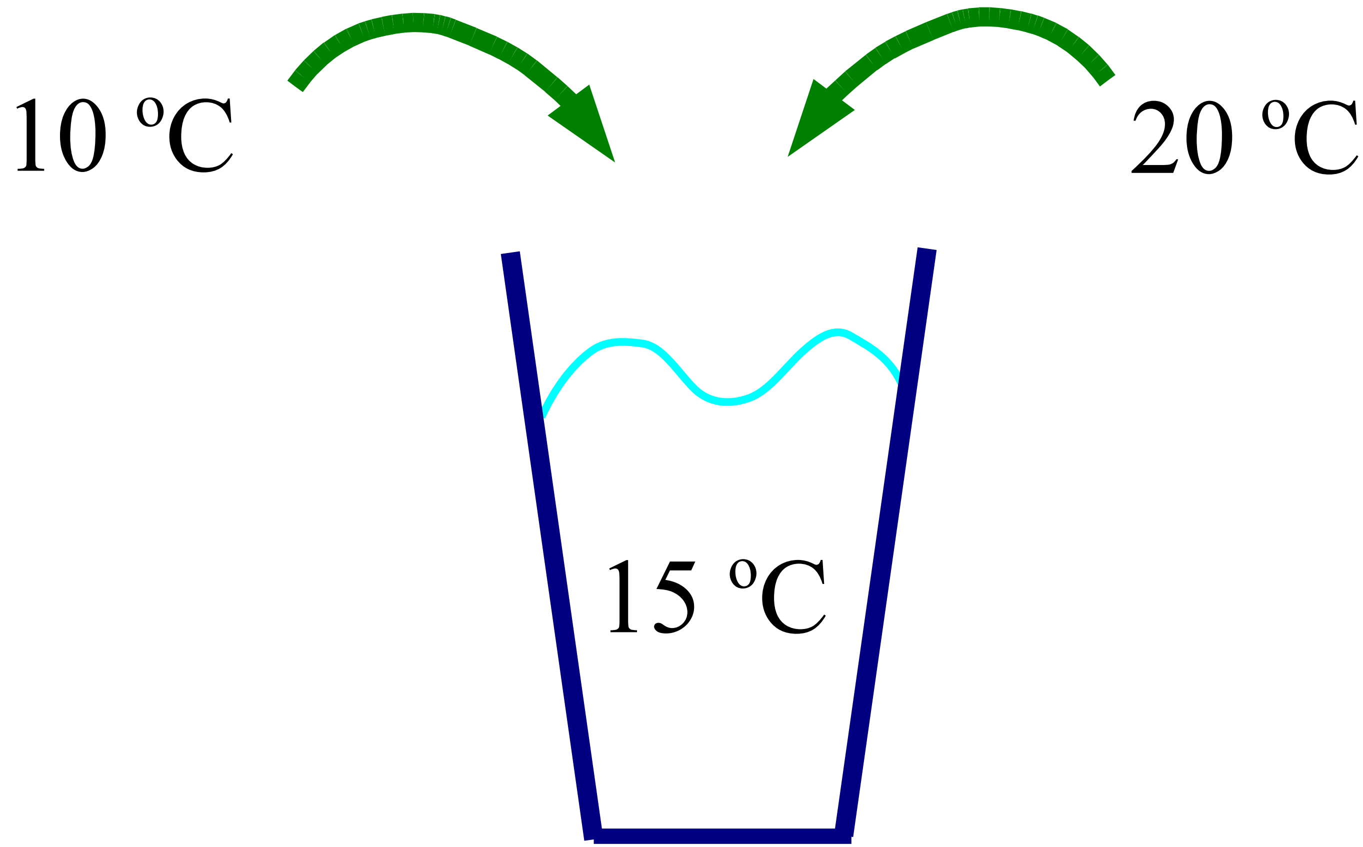
Why Water Freezes (A probabilistic view of phase transitions)

Mark Huber
Dept. of Mathematics and Institute of Statistics and Decision Sciences
Duke University
mhuber@math.duke.edu
www.math.duke.edu/~mhuber

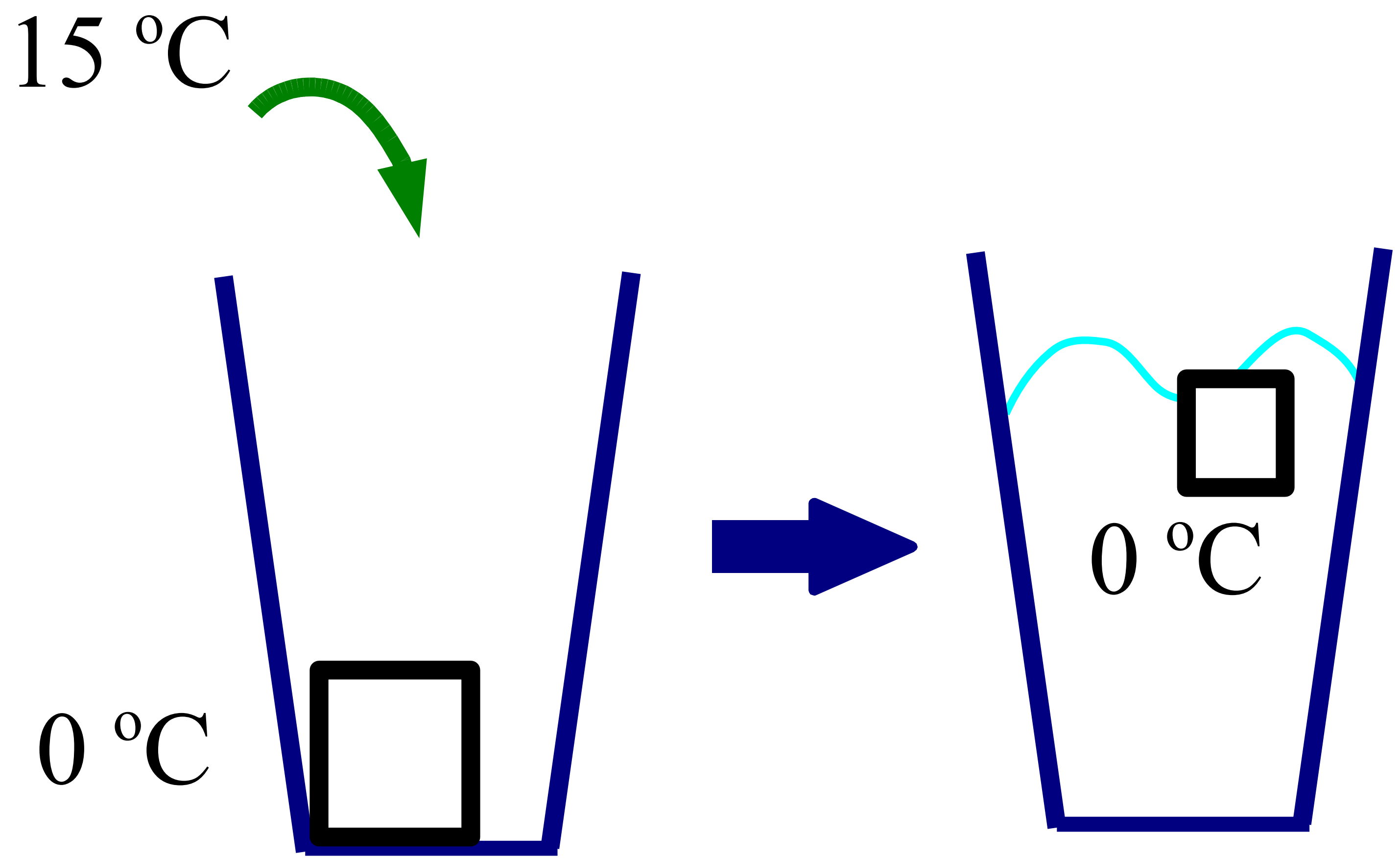
Mom's Old Fashioned Ice Water

1: Get water, cubes of ice
2: Place ice in water
3: Wait until water is cold
4: Drink and enjoy!

Mixing liquids



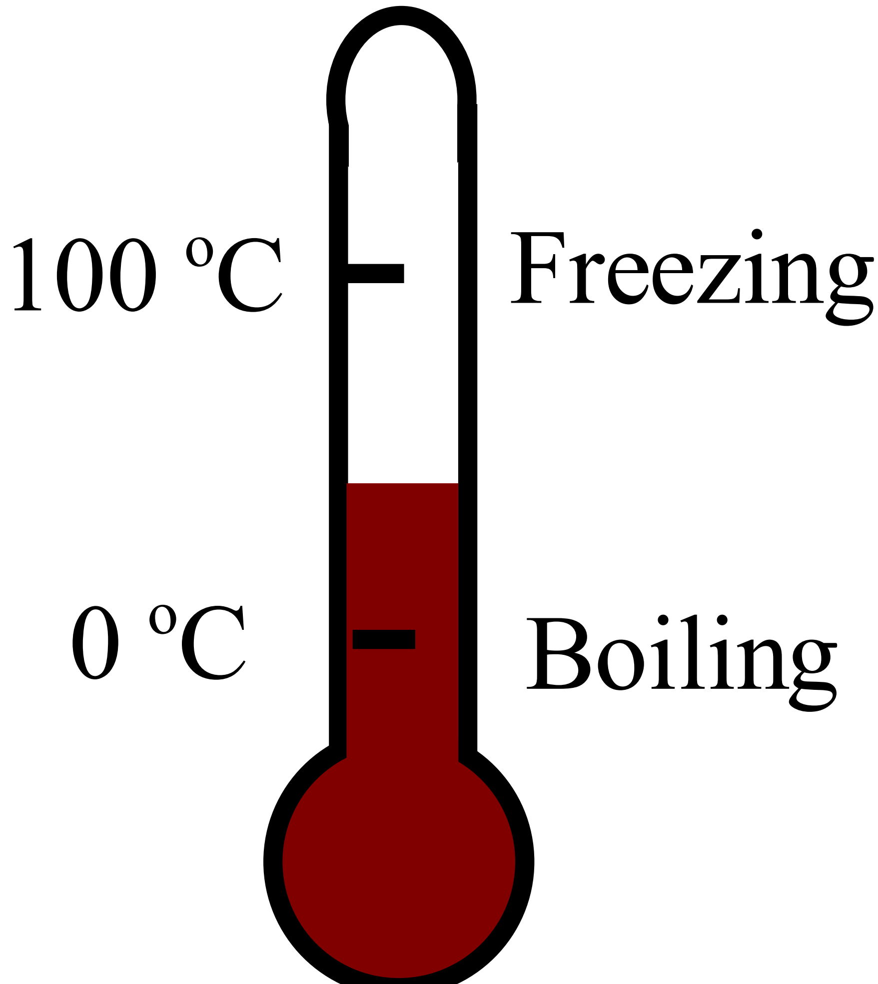
Not so with ice water



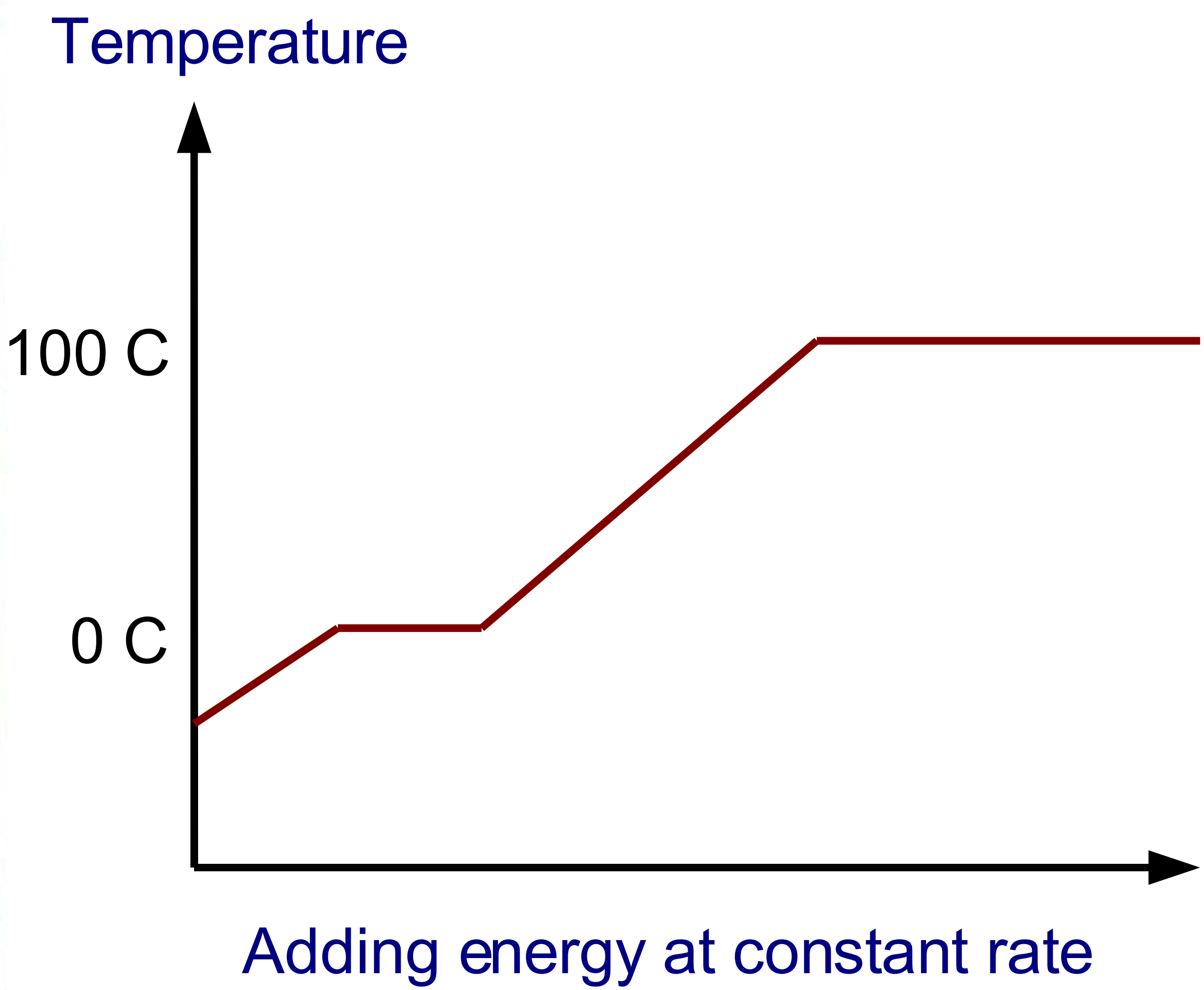
Thermometer calibration

First to notice this: Anders Celsius (1701-1744)

(Freezing point independent of latitude)



Phase Transition



Takes extra energy to complete phase transition from ice to water

Properties

Ice

Long Range Behaviour

Molecules in lockstep

Keeps its shape

Water

Short Range Behaviour

Molecules loosely bound

Loses shape almost instantly

A short history of physics

Newton
(1642-1727)

?

Einstein
(1879-1955)

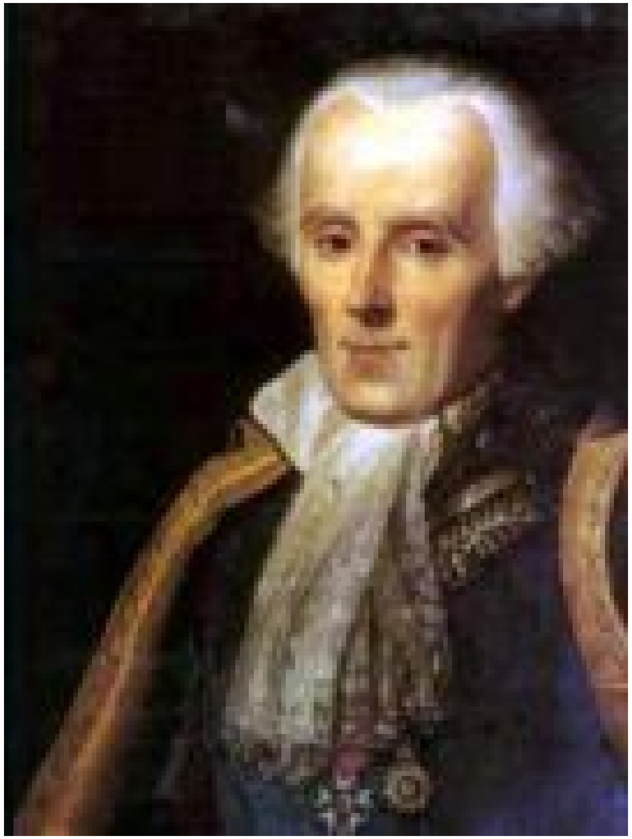
A slightly longer history of physics

Newton
(1642-1727)

Laplace
(1749-1827)

Einstein
(1879-1955)

"The most important questions of life are, for the most part, really only problems of probability."



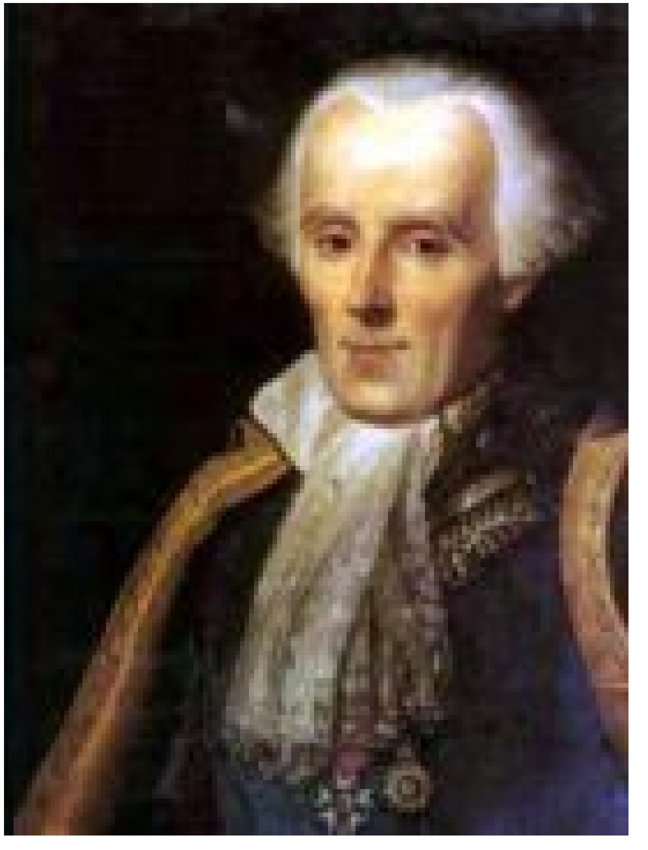
A slightly longer history of physics

Newton
(1642-1727)

Laplace
(1749-1827)

Einstein
(1879-1955)

"... I have sought to establish that the phenomena of nature can be reduced in the last analysis to actions at a distance between molecule and molecule, and that the consideration of these actions must serve as the basis of the mathematical theory of these phenomena."



The original: the Ising model

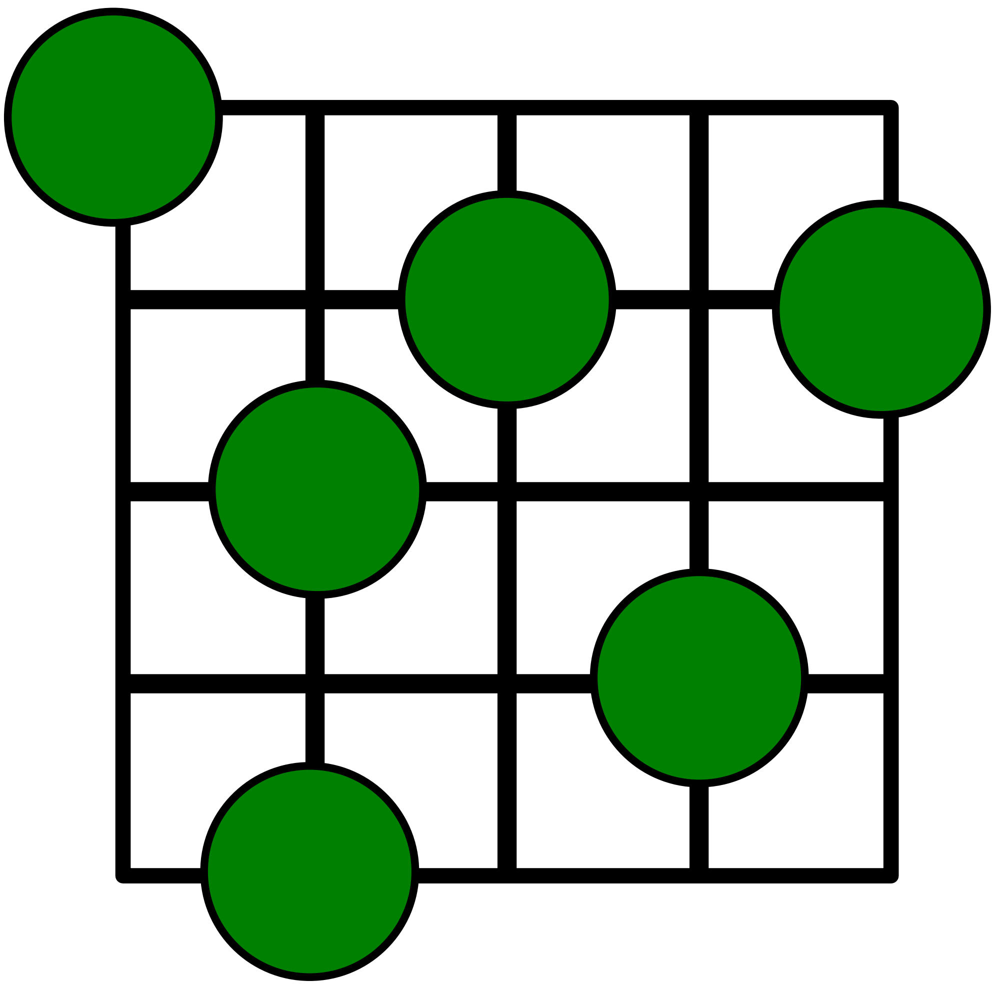
Simple probabilistic model

First to exhibit a phase transition (1924)

Originally used for magnets—currently used to describe alloys

The Hard Core Gas Model

Configuration x: a placement of molecules



No two molecules can be adjacent to each other

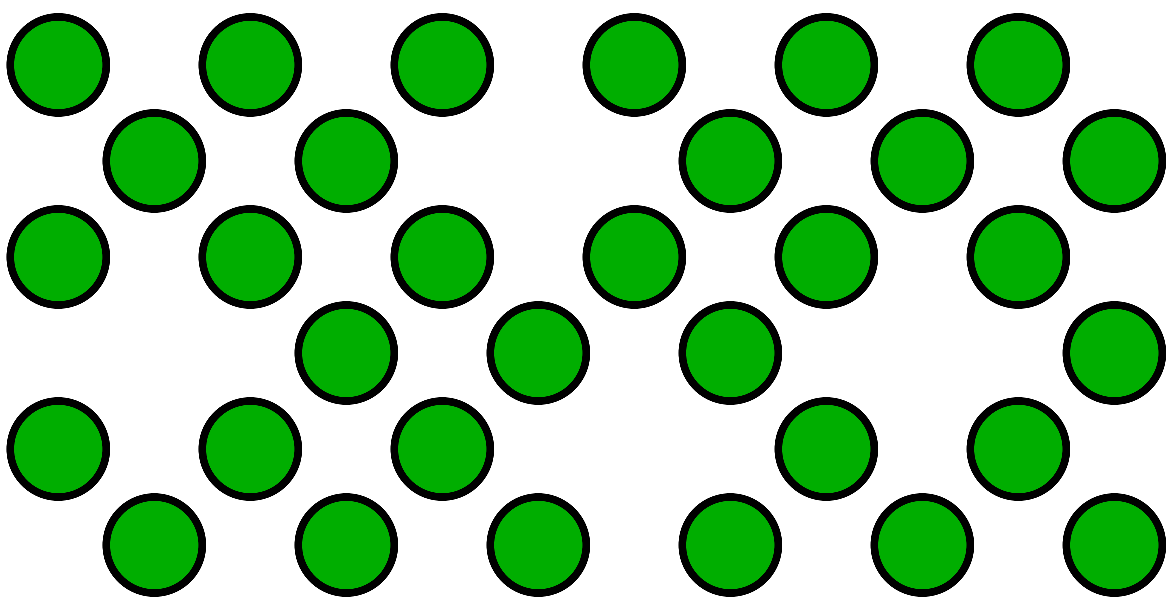
$$\pi(x) = \frac{\lambda^{|x|}}{Z}$$

Hard Core has phase transition!

Distribution looks "smooth" in λ

When λ small, short range interactions

Past critical point, long range ("checkerboard")



Moving up to the 1950's...

Computers speed increasing exponentially

Physicists begin simulating Ising, Hard Core gas model (Monte Carlo Markov Chain approach)

Algorithms for combinatorial optimization problems become feasible

Monte Carlo Markov chain

Goal: generate samples from distribution

Start at an arbitrary configuration
Make "lots" of small random changes to the configuration
Hope that final configuration has distribution close to the target

Example: shuffling cards

The Problem: How many is "lots"?

Upper bounding "lots"

Use bounding chain to experimentally bound "lots" (H. '96)

Start at all configurations simultaneously

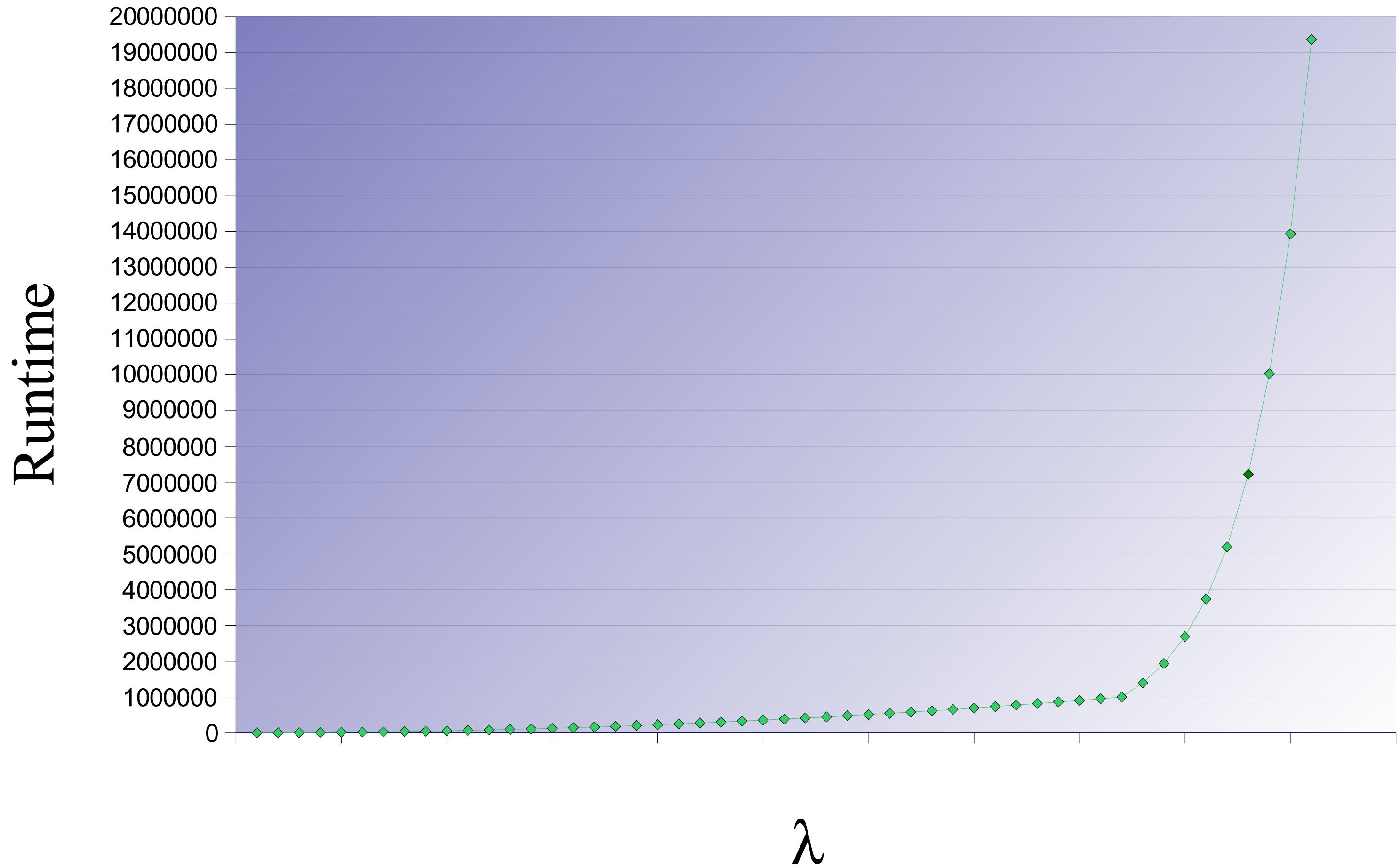
Make "lots" of small random changes to all these configurations at same time

Merge configurations as they run into each other

Time needed to merge into one configuration is an upper bound on "lots" (Doeblin '33, Aldous '82)

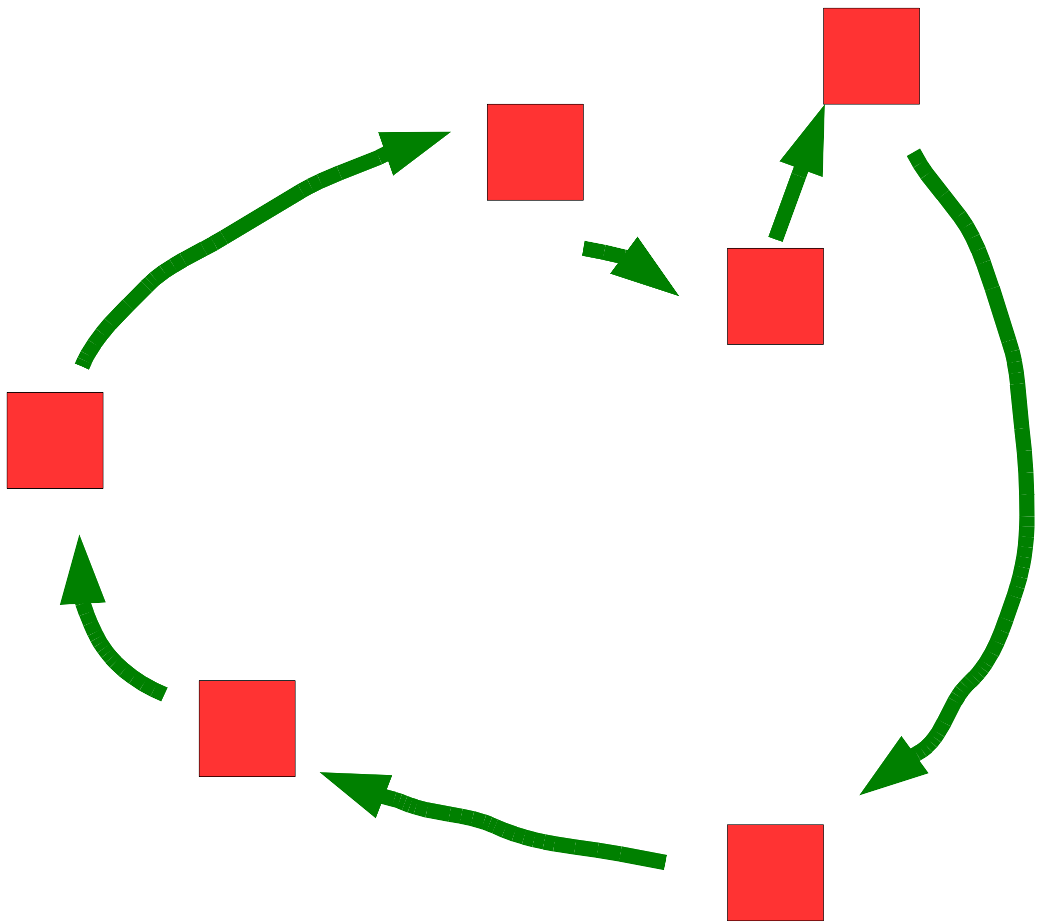
The Results

Time needed for Markov chain to mix undergoes a phase transition at the same λ

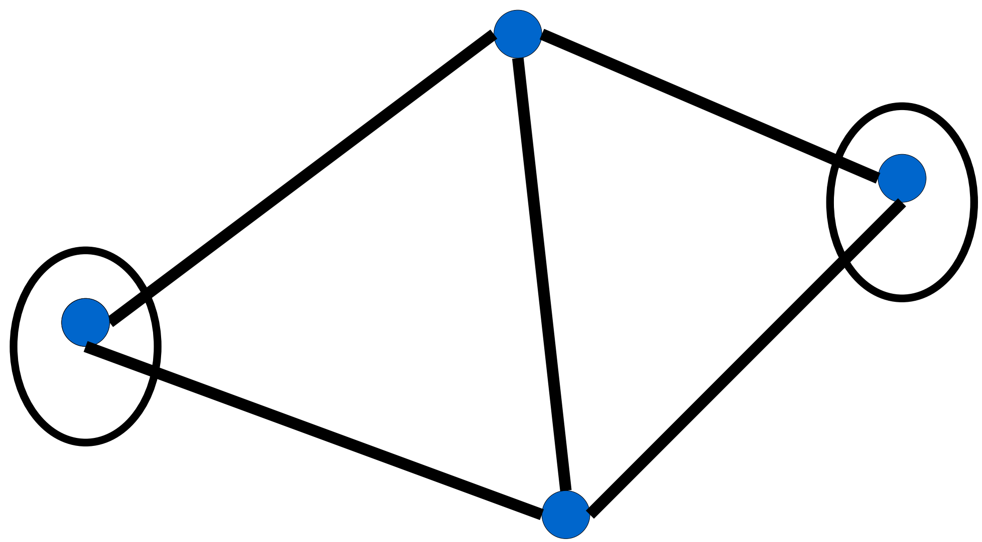


Combinatorial Optimization

The Traveling Salesman Problem



Independent Sets of a graph



MAX independent set problem: Find the largest set of vertices such that no two are adj.

Both TSP and MAX IND SET are *NP*-complete

Simulated Annealing

Sneak up on answer:

Small λ gives small ind sets, MC quick

Large λ gives large ind sets, MC slower

$$\pi(x) = \frac{\lambda^{|x|}}{Z}$$

The Problem:

Below phase transition, MC quick

Above phase transition, MC very slow

Even sampling hard

Let Δ be maximum degree of a graph

Dyer, Frieze, Jerrum ('98) showed:

if you can sample from π for any graph with parameters

$$\lambda > \frac{25}{\Delta}$$

then NP = RP

Markov chain for Independent Sets

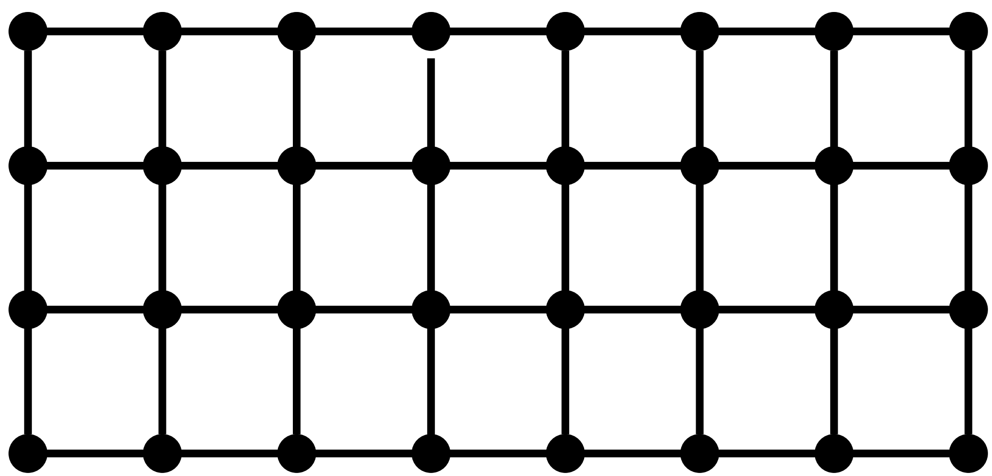
Choose a site uniformly at random

If a neighbor is occupied
    leave the site unoccupied
Otherwise
    With probability $\dfrac{\lambda}{\lambda+1}$
        Make the site occcupied

    With probability $\dfrac{1}{\lambda+1}$
        Make the site unoccupied

Graph structure determins phase transition

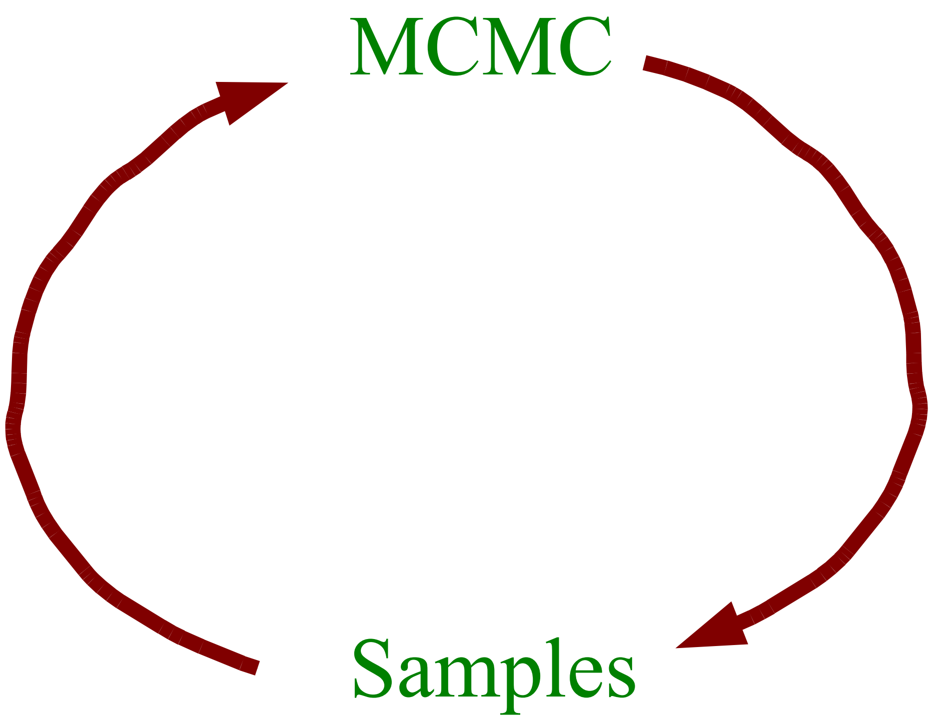
1 Dimensional
No phase transition



2 Dimensional
Phase transition

Expander graphs
Worst case

The Vicious Circle



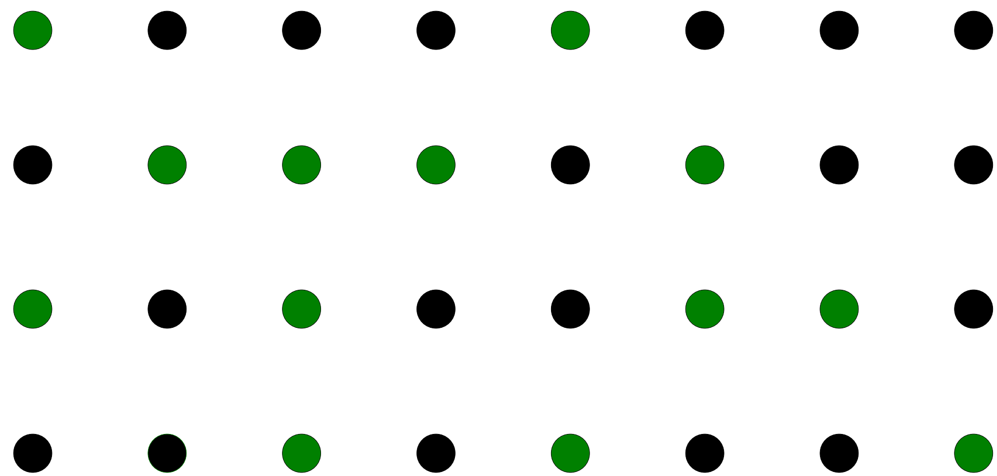
Breaking the cycle of dependence: perfect samplers

Perfect sampling algorithms can sample from:

$$\pi(x) = \frac{weight(x)}{Z}$$

without the need to know Z

Idea: modify graph to make problem easy

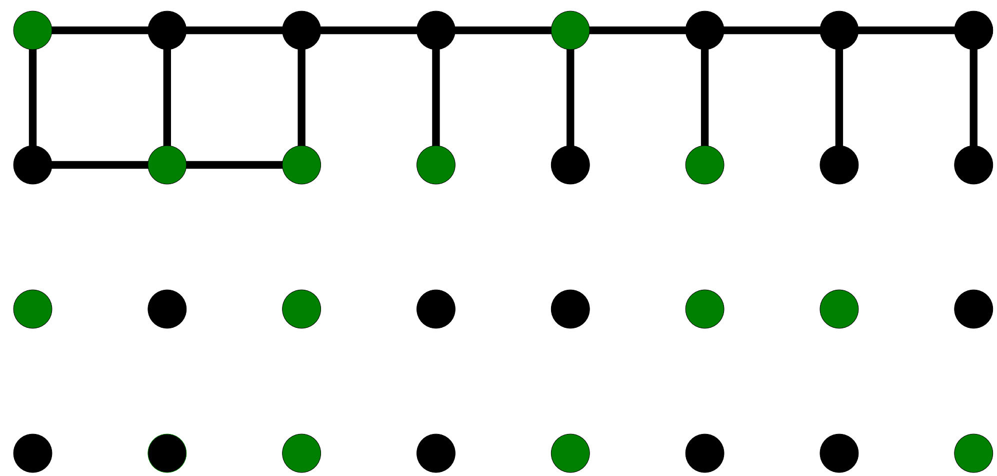


(H., Fill '98)

Step 1: Remove all the edges in the graph

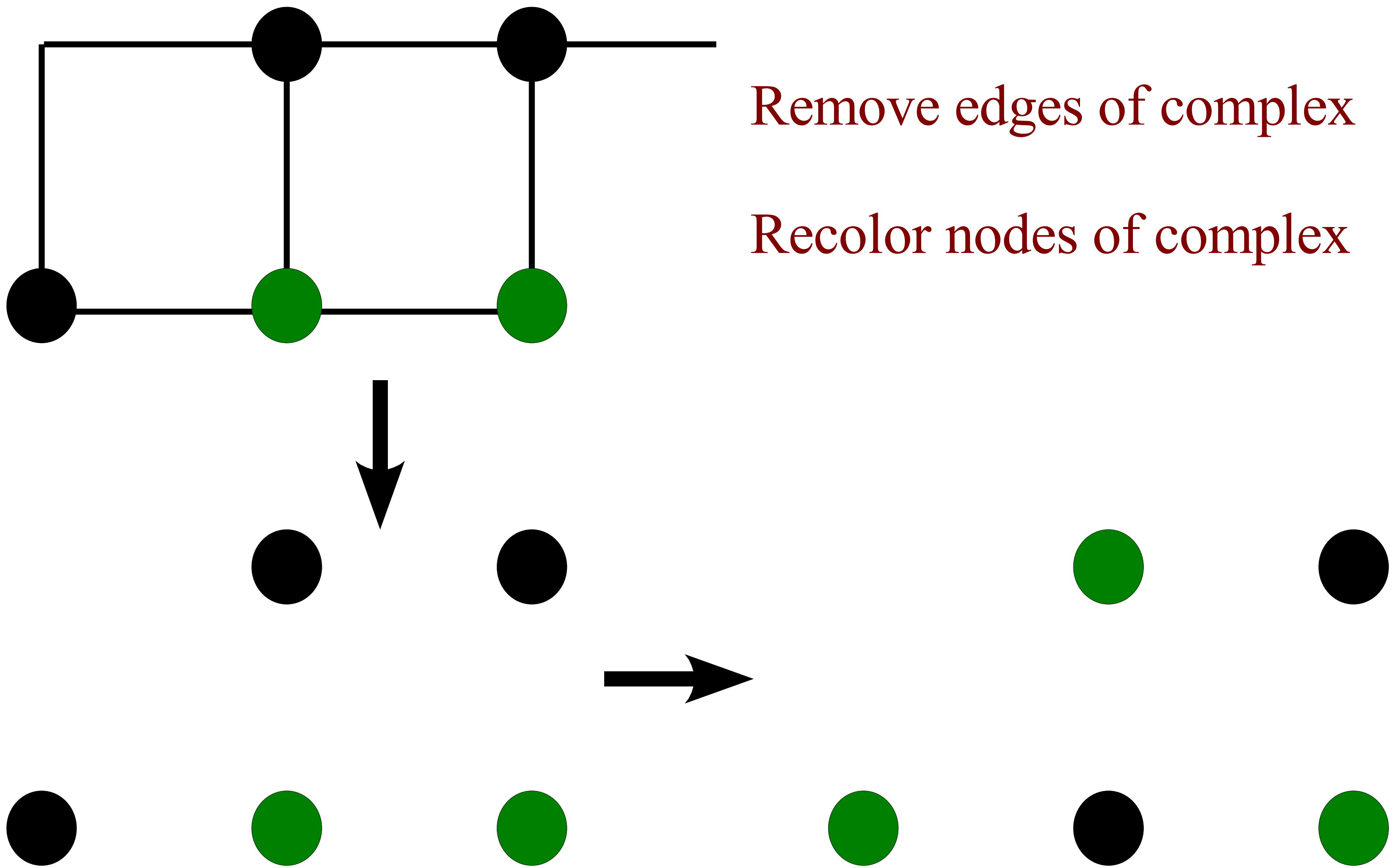
Step 2: Randomly include each node in independent set with probability $\dfrac{\lambda}{1+\lambda}$

Add edges back one at a time



Step 3: Keep adding edges until get conflict

Dealing with conflict



Remove edges of complex

Recolor nodes of complex

Conclusions

Phase transitions pop up everywhere

The physics behind ice also make the traveling salesman problem difficult

What they have in common are long range interactions—can't just look locally

Markov chains (that were supposed to simulate the models) also have phase transitions

Perfect sampling techniques can indicate where these phase transitions lie