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 $\iff$ water

(3) Ferromagnetism in materials such as iron

\[
\begin{array}{cc}
\text{ferromagnetic} & \text{non-ferromagnetic} \\
T_c & \sim 1000 \text{ K for iron}
\end{array}
\]

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 $\alpha$ is

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

  — $E_\alpha$ is the energy of a (microscopic) state $\alpha$
  — $k$ 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 $E_\alpha$ 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 \( s_i = \pm 1 \) (↑ or ↓)
- *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 equilibration 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”: $x = -\log(\text{rand}())$

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 $p = f(x')/f(x)$.

3. If $p \geq 1$, 
   accept $x'$, i.e., set $x = x'$
   otherwise 
   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 $\alpha$ from the Boltzmann distribution $P_\alpha \propto e^{-E_\alpha/kT}$

Given states distributed according to the PDF $P_\alpha$, macroscopic quantities can be computed, e.g., the total energy:

$$E_{\text{tot}} = \sum_\alpha P_\alpha E_\alpha$$

weighted average

is given by the average of $E_\alpha$ w.r.t. the samples
(Monte Carlo integration)

The Metropolis Algorithm — grown-ups’ game

0. Start random walk at any state $\alpha = \{s_1, s_2, \ldots, s_N\}$

1. Propose to move current state $\alpha$ to a new state $\alpha'$ by
   (a) randomly selecting a site (say, $i$)
   (b) flipping its spin (i.e., letting $s'_i = -s_i$)

2. Compute $p = P_{\alpha'}/P_\alpha$.

3a. If $P_{\alpha'}/P_\alpha \geq 1$, accept $\alpha'$ as new state, i.e., set $\alpha = \alpha'$;
    otherwise, accept $\alpha'$ with probability $P_{\alpha'}/P_\alpha$.
    — if accept, set $\alpha = \alpha'$
    — if not accept, set $\alpha = \alpha$

3b. Accumulate measurements (e.g., $E_\alpha$).

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.