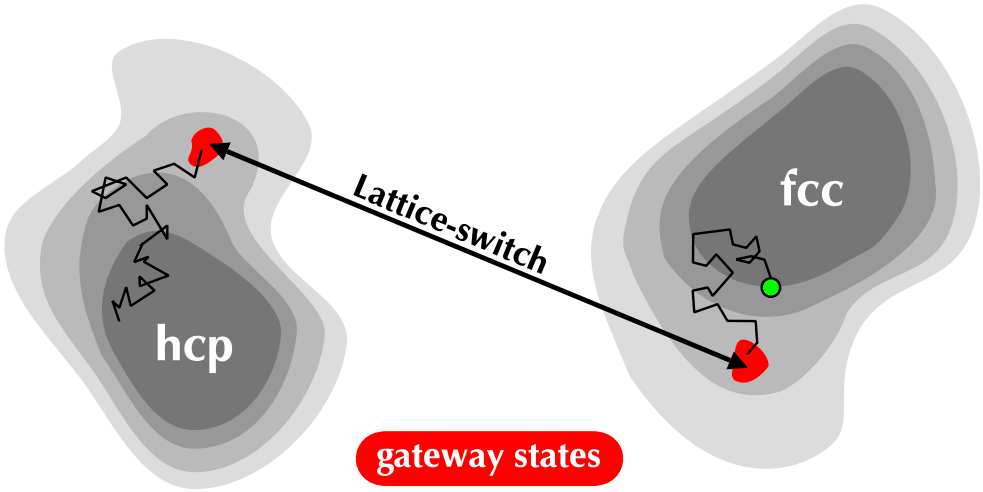


Face-Centered Cubic



ABABAB versus ABCABC

(sadly, not ABBAABBA)



$\mathcal{M} < 0$ $\mathcal{M} = 0$ $\mathcal{M} > 0$

The pun possibilities:

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ABBA were: Bj:orn, Benny, Agnetha and Anni-Frid (Frida). Swedish.

Songs:

Dancing Queen - Having the time of your life,
looking out for place to go,
hiiiiiigh,
watch that scene,

Knowing me, knowing you ‘ah-aaa’
There is nothing we can do.
Breaking up is never easy I know, but I have to go.

Take a chance on me,
if you change your mind I’ll be first in line,
honey I’m still free
if you got no place to go, when you feeling down
If you put me to the test, if you let me try.
So much that I want to do
It’s magic
but I can’t let go.
Bababaha-ba bababa-ba-ba

Mamma mia - here i go again.

Lay all you love on me
don’t go wasting your emotion

Super Trouper
And somewhere in the crowd there’s Sue.

I have a dream, a fantasy, to help me through reality
If you’ve see the wonder of the fairytale.
I believe in Angels.

I’ve crossed the stream

The winner takes it all, the loser’s standing small/has to fall.
nothing else to say, no other ace to play.

Money, money, money it must be funny in a rich man’s world. always sunny. Aha--aaah ah ahhh
all the things I had I could do.

S.O.S. it use to be so nice, it used to be so good.
when your gone, how can i even try to go on.

Chiquitita you and I know.

Fernando
can you hear the drums, fernando
if I had to do the same again, i would my friend

Voulez Vous

Gimme! Gimme! Gimme! (a man after midnight)

Does your mother know that your out.
i could dance with you honey, if you think that it’s funny.

One of us

whats the The name of the game?

so i say Thank you for the music, the songs i’m singing, the joy their bringing. for giving it to me.

Waterloo - My my, at Waterloo Napolean did surrender. Yeah yeah.
couldn’t escape if I wanted to.
i feel like i win when i lose.
finally facing my waterloo.
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