Materials Modeling
— An Illustration with Magnetism

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Outline:

Ferromagnetism in Fe, Ni, etc. (existence of T_c)

Can we develop a simple model for it?

- Phase transitions
- A bit of statistical mechanics
  - Boltzmann distribution
- The Ising Model for Ferromagnetism
- Grown-up's π game
  - allows actual calculations based on Boltzmann distribution
- Simulating the Ising Model

Phase transitions

(1) Percolation

- Each site of lattice is occupied with probability p
- There exists p_c at which a *spanning* cluster first appears
  - For 2-D square lattice, $p_c \approx 0.593$
- At p_c, a phase transition occurs
  - *Fundamentally* different behaviors at $p > p_c$ and $p < p_c$, *e.g.*, conductivity in materials
- An example to see that p_c is special — forest fire model:

  * Occupied site $-\rightarrow$ a tree
  * All trees at one edge catch fire at $t_0 = 0$
  * In each clock cycle, all trees adjacent to burning trees will start to burn
  * Trees burning at t_{n-1} will burn out at t_n

  Q: What is the time it takes for entire fire to burn out?

Phase transitions

(2) ice $\Longleftrightarrow$ water

(3) Ferromagnetism in materials such as iron

ferromagnetic non-ferromagnetic

$$T_c \sim 1000\,\mathrm{K} \text{ for iron}$$

In both 2 and 3:

- Interactions between particles play a key role
- Phase transition occurs as a function of *temperature* T

In all cases, 1, 2, and 3, tuning of a parameter is involved, as opposed to self-organized critical phenomena.

The Boltzmann distribution

- For a system in equilibrium at temperature T, the probability for finding the system in any particular state α is

  $$P_\alpha \propto e^{-E_\alpha/kT},$$

  — E_α is the energy of a (microscopic) state α

  — k is a universal constant (Boltzmann's constant)

- Any macroscopic quantity of the system is given by the *weighted average* of microscopic states, *e.g.*,

  $$E = \sum_\alpha P_\alpha E_\alpha = \frac{\sum_\alpha E_\alpha e^{-E_\alpha/kT}}{\sum_\alpha e^{-E_\alpha/kT}}$$

Note:

- state $\longleftrightarrow$ 'snapshot'
- energy E_α comes from particle interaction
- As T is lowered, high-energy states are occupied less and less

The Ising model for ferromagnetism

The Ising model:

- Square lattice of magnetic moments (think of as atoms with spin)
- Each lattice site has one spin
- Each spin can have one of two possible values $s_i = \pm 1$ ($\uparrow$ or $\downarrow$)
- *Near-neighbor* spins interact

$$E_\alpha = -J \sum_{\langle ij \rangle} s_i \, s_j$$

$\langle ij \rangle$: a pair of *near-neighbor* spins i and j
$J > 0$: a known constant

- Periodic boundary condition is imposed

Qualitatively:

- Aligned spins lower the energy

- High T, random;
  low T, aligned

Grown-up's π game

Goal:

To generate a *uniform* distribution of stones inside (big) square

Algorithm:

1. Throw stone in random direction

2. If stone landed *inside* square,
   walk to stone, take out a new one from bag, and repeat 1

   otherwise (stone landed *outside* square),
   take out a new stone from bag and drop it at current position;
   take out (yet another!) new stone and repeat 1

What's the point?

It's possible to create a Markov chain random walk with simple rules whose asymptotic distribution is the desired PDF

Note:

- Kids' game is *always* the better algorithm
- Specific drawbacks of grown-up's game:
  - requires equlibration time
  - successive samples are correlated (memory effect)
- But, unlike in this simple case, often there is no algorithm to *directly* sample a complicated, many-dimensional PDF
- Grown-up's game contains the essence of a *general* solution

  — **the Metropolis Algorithm**

Extension of the grown-up's game

Another example:

How to sample x from the PDF $f(x) = e^{-x}$ where x is on $(0, \infty)$?

"Kids' algorithm": `x=-log(rand())`

The following algorithm *also* works: — Metropolis algorithm

0. Start random walk at any position $x > 0$

1. *Propose* to move x to a new position x',
   where x' is selected randomly and uniformly
   inside a 1-d box of length L centered at x.

2. Compute $p \equiv f(x')/f(x)$.

3. <u>If</u> $p \geq 1$,
   accept x', *i.e.*, set $x = x'$

   <u>otherwise</u>
   accept x' with probability p
   accept: $x = x'$
   not accept: $x = x$

4. Repeat from 1.

- How to choose L?

Simulating the Ising Model

What exactly is it that we want to do?

- to generate states α from the Boltzmann distribution $P_\alpha \propto e^{-E_\alpha/kT}$

Given states distributed according to the PDF P_α, macroscopic quantities can be computed, e.g., the total energy:

$$E_{\text{tot}} = \sum_\alpha P_\alpha E_\alpha \qquad \text{weighted average}$$

is given by the average of E_α w.r.t. the samples (Monte Carlo integration)

The Metropolis Algorithm — grown-ups' game

0. Start random walk at any state $\alpha = \{s_1, s_2, \cdots, s_N\}$
1. *Propose* to move current state α to a new state α' by
   (a) randomly selecting a site (say, i)
   (b) flipping its spin (i.e., letting $s_i' = -s_i$)
2. Compute $p \equiv P_{\alpha'}/P_\alpha$.

3a. If $P_{\alpha'}/P_\alpha \geq 1$, accept α' as new state, i.e., set $\alpha = \alpha'$; otherwise, accept α' with probability $P_{\alpha'}/P_\alpha$.

— if accept, set $\alpha = \alpha'$

— if not accept, set $\alpha = \alpha$

3b. Accumulate measurements ($e.g.$, E_α).

4. Repeat from 1.

Simulating the Ising Model

Note:

1. In proposing new state:

   - $N = L \times L$ attempted flips is considered one step

   - sweeping thru lattice also ok (vs. random site selection)

2 a. Computation of $p \equiv P_{\alpha'}/P_\alpha$ is fast (local interaction).

Actual Simulation — and what can we learn from it?

`http://bartok.ucsc.edu/peter/java/ising/keep/ising.html`

Summary:

- Phase transitions are common and important.
- Statistical mechanics provides framework to relate microscopic quantities to equilibrium macroscopic properties.
  - Boltzmann distribution
  - Phase transitions, as well as other equilibrium phenomena, directly arise from this framework
- The Ising model — a simple microscopic model for magnetism
  - Has applications in magnetism, binary alloys, liquid-gas transitions, etc.
  - Has played an important role in furthering our understanding of the quantitative aspect of phase transitions
- The algorithm of Metropolis *et. al.*
  - A Markov chain random walk which generates random variables according to essentially any PDF.
  - Provides a general approach to simulating systems in thermal equilibrium, and allows detailed calculations according to the laws of statistical physics.
  - Is widely applied in many disciplines — problems include polymers, protein folding, quantum electronics, etc.