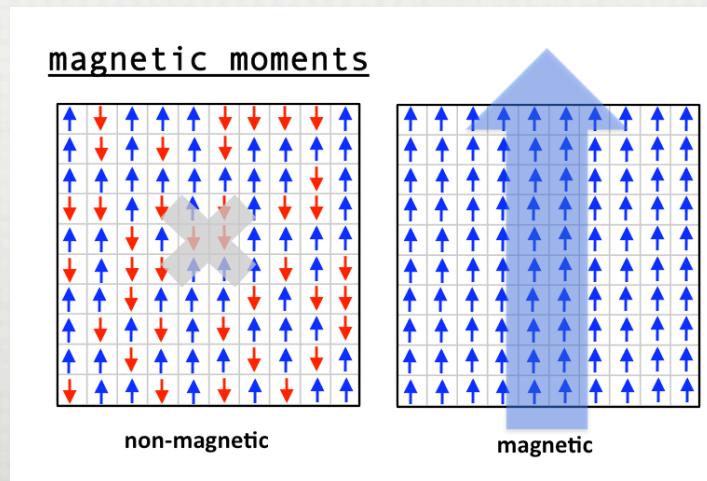


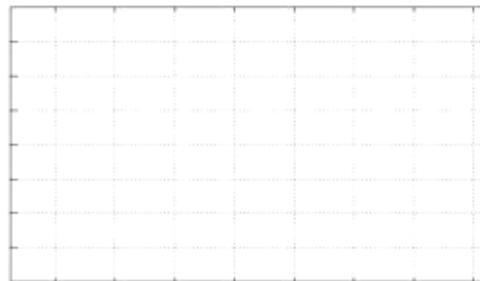
PHY-4810

COMPUTATIONAL PHYSICS

LECTURE 6: METROPOLIS ALGORITHM AND ISING MODEL



Random Walk in 3D



GENERAL PHILOSOPHY

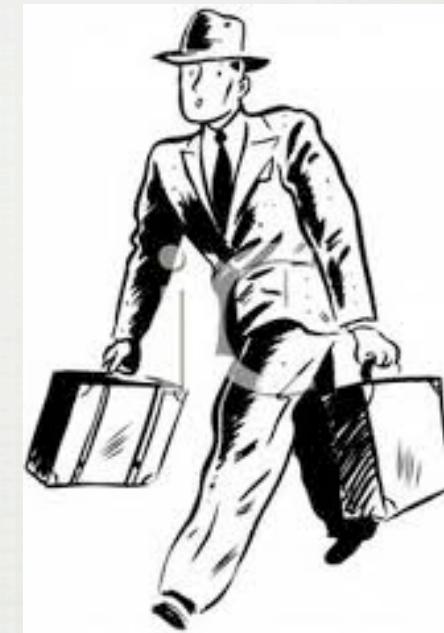
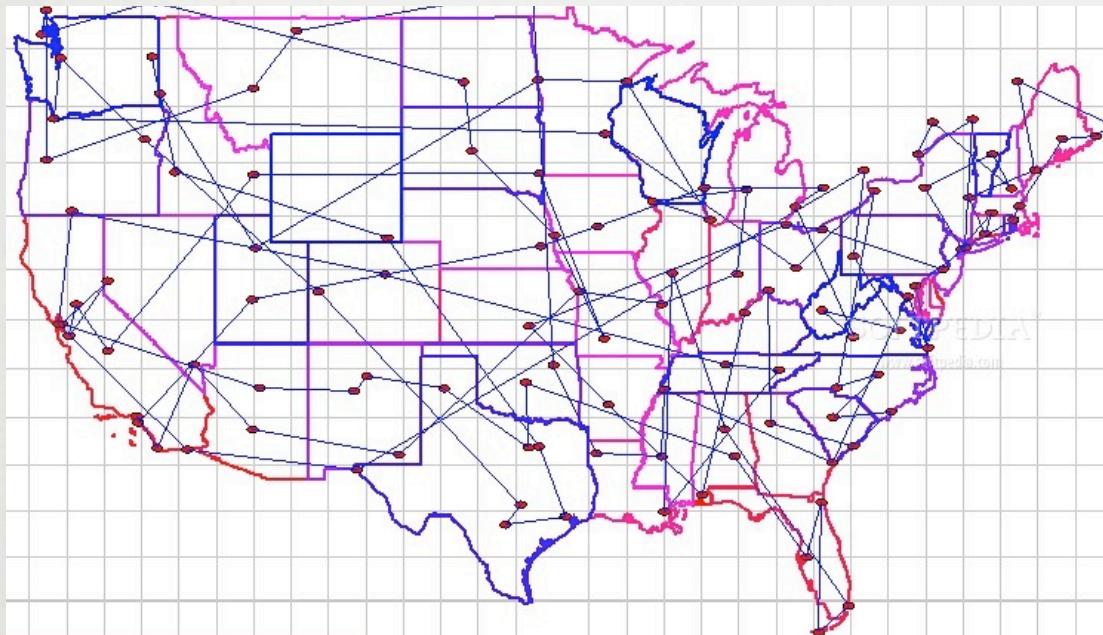
- Why reinvent the wheel?
- Let's rather try to mimic tricks Nature slowly developed to reach some kind of equilibrium
- *Computational physics is a lot about that. The difficulty is to use mathematical language to translate Nature's rules and behavior into a set of tractable methods on computers*

Computational physics is a lot about that. The difficulty is to use mathematical language to translate Nature's rules and behavior into a set of tractable methods on computers

ON THE MENU TODAY

- Introduction to Metropolis Algorithm:
 - The traveling salesman
 - Simulated annealing
 - Ising model
 - Ferromagnetism
 - Antiferromagnetism
 - 2D visualization demonstrations

PROBLEM I: THE TRAVELING SALESMAN



A salesman must visit some large number of cities while minimizing the total mileage traveled.

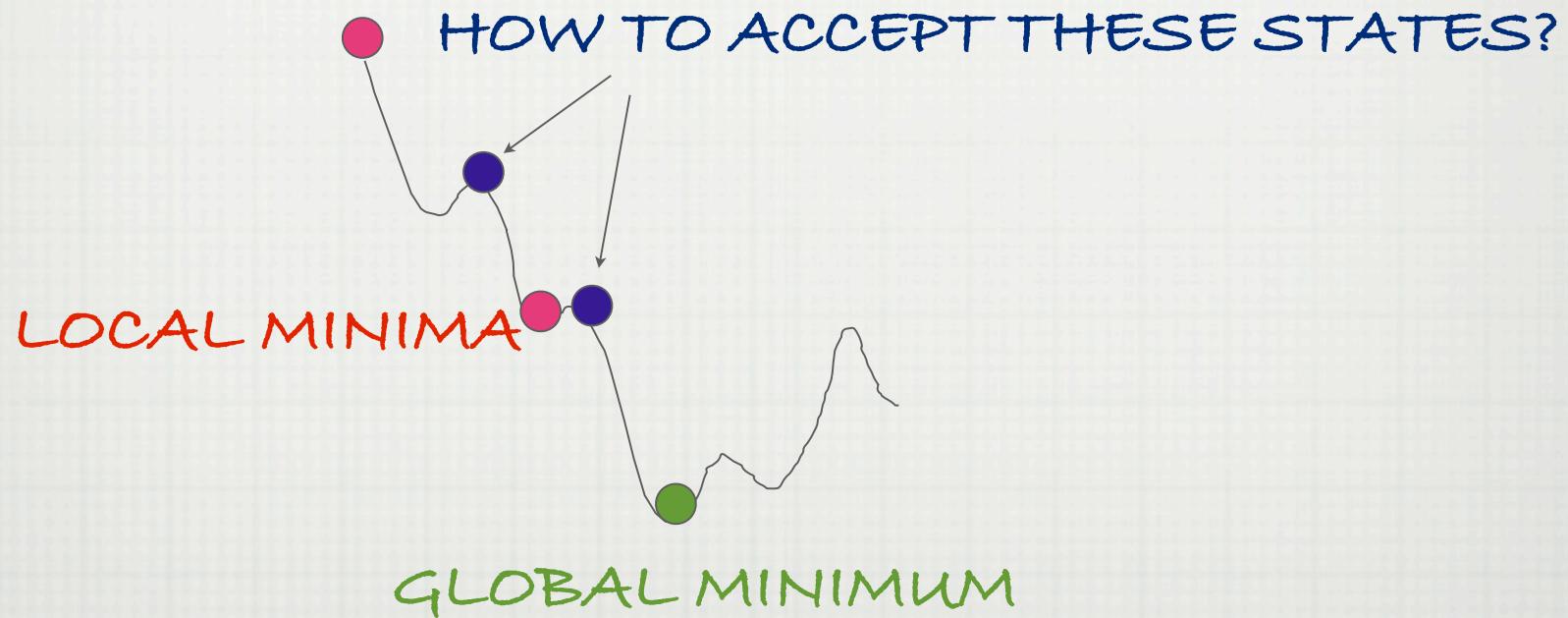
TRAVELING SALESMAN: THE PROBLEM

- If the salesman starts with a random itinerary, he can then pairwise trade the order of visits to cities, hoping to reduce the mileage with each exchange.
- The difficulty with this approach is that while it rapidly finds a local minimum, it cannot get from there to the global minimum.

SOLUTION TO THE TRAVELING SALESMAN: SIMULATED ANNEALING

- Simulated annealing improves this strategy using the following tricks:
 - The "Metropolis algorithm" (1953), in which some trades that do not lower the mileage are accepted when they serve to allow the solver to "explore" more of the possible space of solutions.

HOW TO CHOOSE “BAD TRADES”?



VIRTUAL TEMPERATURE

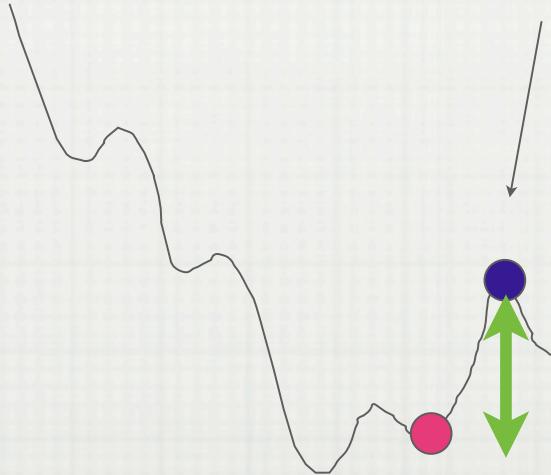
- Such "bad" trades are allowed using the criterion that (ARHENIUS)

$$e^{-\Delta D/T} > R(0, 1)$$

- ΔD is the change in distance implied by the trade (negative for a "good" trade; positive for a "bad" trade),
- T is a "virtual temperature," and
- R is a random number in the interval [0,1].
- If T is large, many "bad" trades are accepted, and a large part of solution space is accessed.
- [this is related to Boltzman constant and distribution]

BACK TO PREVIOUS QUESTION: HOW TO CHOOSE “BAD TRADES”?

HOW TO ACCEPT THIS STATE?



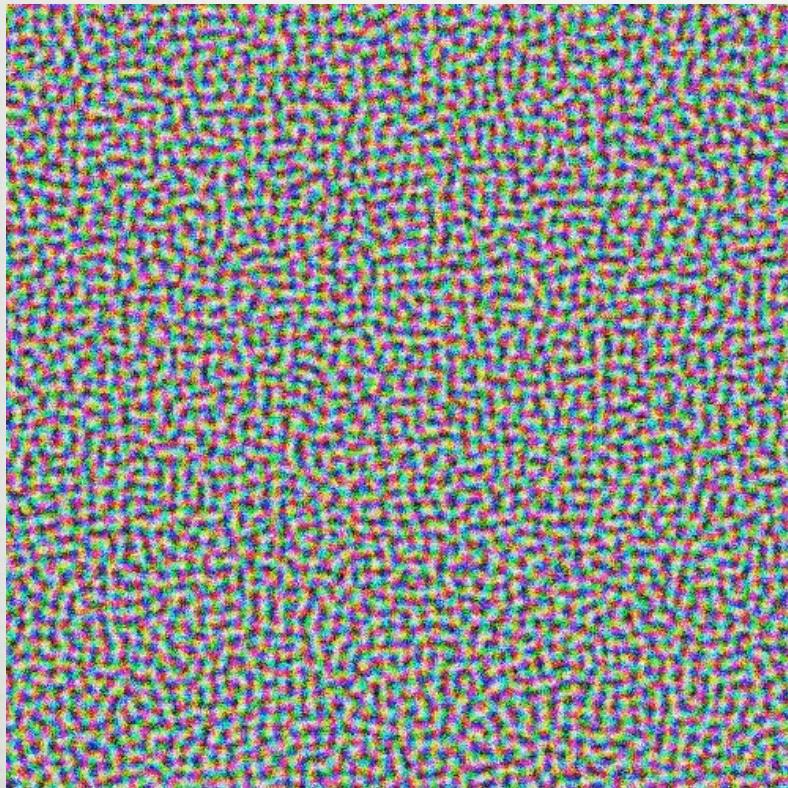
$$kT \approx \Delta D \Rightarrow P(\text{accept}) \uparrow$$

ANNEALING PART: SLOWLY DECREASE THE TEMPERATURE

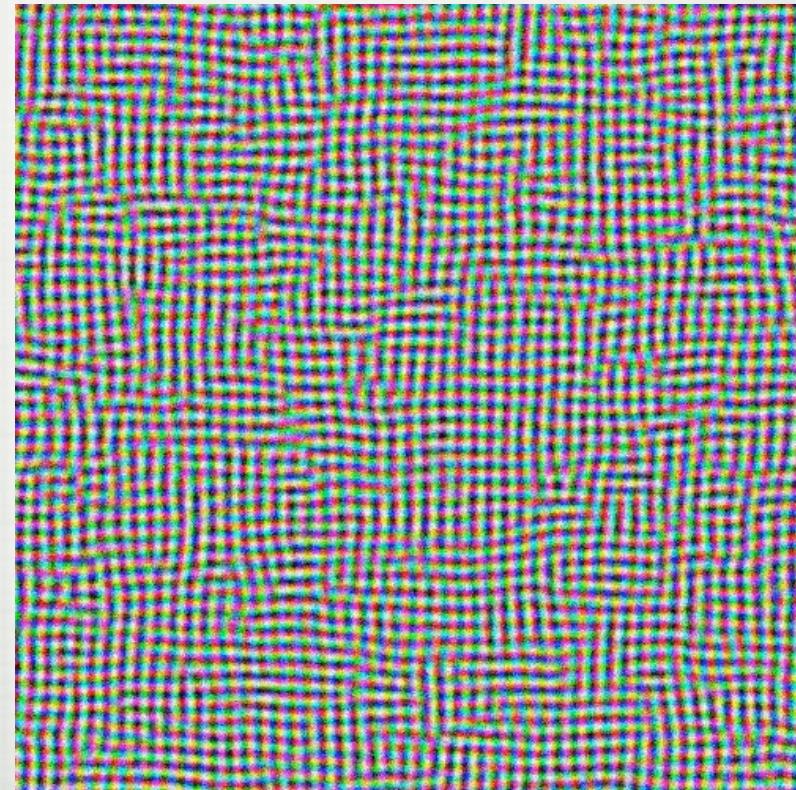
$$e^{-\Delta D/T} > R(0, 1)$$

- The second trick is to lower the "temperature." After making many trades and observing that the cost function declines only slowly, one lowers the temperature, and **thus limits the size of allowed "bad" trades.**
- After lowering the temperature several times to a low value, one may then "quench" the process by accepting only "good" trades in order to find the local minimum of the cost function.
- There are various "annealing schedules" for lowering the temperature, but the results are generally not very sensitive to the details.

SLOW VERSUS FAST SCHEDULE: BACK TO NATURE!

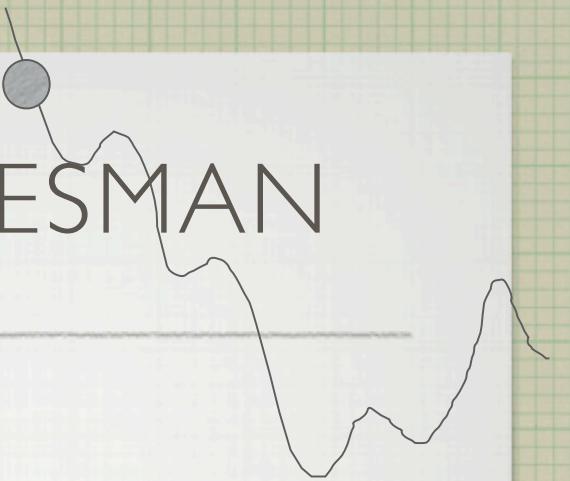


AMORPHOUS



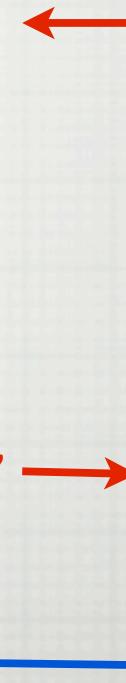
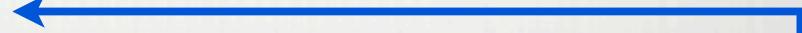
CRYSTALLINE

PSEUDO-CODE FOR SALESMAN

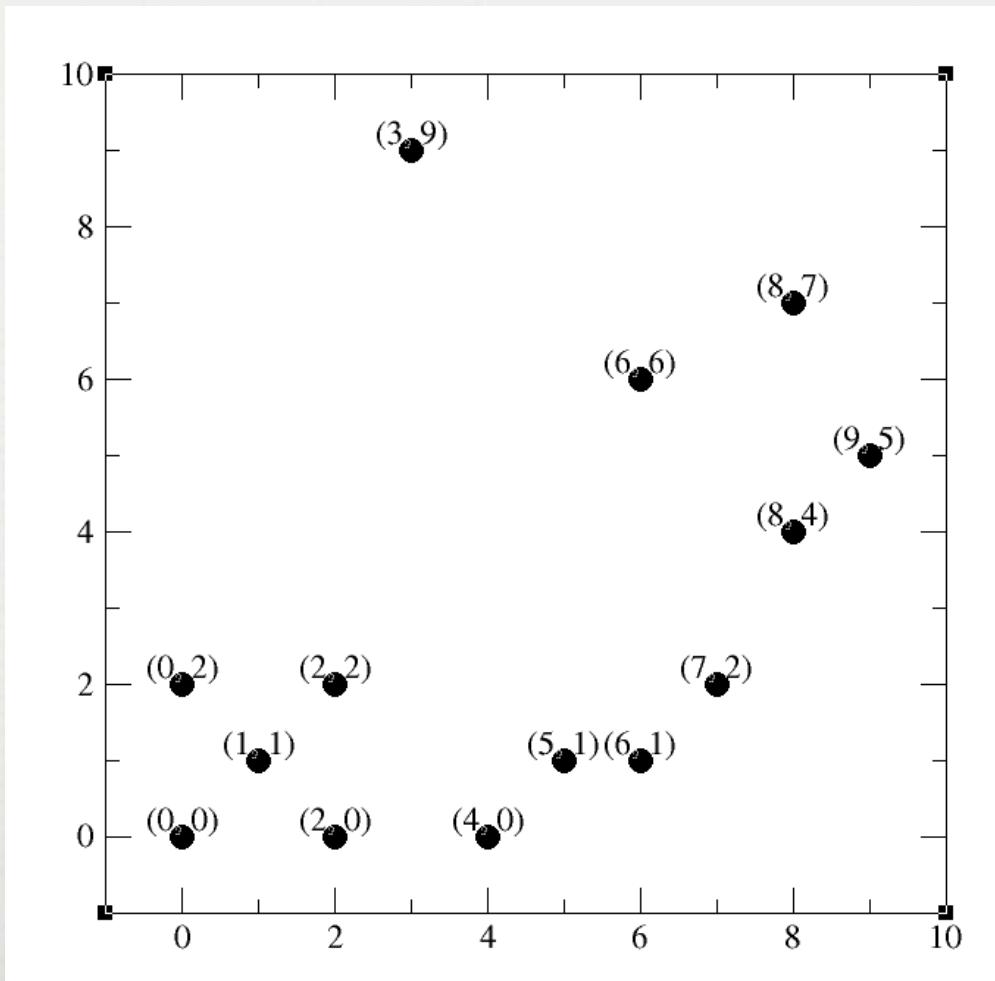


- Start with some finite temperature value T_0 ;
- Pick an “initial state” S_0 , with “potential energy” E_0
- $S_{\text{current}}=S_0$ and $E_{\text{current}}=E_0$ (initialization)
- Start loop on potential energy evaluation and system modifications
 - Pick two-neighboring cities randomly
 - if $(E_{\text{swap}} < E_{\text{current}} \text{ OR } \exp(-(E_{\text{swap}} - E_{\text{current}})/T) > R(0,1))$ then
 - $S_{\text{current}}=S_{\text{swap}}$ and $E_{\text{current}}=E_{\text{swap}}$
- Repeat process until energy is “low enough” or “enough iterations” done
- Repeat with lower temperature, using S_{current} as S_0

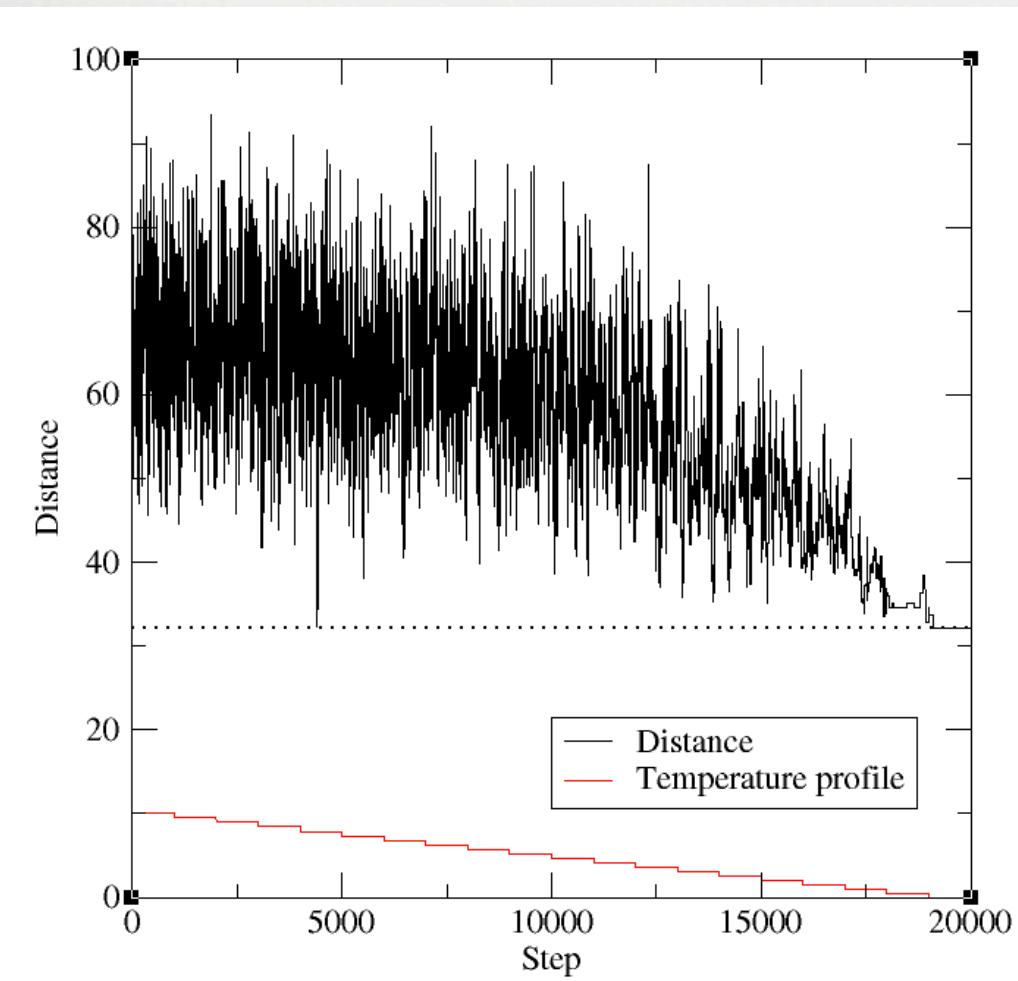
TEMPERATURE LOOP



CITY LAYOUT



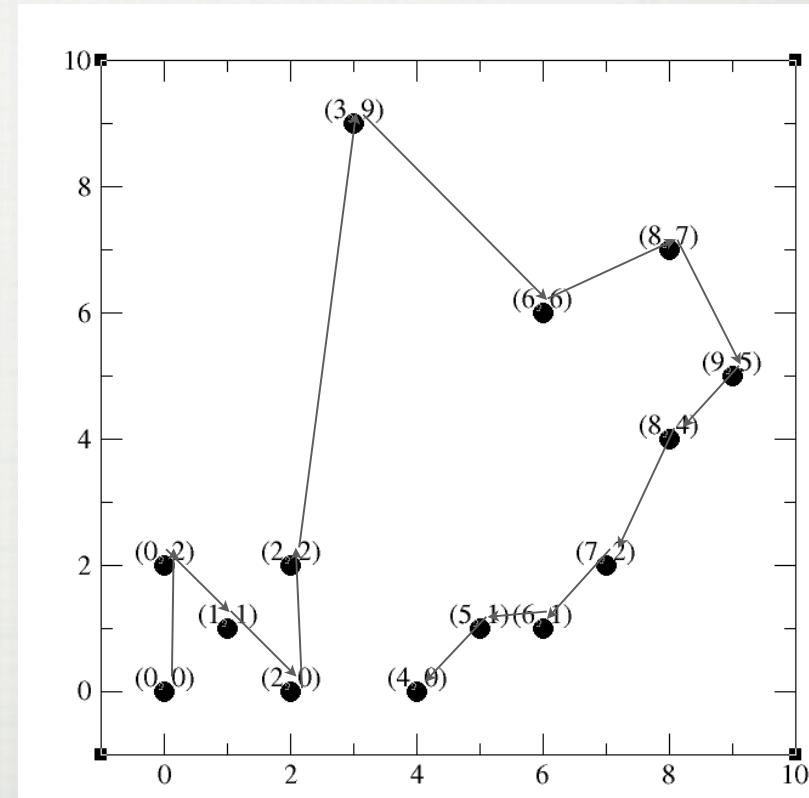
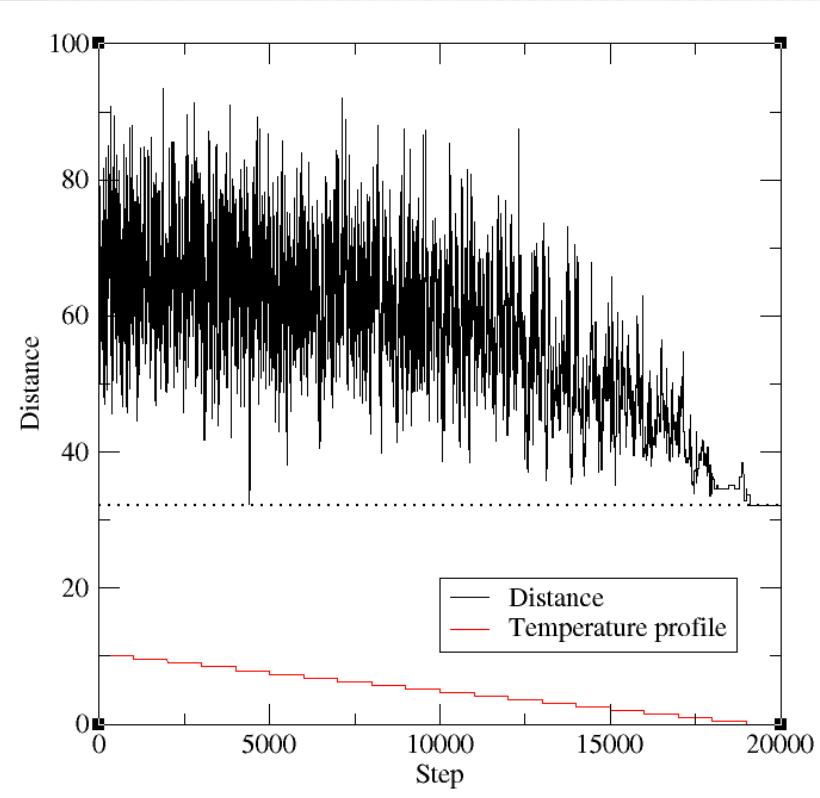
TOTAL DISTANCE AS FUNCTION OF TEMPERATURE



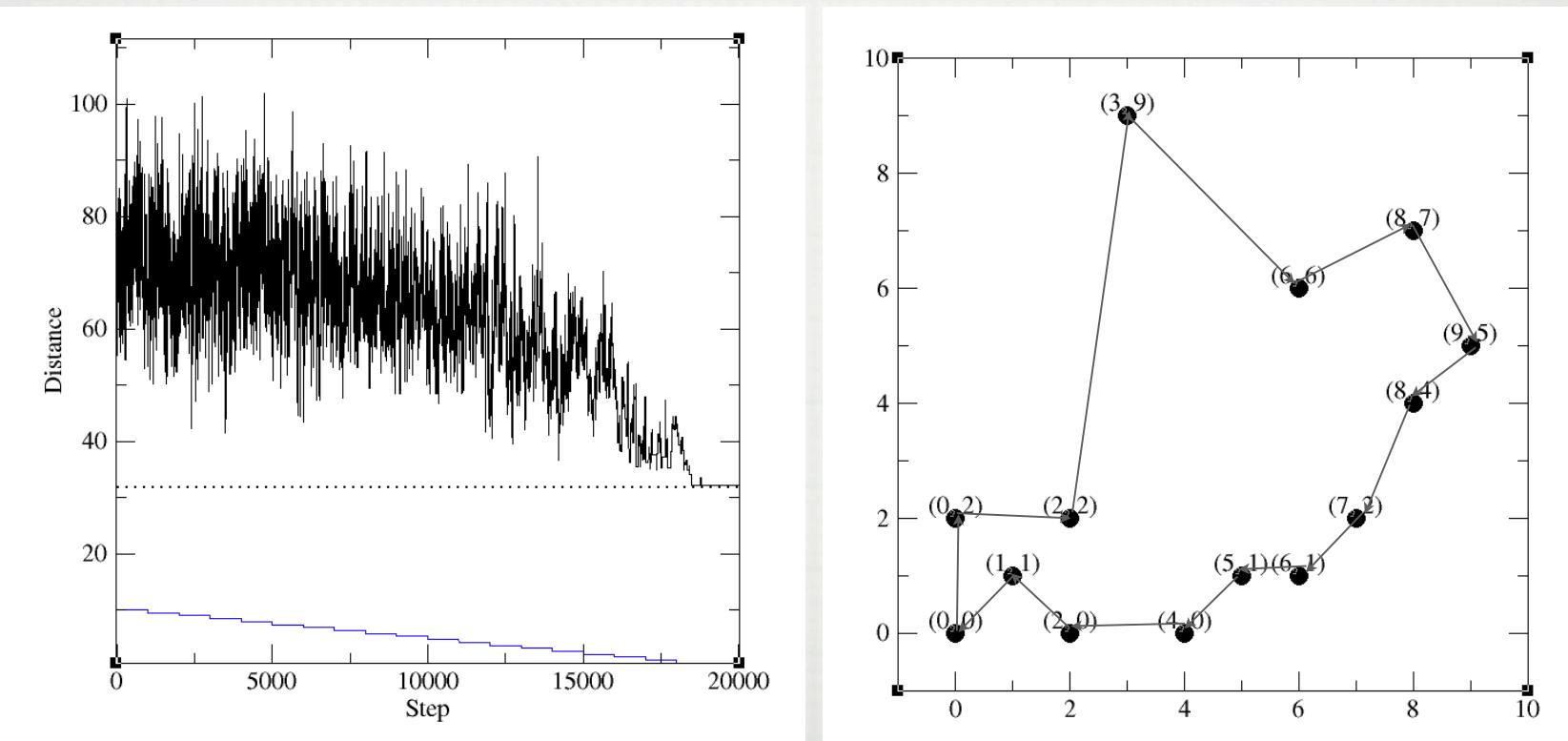
WE EXPLORE MANY
LOCAL MAXIMA

WE LOWER THE
TEMPERATURE
GRADUALLY

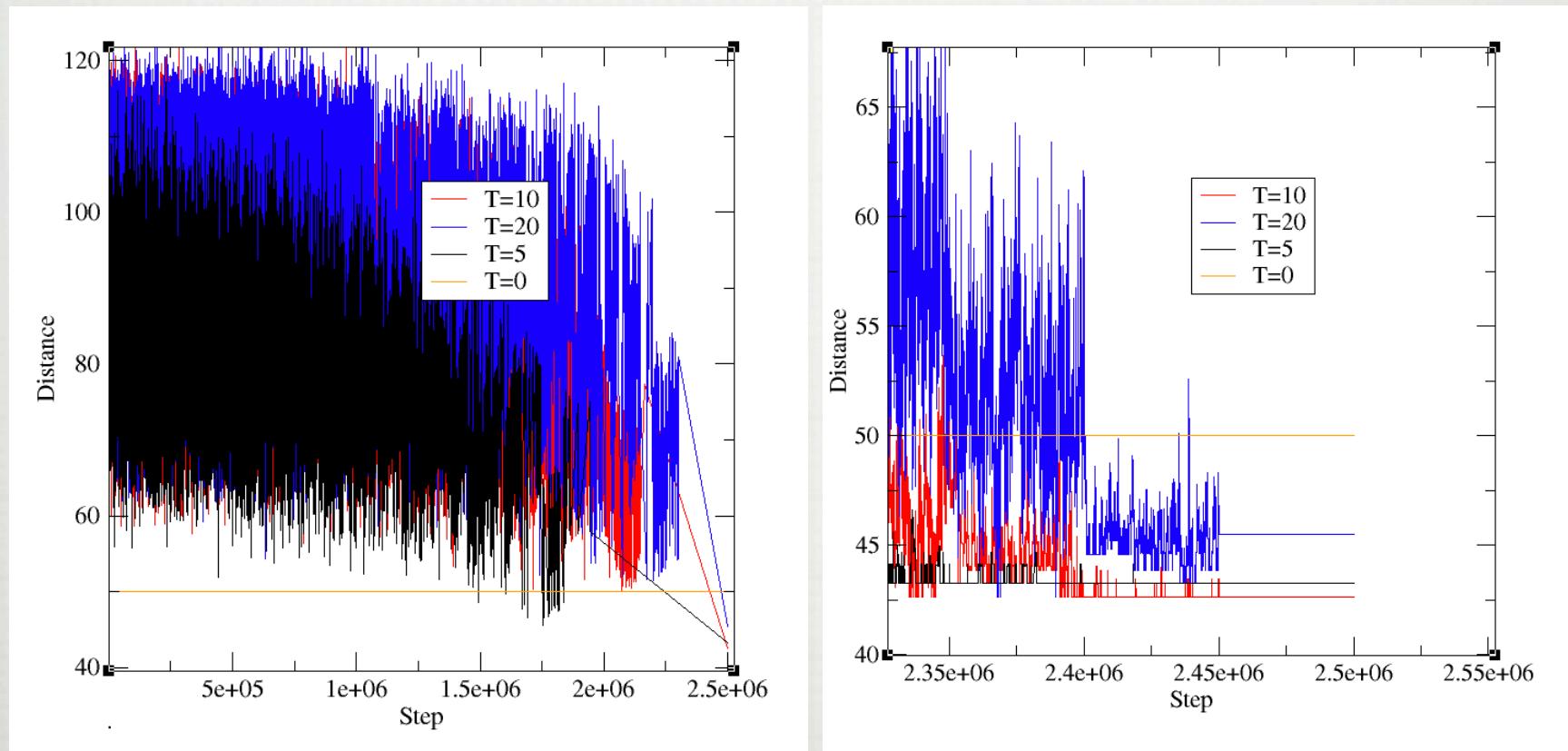
CORRESPONDING SOLUTION



INCLUDING GOING BACK HOME

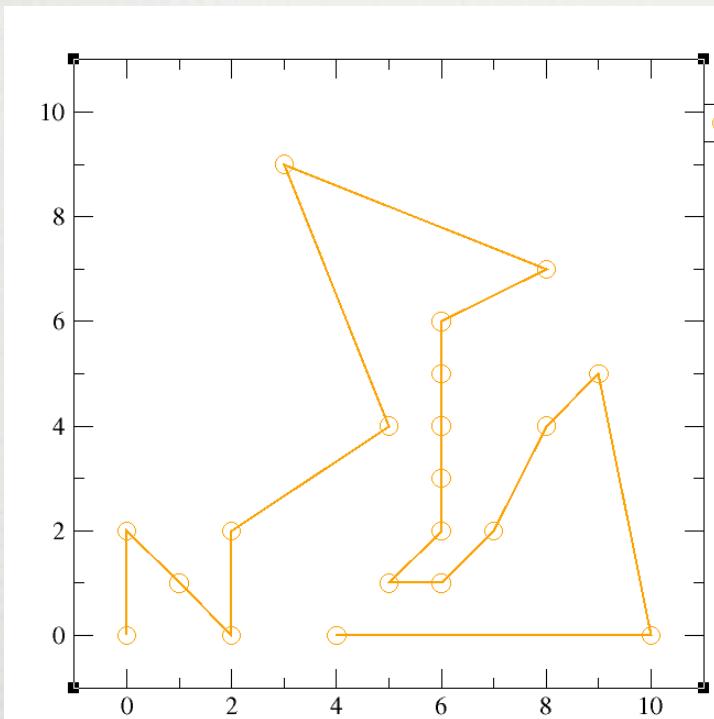


IMPORTANCE OF ANNEALING TEMPERATURE

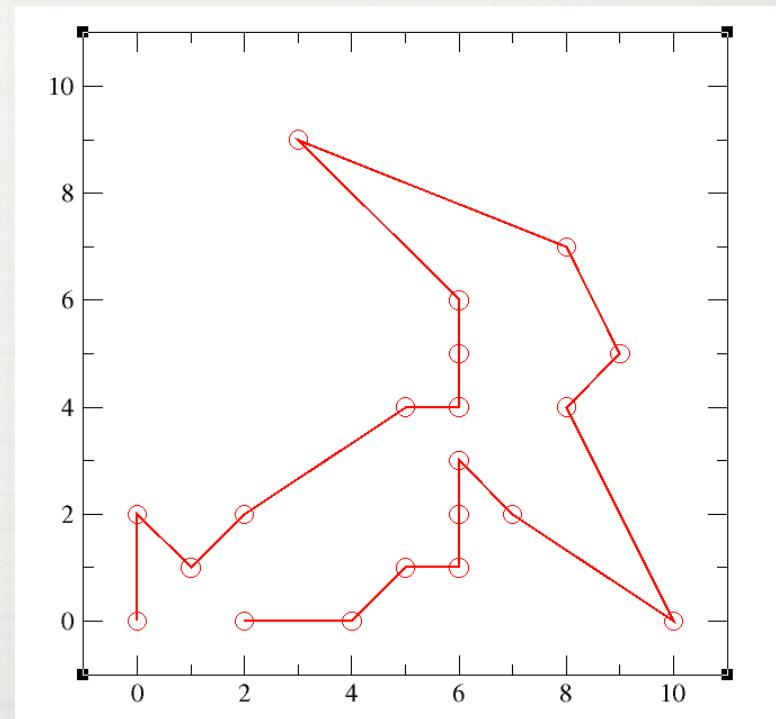


'BAD' CHOICE OF T CAN LEAD TO A LOCAL MINIMUM

$T=0$ AND $T=15$



Not the global minimum



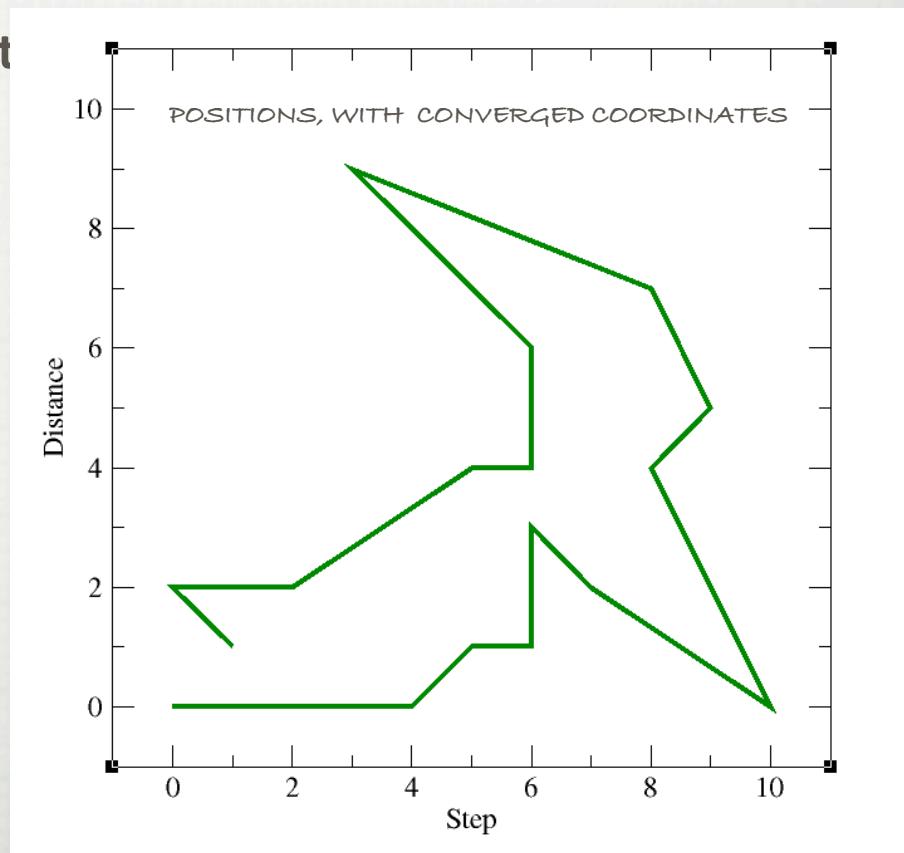
The global minimum

YOU CAN PLAY WITH IT

- Write code
- Create an input is file “cities.dat”

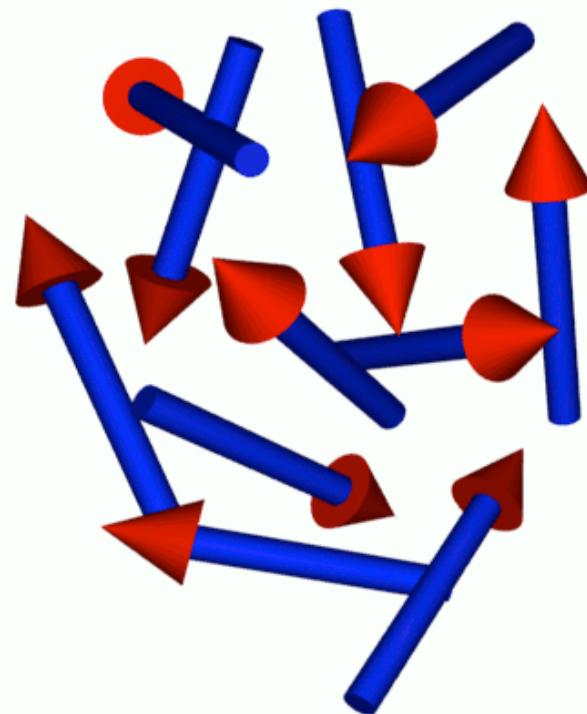
(1) 20 (NUMBER OF CITIES)

(2) 0 0
(3) 2 0
(4) 2 2
(5) 0 2
(6) 1 1
(7) 10 0
(8) 5 1
(9) 9 5
(10) 8 7
(11) 4 0
(12) 6 6
(13) 3 9
(14) 8 4
(15) 7 2
(16) 6 1
(17) 5 4
(18) 6 3
(19) 6 2
(20) 6 4
(21) 6 5

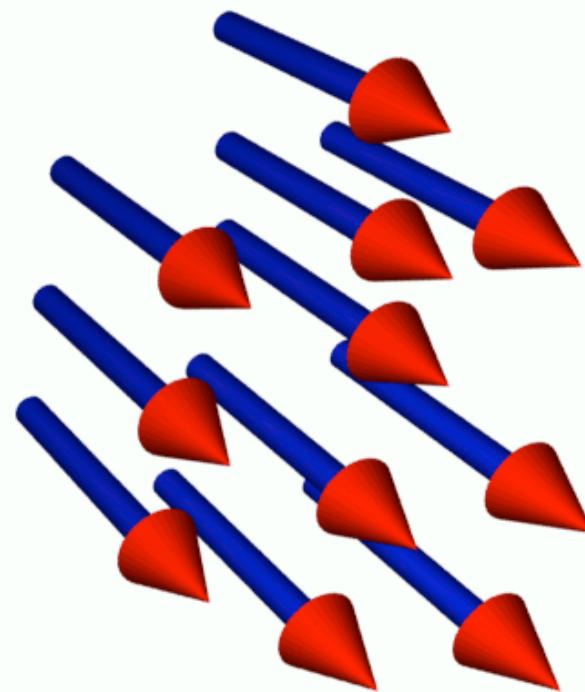


PROBLEM 2: MAGNETISM

Weak interactions

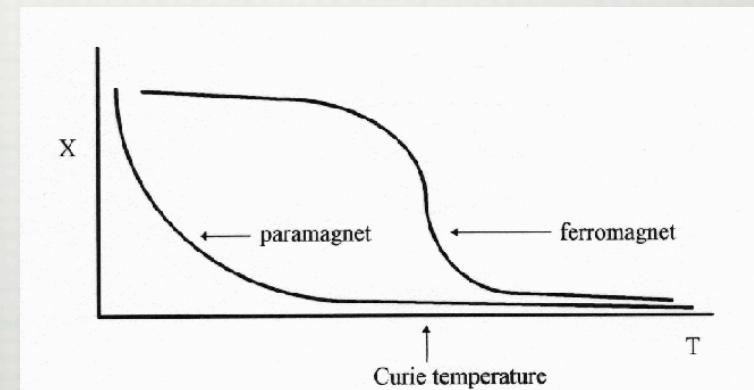
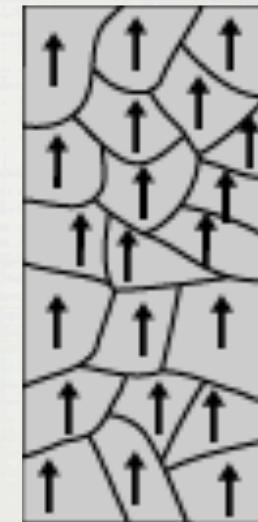


Strong interactions



FERROMAGNETISM

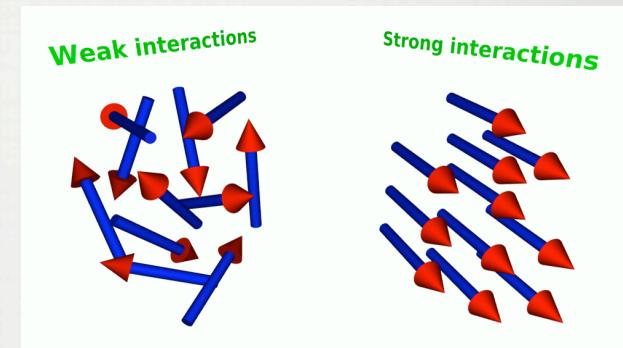
- Ferromagnetic materials contain finite-size domains in which, even in the absence of an external magnetic field, the spins of all the atoms are aligned in the same direction.
- When an external magnetic field is applied to these materials at low temperatures, the different domains align and the material becomes “magnetized.”
- Yet, as the temperature is raised, the magnetism decreases and then goes through a phase transition at the Curie temperature, beyond which all magnetization vanishes.



FERROMAGNETISM (2)

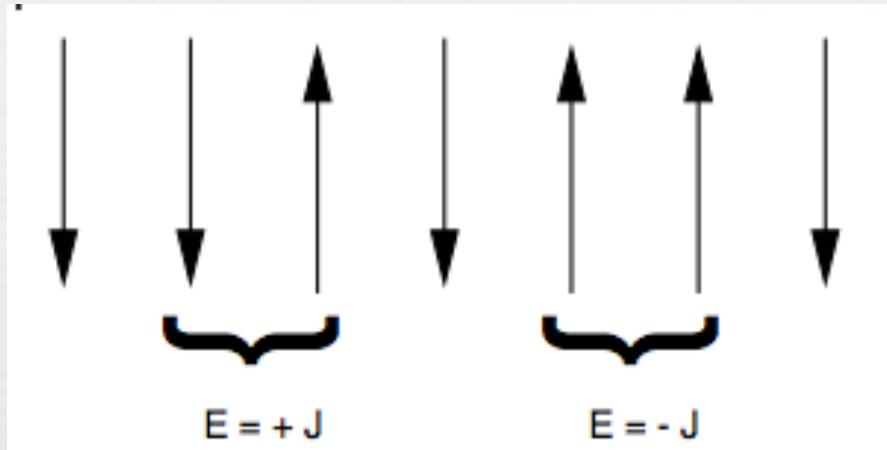
- When we say that an object is at a temperature T , we mean that the object's atoms are in thermodynamic equilibrium at temperature T . While this may be an equilibrium state, it is a dynamic one in which system's energy is fluctuating as it exchanges energy with the environment.

- In the present problem we deal with the thermal properties of magnetized materials. The magnetism arises from the alignment of the spins of the atoms within domains. When the number of atoms is large, the problem is too big to solve completely, and so statistical methods are used to obtain average quantities.



WHY DO SPINS ALIGN?

- A 1D lattice of N spins. The interaction energy $V = \pm J$ between nearest-neighbor pairs is shown for aligned and opposing spins. (“exchange energy”)



STATISTICAL MECHANICS

- Statistical mechanics starts with the elementary interactions among particles of a system and constructs the macroscopic thermodynamic properties such as temperature T and internal energy U.
- The essential assumption is that all configurations of the system consistent with the constraints are possible.
- Because we have the temperature, volume, and number of particles fixed, we have a canonical ensemble or Boltzmann distribution.

STATISTICAL MECHANICS: BOLTZMANN

- The population of a state α_j of energy $E(\alpha_j)$ in a canonical ensemble is not fixed, but rather is distributed with probabilities $P(\alpha_j)$ according to the Boltzmann distribution:

$$P(\alpha_j) = \frac{e^{-E(\alpha_j)/kT}}{Z(T)} \quad Z(T) = \sum_{\alpha_j} e^{-E_j/kT}$$

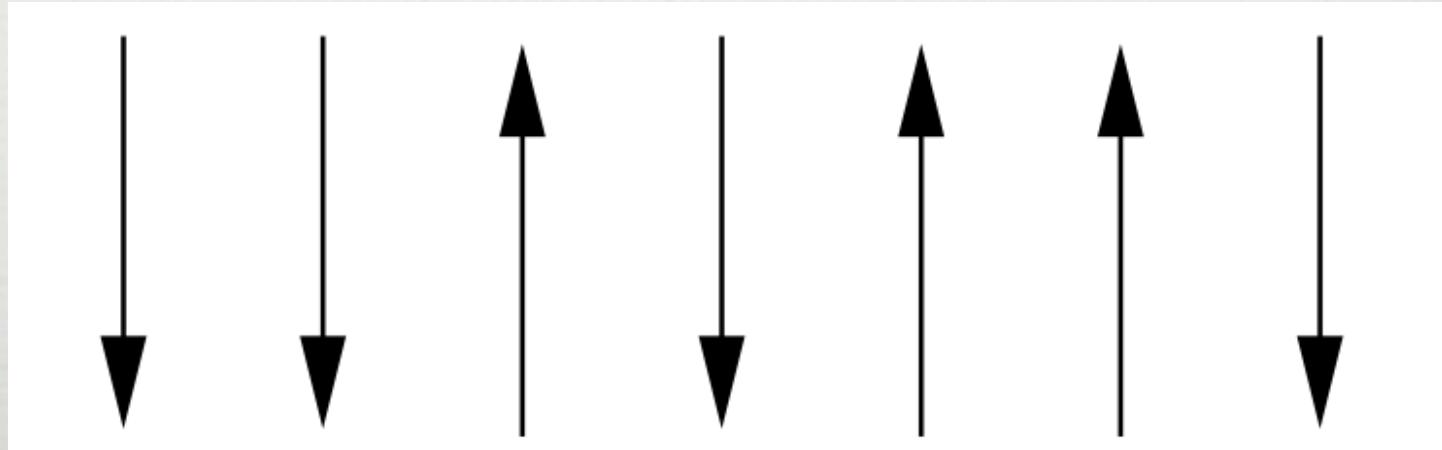
where k is Boltzmann's constant and T is the temperature.

- The **partition function $Z(T)$** is a weighted sum over states.
- Notice that P can be non-zero even for states with non-minimal energy

APPLICATION: ISING CHAIN

- **Model**

- **N magnetic dipoles fixed on the links of a linear chain.**
- **Because the particles are fixed, their positions and momenta are not dynamical variables: we need to worry only about their spins.**



ASSUMPTIONS

- We assume that the particle at site i has spin s_i , which is either up or down:

$$s_i \equiv s_{z,i} = \pm \frac{1}{2}$$

- Each possible configuration or state of the N particles is described by the quantum state vector

$$|\alpha_j\rangle = |s_1, s_2, \dots, s_N\rangle = \{\pm \frac{1}{2}, \pm \frac{1}{2}, \dots\} \quad j = 1, 2^N$$

- Because the spin of each particle can assume any one of the two values, there are 2^N different possible states of the N particles in the system.
- Bonus question: (Pauli Principle) Should we worry about symmetry of the wavefunction?

ENERGY

- The energy of the system arises from the interaction of the spins with each other and with the **external magnetic field B** .
- In quantum mechanics, an electron's spin and magnetic moment are proportional to each other, so a “dipole–dipole” interaction is equivalent to a “spin–spin” interaction.
- We assume that each dipole interacts with the external magnetic field and with its nearest neighbor through the potential:

$$V_i = -J \mathbf{s}_i \cdot \mathbf{s}_{i+1} - g\mu_b \mathbf{s}_i \cdot \mathbf{B}$$

- The constant J is called the **exchange energy** and is a measure of the strength of the spin–spin interaction.
- The constant g is the **gyromagnetic ratio**, that is, the proportionality constant between the angular momentum and magnetic moment. The constant μ_b is the Bohr magneton, the unit for magnetic moments.

NOW SUPPOSE WE HAVE ONE MOLE OF MATERIALS...

- $N=6.02 \times 10^{23}$, therefore, the number of states is 2^N :

$$N_{\text{state}} = 2^N = 2^{6.02 \times 10^{23}}$$

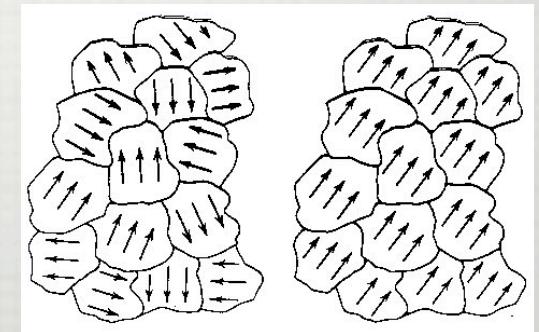
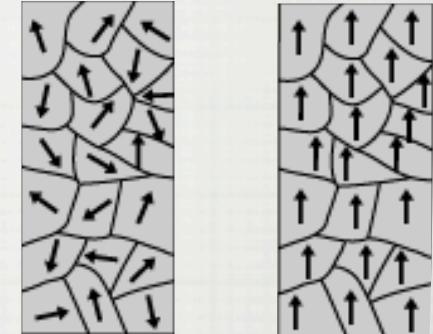
that's a...big number.

- We have to rely on statistical approach, but our knowledge of physics can come to the rescue...
- Be careful, that for a "statistics" to be really "statistical", the sample size should be "large enough".
- What is large enough?

TOTAL ENERGY OF THE SYSTEM

$$E(\alpha) = \langle \alpha | \sum_i V_i | \alpha \rangle = -J \sum_{i=1}^{N-1} s_i s_{i+1} - B \mu_b \sum_{i=1}^N s_i$$

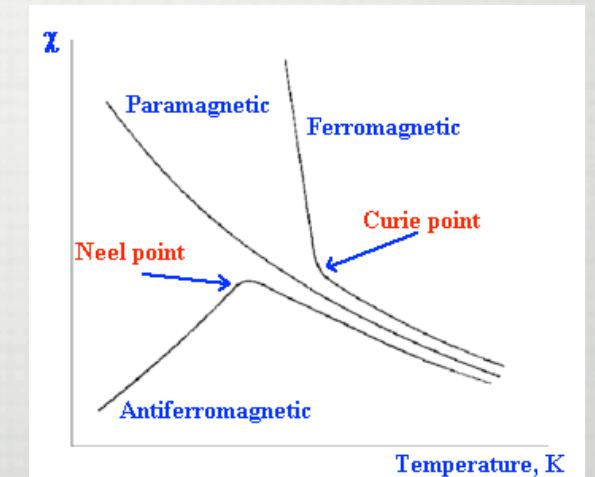
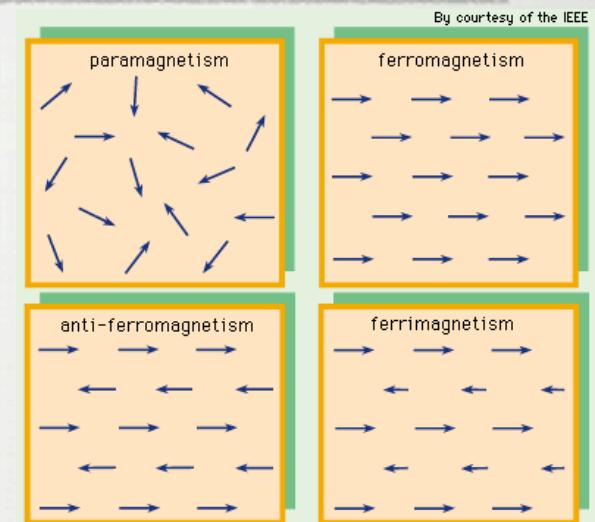
- **Paradox:** if $B=0$, the system should not have a preferred direction for spins.
- However, $B=0$ is a metastable situation and any small B would turn the system to an aligned materials (think about a ball balanced on top of a pole)
- In real materials, we have domains, pointing in various directions



MORE ABOUT J

$$E(\alpha) = \langle \alpha | \sum_i V_i | \alpha \rangle = -J \sum_{i=1}^{N-1} s_i s_{i+1}$$

- The equilibrium alignment of the spins depends critically on the sign of the exchange energy J .
- If $J > 0$, the lowest energy state will tend to have neighboring **spins aligned**. If the temperature is low enough, the ground state will be a **ferromagnet** with all spins aligned.
- If $J < 0$, the lowest energy state will tend to have neighbors with **opposite** spins. If the temperature is low enough, the ground state will be a **antiferromagnet** with alternating spins.



CURIE TEMPERATURE

- A fascinating aspect of magnetic materials is the existence of a critical temperature, the Curie temperature, above which the gross magnetization essentially vanishes.
- Below the Curie temperature the quantum state of the material has long-range order extending over macroscopic dimensions;
- Above the Curie temperature there is only short-range order extending over atomic dimensions.
- *Even though the 1D Ising model predicts realistic temperature dependences for the thermodynamic quantities, the model is too simple to support a phase transition.*
- However, the 2D and 3D Ising models does support the Curie-temperature phase transition.

ANALYTICAL SOLUTION: 1D

- For very large numbers of particles, the thermodynamic properties of the 1D Ising model can be solved analytically. The solution tells us that the average energy U is

$$\frac{U}{J} = -N \tanh \frac{J}{kT} = -N \frac{e^{J/kT} - e^{-J/kT}}{e^{J/kT} + e^{-J/kT}} = \begin{cases} N & kT \rightarrow 0 \\ 0 & kT \rightarrow \infty \end{cases}$$

- Specific heat per particle and magnetization are

$$C(kT) = \frac{1}{N} \frac{dU}{dT} = \frac{(J/kT)^2}{\cosh^2(J/kT)}$$

$$M(kT) = \frac{Ne^{J/kT} \sinh(B/kT)}{\sqrt{e^{2J/kT} \sinh^2(B/kT) + e^{-2J/kT}}}.$$

ANALYTICAL SOLUTION 2D

- Spontaneous magnetization:

$$\mathcal{M}(T) = \begin{cases} 0 & T > T_c \\ \frac{(1+z^2)^{1/4}(1-6z^2+z^4)^{1/8}}{\sqrt{1-z^2}} & T < T_c \end{cases}$$

$kT_c \simeq 2.269185J$
 $z = e^{-2J/kT}$

where the temperature is measured in units of the Curie temperature T_c , and z is a dimensionless variable.

METROPOLIS ALGORITHM

- Remember multidimensional integrals using Monte Carlo
- We mentioned that increasing sampling at areas of interest DOES increase speed and accuracy.
- The idea of the Metropolis algorithm is just that: trying to sample those systems that are most relevant, i.e. those with large probability of existing.
- We know from physics how to do that, i.e. by using the Boltzmann distribution!
- If we work at high T, we stimulate many spin flips, but we only keep those with finite probability, just as for the salesman problem.
- Then we reduce T until we reach global minimum

PSEUDO-CODE FOR ISING MODEL

1. Start with an arbitrary spin configuration $\alpha_k = \{s_1, s_2, \dots, s_N\}$.
2. Generate a trial configuration α_{k+1} :
 1. Pick particle i randomly.
 2. Reverse i 's spin direction.
3. Calculate the energy $E(\alpha_{tr})$ of the trial configuration.
 1. If $E(\alpha_{tr}) \leq E(\alpha_k)$, accept by setting $\alpha_{k+1} = \alpha_{tr}$.
 2. If $E(\alpha_{tr}) > E(\alpha_k)$, accept with relative probability $P = \exp(-\Delta E/kT)$:
2. Choose a uniform random r_j , $0 \leq r_j \leq 1$.

$$\alpha_{k+1} = \begin{cases} \alpha_{tr} & \text{if } P \geq r_j \text{ (accept)} \\ \alpha_k & \text{if } P < r_j \text{ (reject)} \end{cases}$$

CORE OF THE ALGORITHM (SAME AS FOR TRAVELING SALESMAN)

- If the trial configuration has a lower energy ($\Delta E \leq 0$), the relative probability will be greater than one and we accept the trial configuration as the new initial configuration.
- However, if the trial configuration has a higher energy ($\Delta E > 0$), we do not reject out of hand because the system has moved away from its lowest energy state.
- Instead, we accept it with relative probability $P_{tr}/P_i = \exp(-\Delta E/kT) < 1$.
- To accept a configuration with a probability, we pick a uniform random number between 0 and 1, and if the probability is greater than this number, we accept the trial configuration; if the probability is smaller than the chosen random number, we reject it.

$$\frac{P_{tr}}{P_i} = e^{-\Delta E/kT} \quad \Delta E = E_{tr} - E_i$$

SUMMARY OF THE ALGORITHM

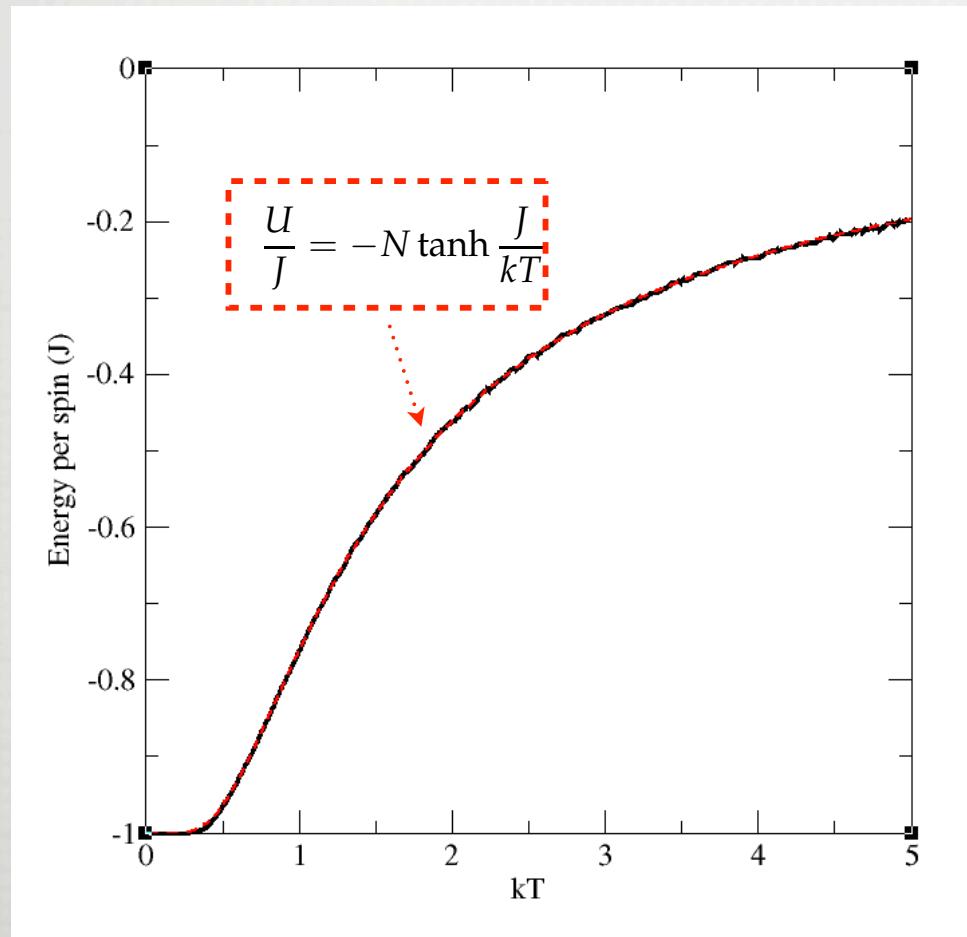
- The key aspect of the Metropolis algorithm is that the weight given to a trial configuration depends on how far it is from the minimum-energy configuration.
- Those configurations that stray far from the minimum-energy configuration are deemphasized but not completely discarded.
- By permitting $\Delta E > 0$, we are permitting the system to go “uphill” for a while.
- This deviation away from a direct path to the minimum-energy configuration permits the algorithm to get away from a local minimum and instead find a global one.
- Its success relies on it not being too quick in “cooling” to the minimum-energy configuration; for this reason the algorithm is sometimes called simulated annealing.

DETAILS ON IMPLEMENTATION

- Periodic boundary conditions
- Different starting configurations should give same final answer
- Total energy and magnetization:

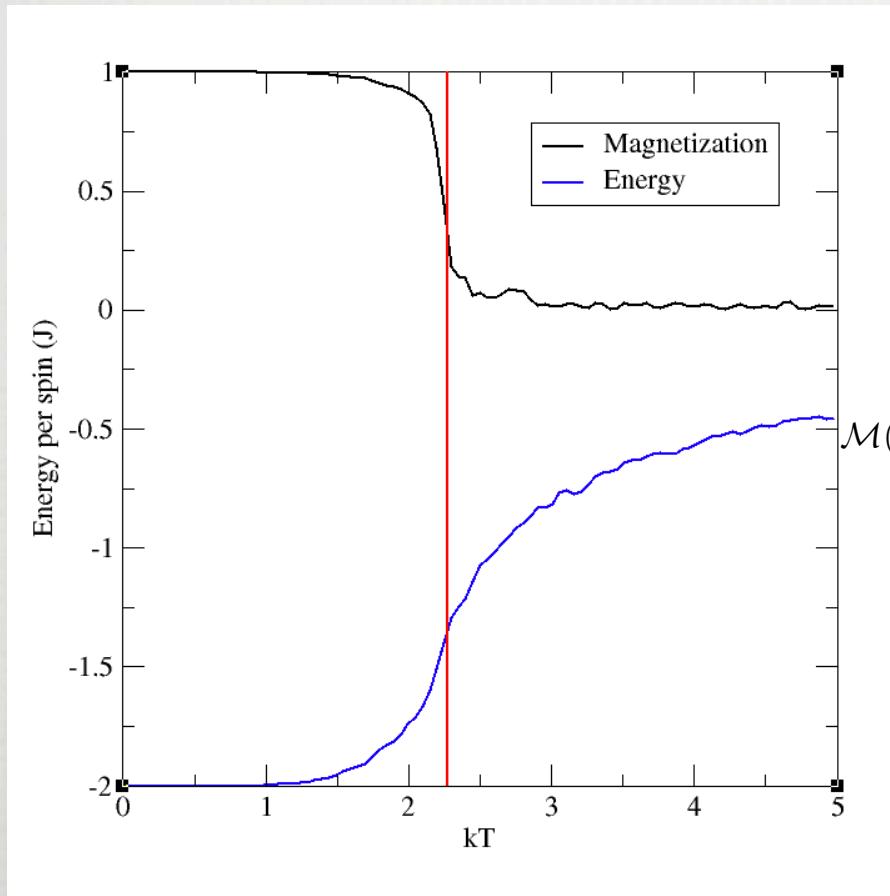
$$E_j = -J \sum_{i=1}^{N-1} s_i s_{i+1} \quad \mathcal{M}_j = \sum_{i=1}^N s_i$$

NUMERICAL EXAMPLE: 1D



- Linear system
- 100 spins
- $J=-1$
- no magnetic field
- average over 500 samples
- cold start (*what is a cold start?*)

ISING IN 2D: FERROMAGNETISM

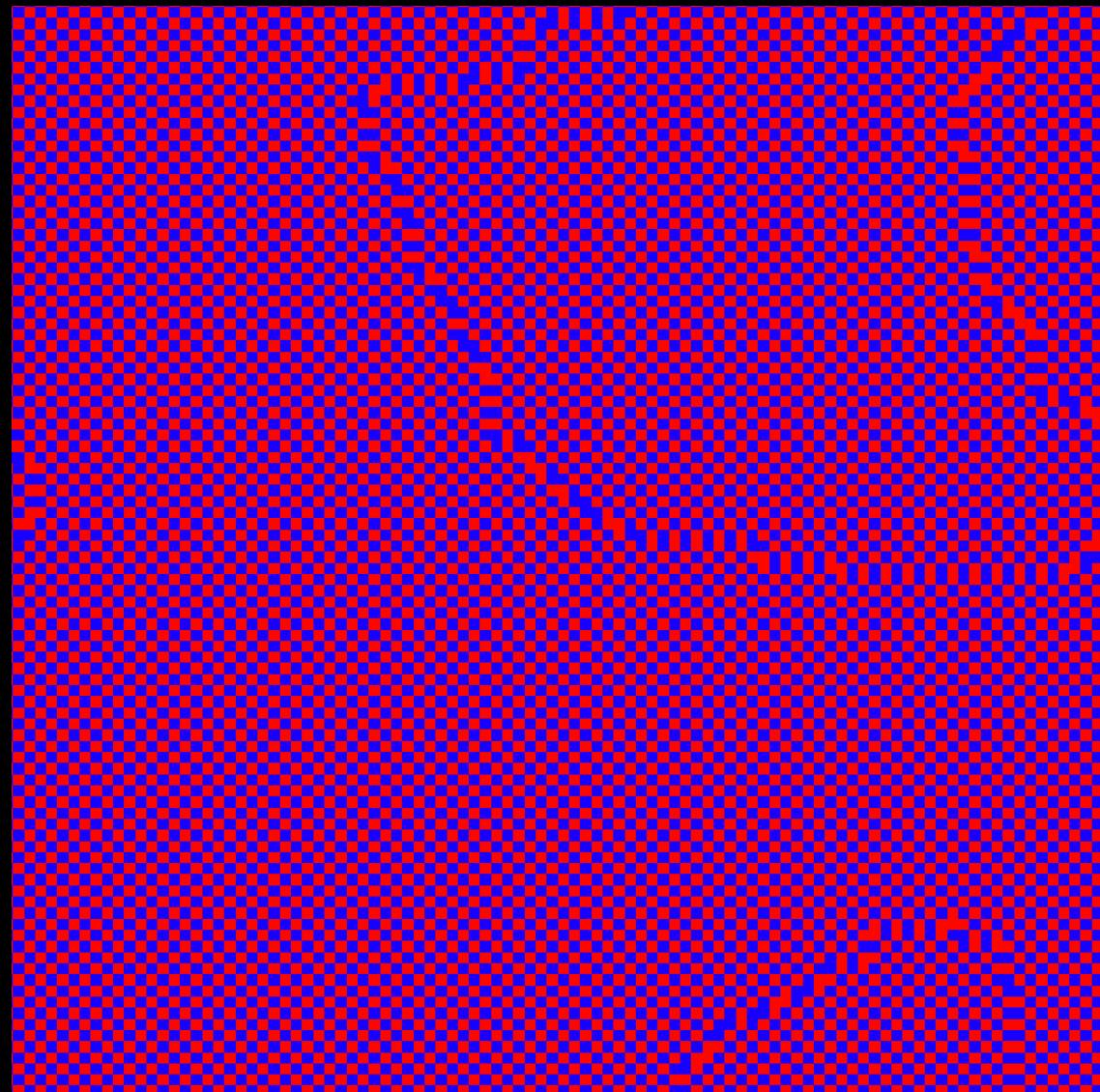


$$\mathcal{M}(T) = \begin{cases} 0 & T > T_c \\ \frac{(1+z^2)^{1/4}(1-6z^2+z^4)^{1/8}}{\sqrt{1-z^2}} & T < T_c \end{cases}$$

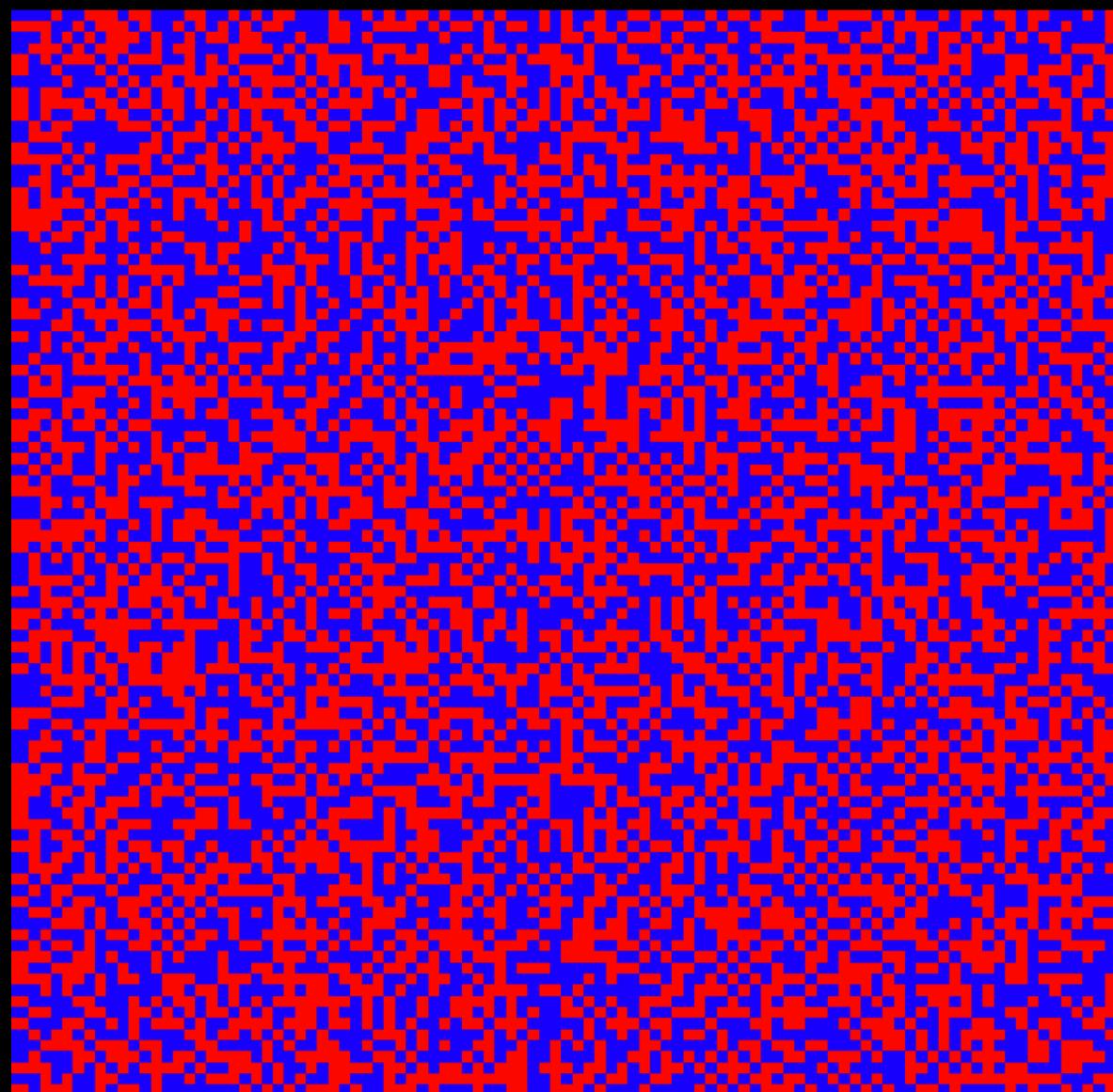
$$kT_c \simeq 2.269185J$$
$$z = e^{-2J/kT}$$

PART 3: SOME VISUALIZATION

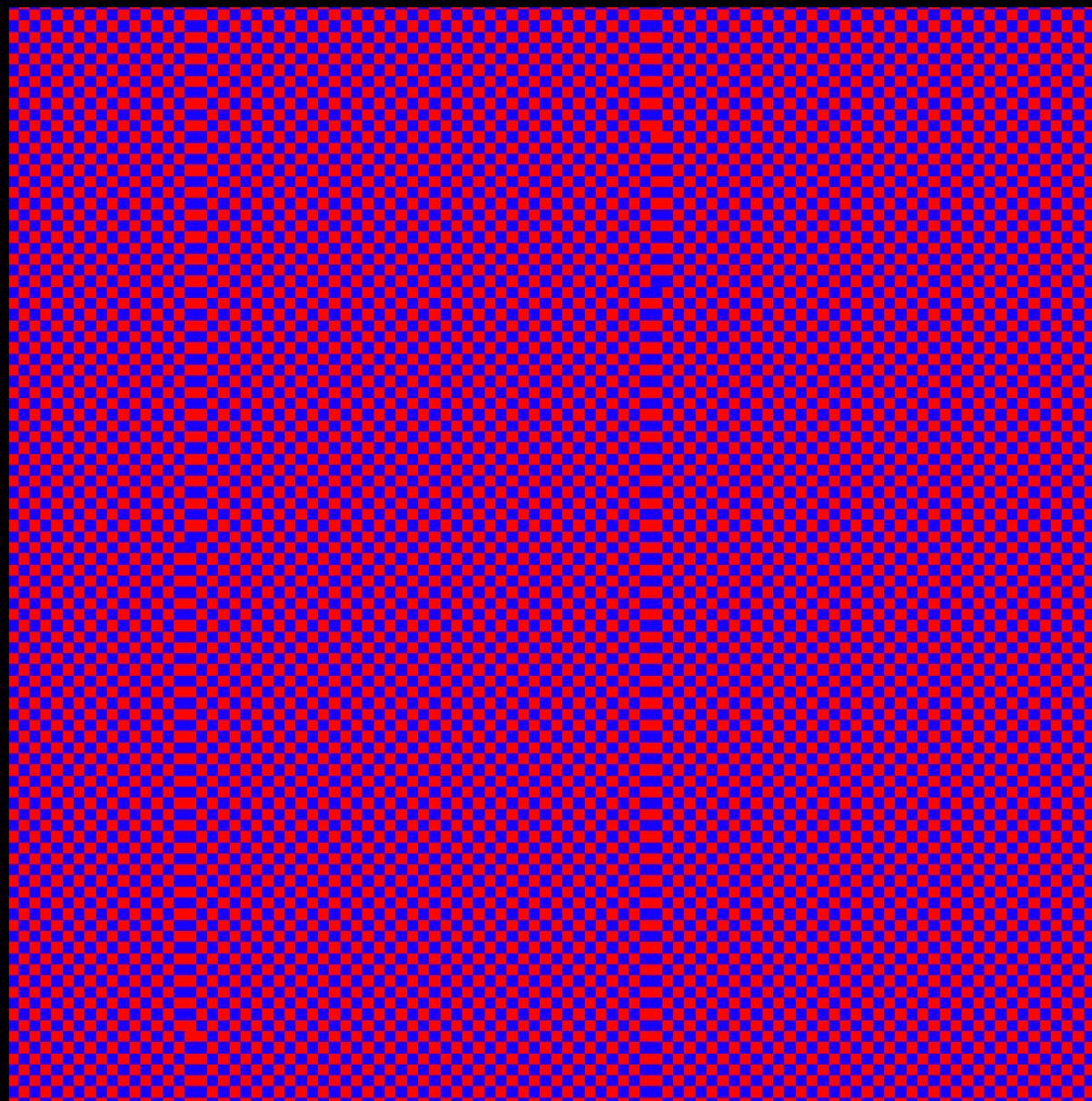
ANTIFERROMAGNETISM: COLD START, T=100



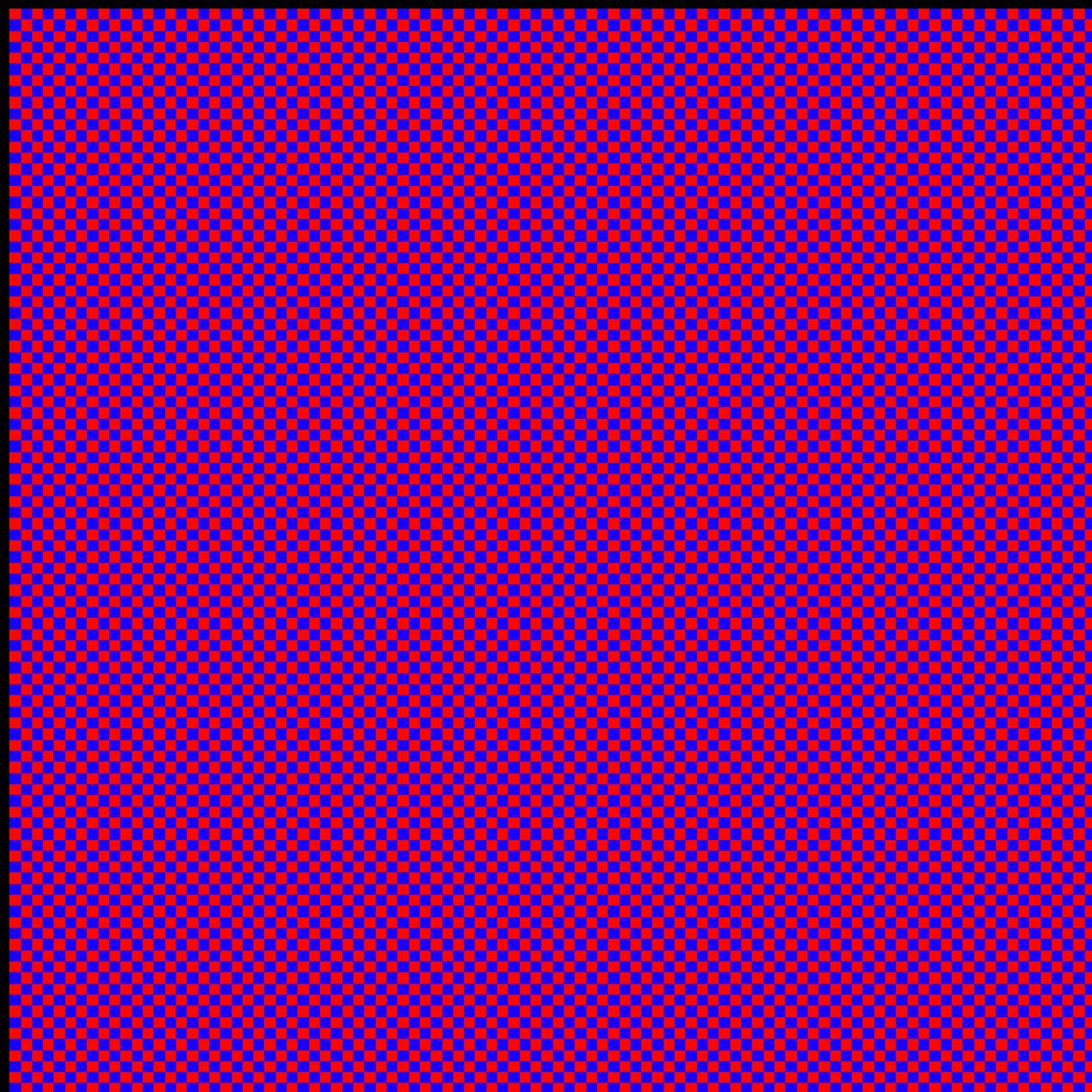
ANTIFERROMAGNETISM: TOO HIGH TEMPERATURE!!!



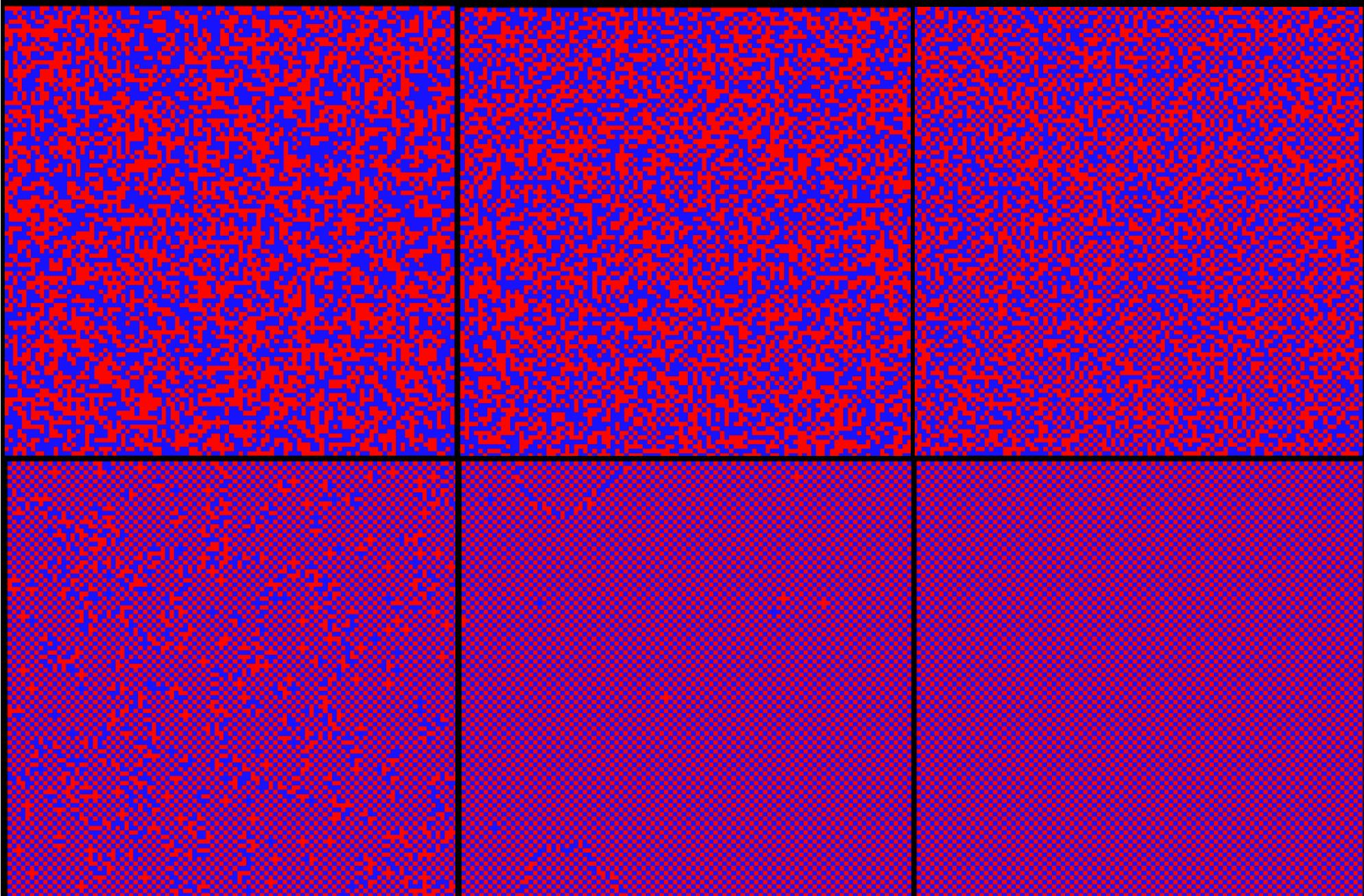
ANTIFERROMAGNETISM: COLD START, T=10



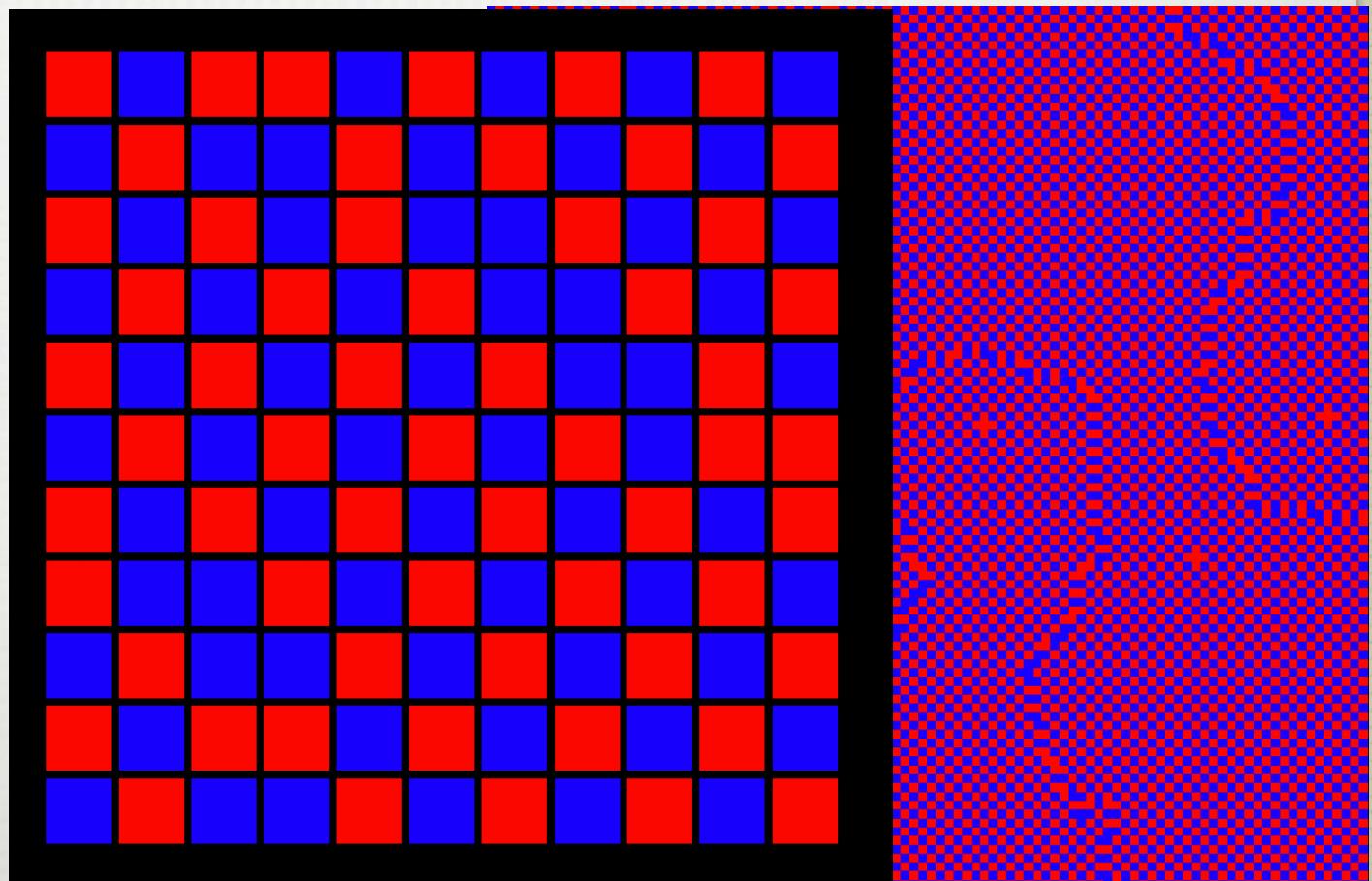
ANTIFERROMAGNETISM: COLD START, T=2

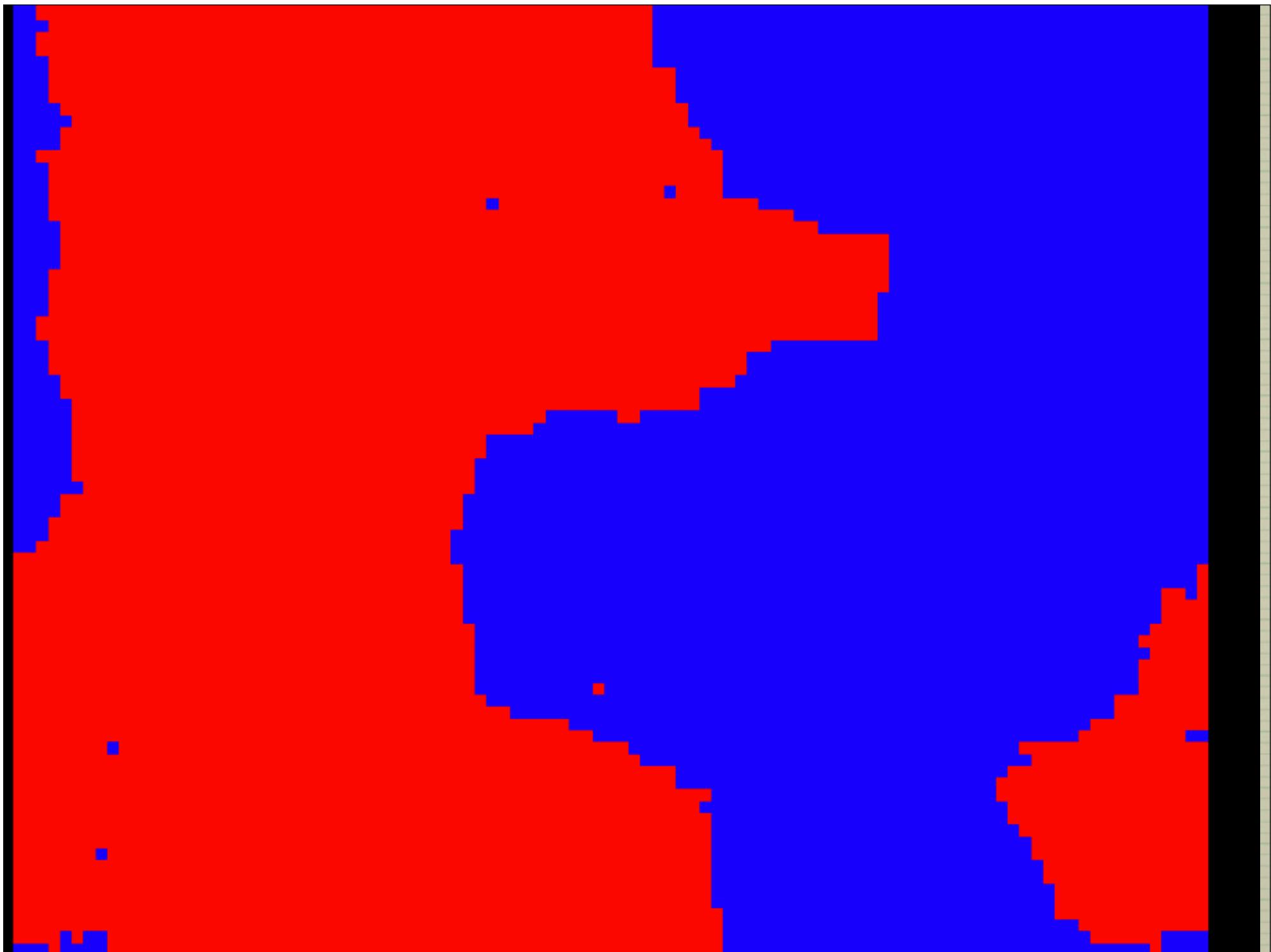


ANTIFERROMAGNETISM

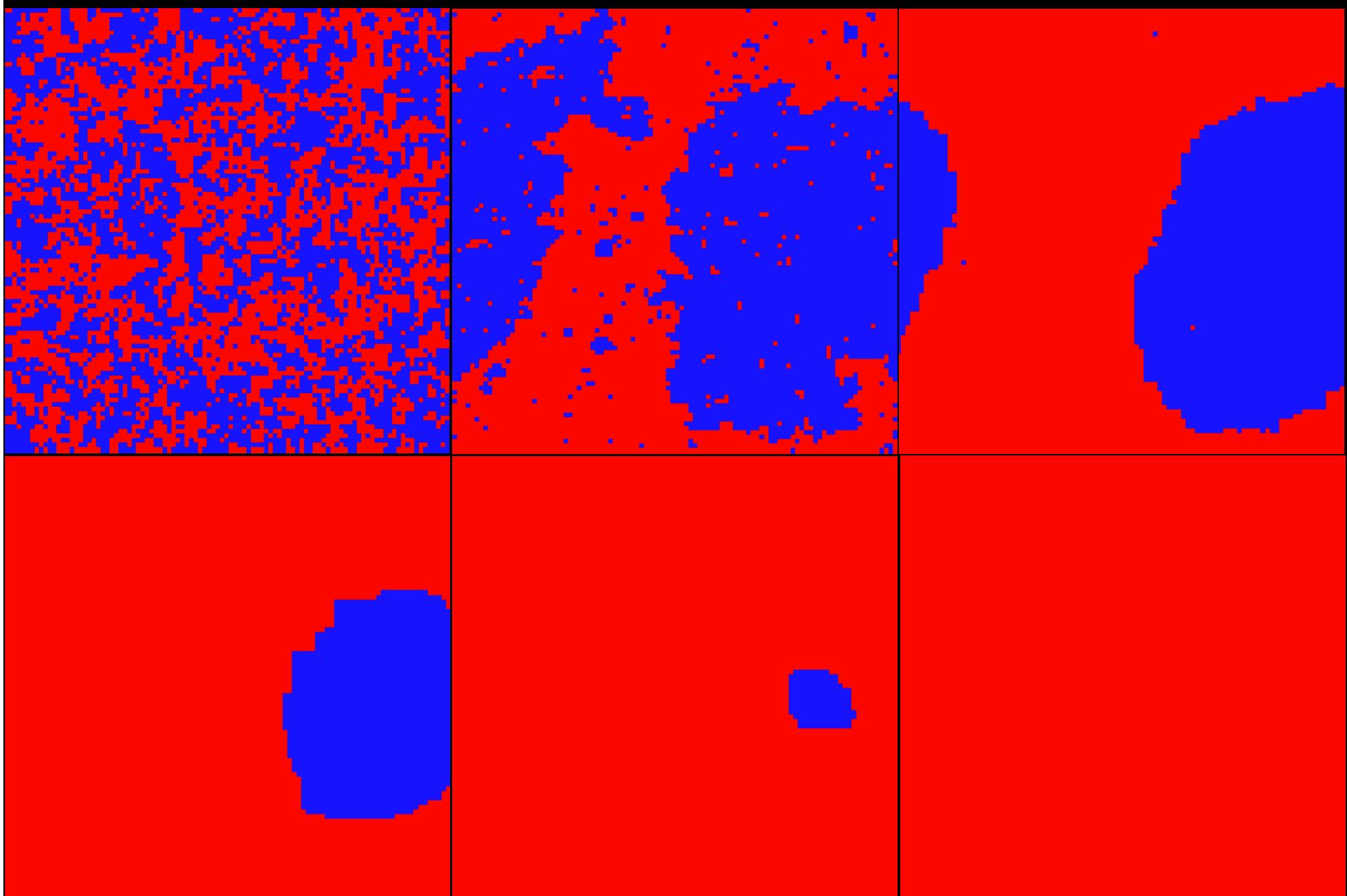


ODD NUMBER OF GRID POINTS

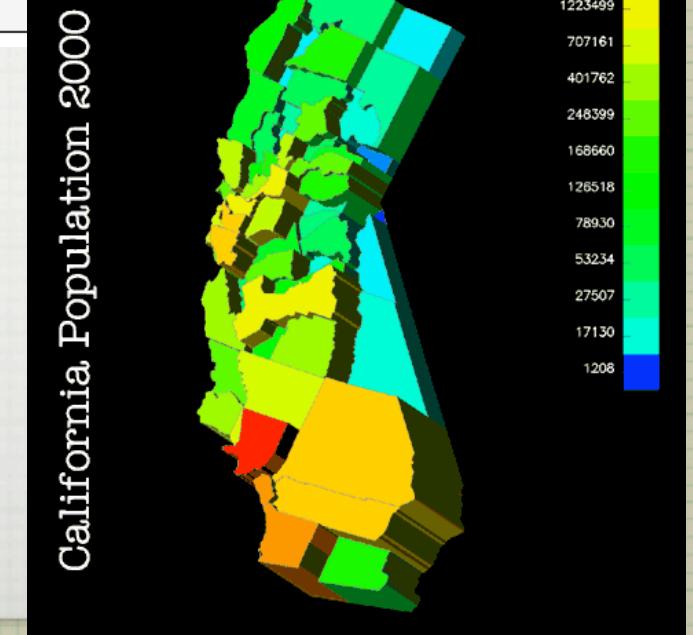
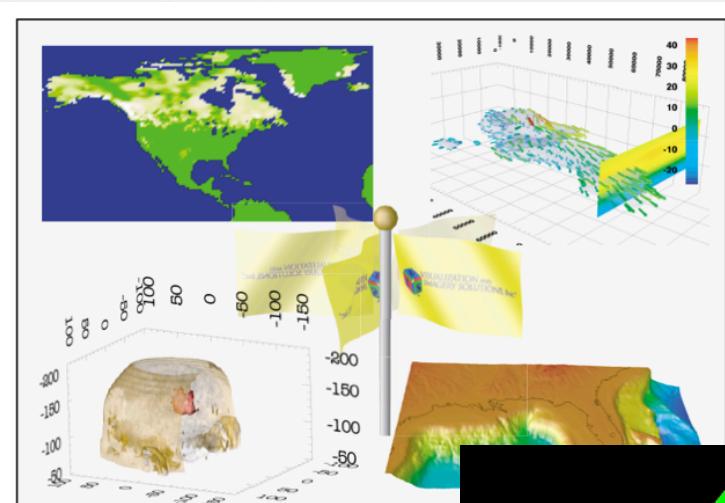
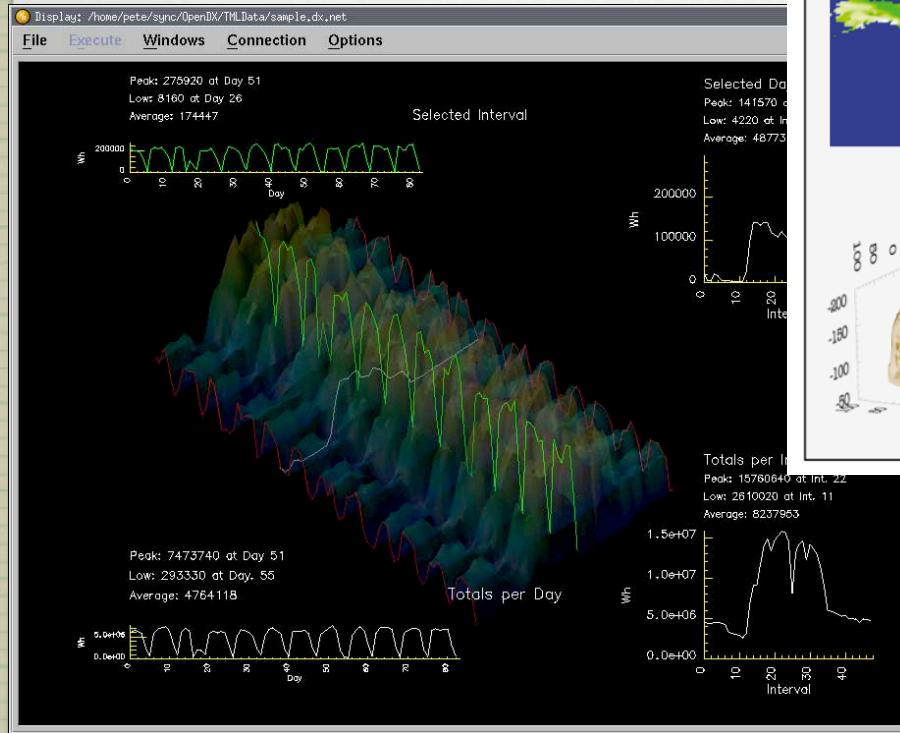




FERROMAGNETISM: ANNEALED AT HIGH T



OPENDX



OpenDX

SUMMARY

- This lecture is the last focusing solely on the use of random number to model natural phenomena
- The **Metropolis algorithm** is very powerful: it permits to find the global minimum of a system of size well too large for a systematic inspection
 - The main idea is that the algorithm restricts itself to searching areas that are most probable of yielding a global minimum
 - However, the main feature remains that the algorithm is not a “down-hill” method: it does allow going up in energy, at least if the relative probability of existence of the new state is “large enough”.
 - The method works because of the calculation of the probability hinges on well-established laws of nature.