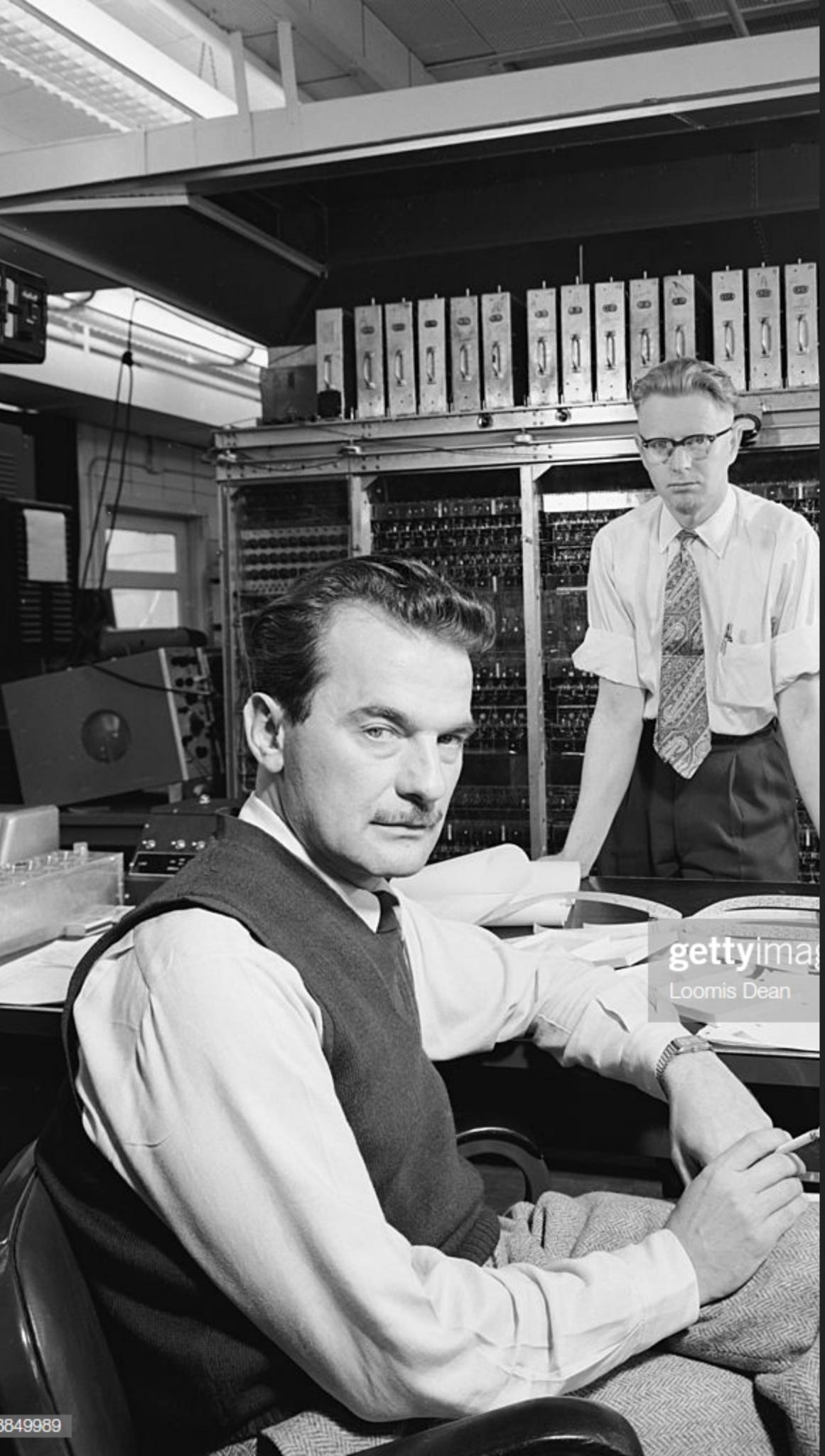


NICOLÁS VERGARA - NANOMAGNETISM
LABORATORY

APPLICATION OF THE METROPOLIS–HASTINGS
ALGORITHM IN 2D AND 3D NANO-MATERIALS
WITH MAGNETIC PROPERTIES.



AT LOS ALAMOS, IN THE 1950S, A GROUP OF RESEARCHERS LED BY METROPOLIS, INCLUDING JOHN VON NEUMANN AND STANISLAW ULAM, DEVELOPED THE MONTE CARLO METHOD.

NICHOLAS METROPOLIS

THE MONTE CARLO METHOD IS A STATISTICAL APPROACH TO SOLVE DETERMINISTIC MANY-BODY PROBLEMS. IN 1953 METROPOLIS CO-AUTHORED THE FIRST PAPER ON A TECHNIQUE THAT WAS CENTRAL TO THE METHOD NOW KNOWN AS SIMULATED ANNEALING.

THIS LANDMARK PAPER SHOWED THE FIRST NUMERICAL SIMULATIONS OF A LIQUID



N. Metropolis; A.W. Rosenbluth; M.N. Rosenbluth; A.H. Teller & E. Teller (1953).

"Equation of State Calculations by Fast Computing Machines". Journal of Chemical Physics. 21 (6): 1087-1092

. Bibcode:1953JChPh..21.1087M.

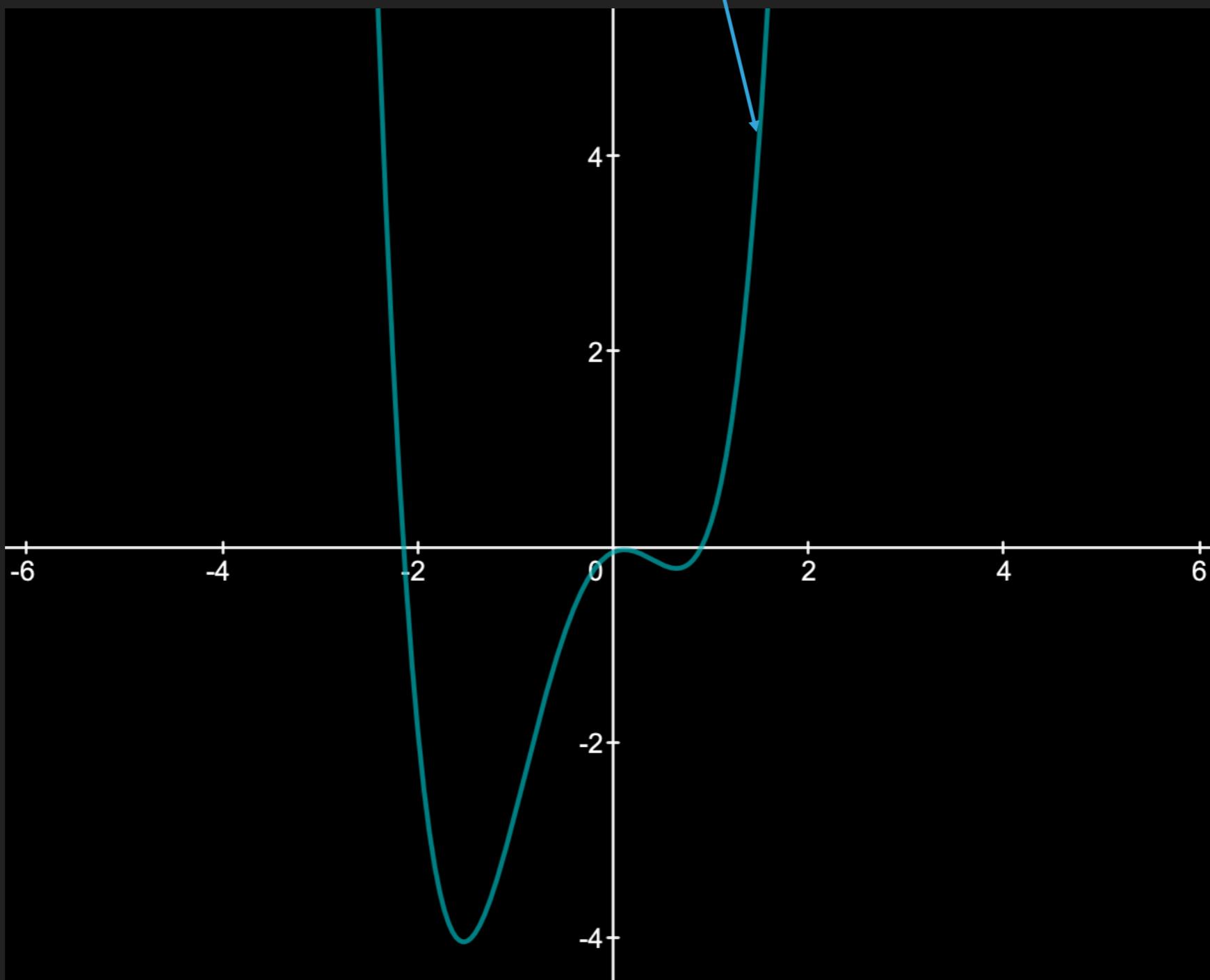


THE ALGORITHM FOR GENERATING SAMPLES FROM THE BOLTZMANN DISTRIBUTION WAS LATER GENERALIZED BY W.K. HASTINGS TO BECOME THE METROPOLIS-HASTINGS ALGORITHM

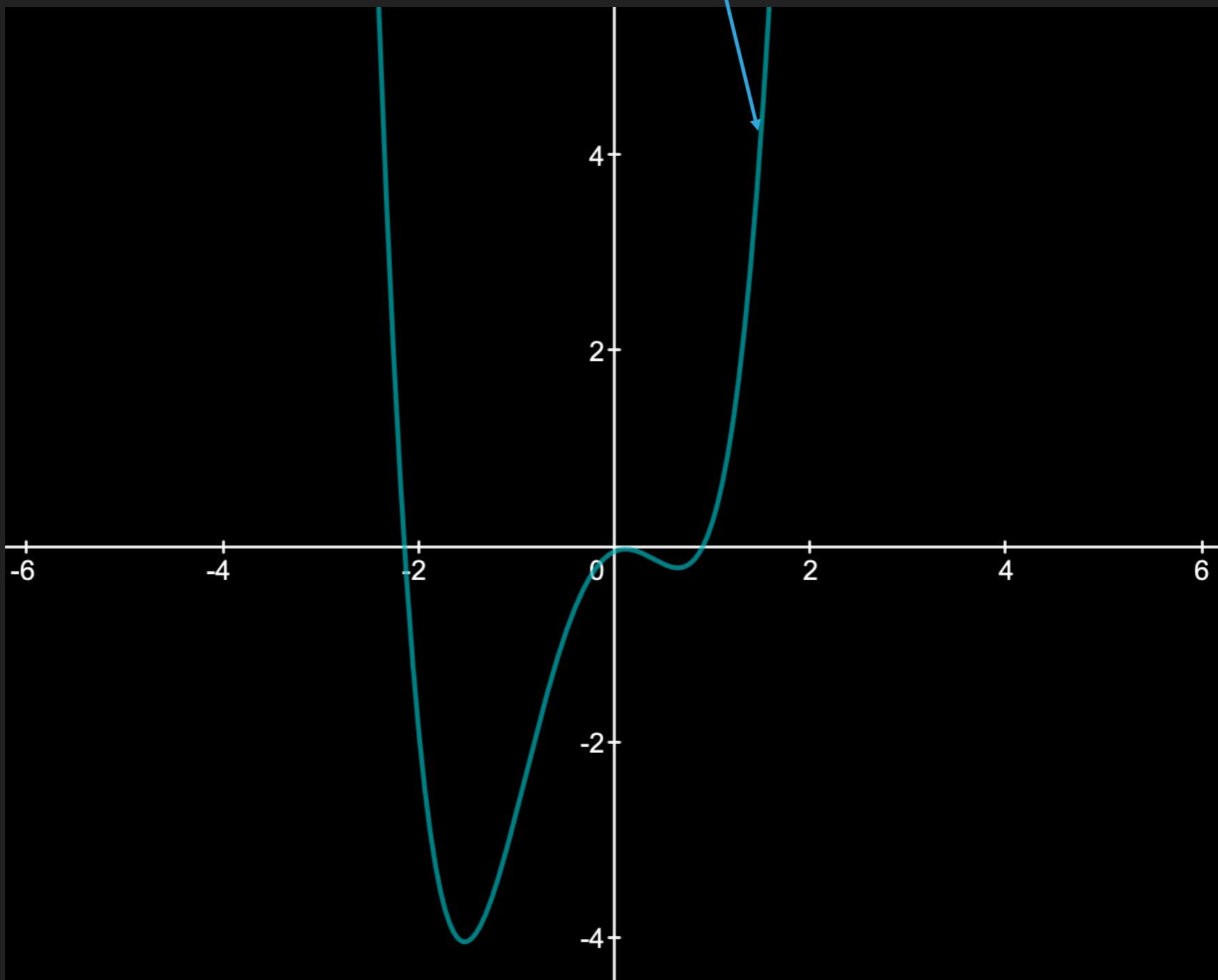
W. K. HASTINGS

**EVERYTHING IS
OPTIMIZATION.**

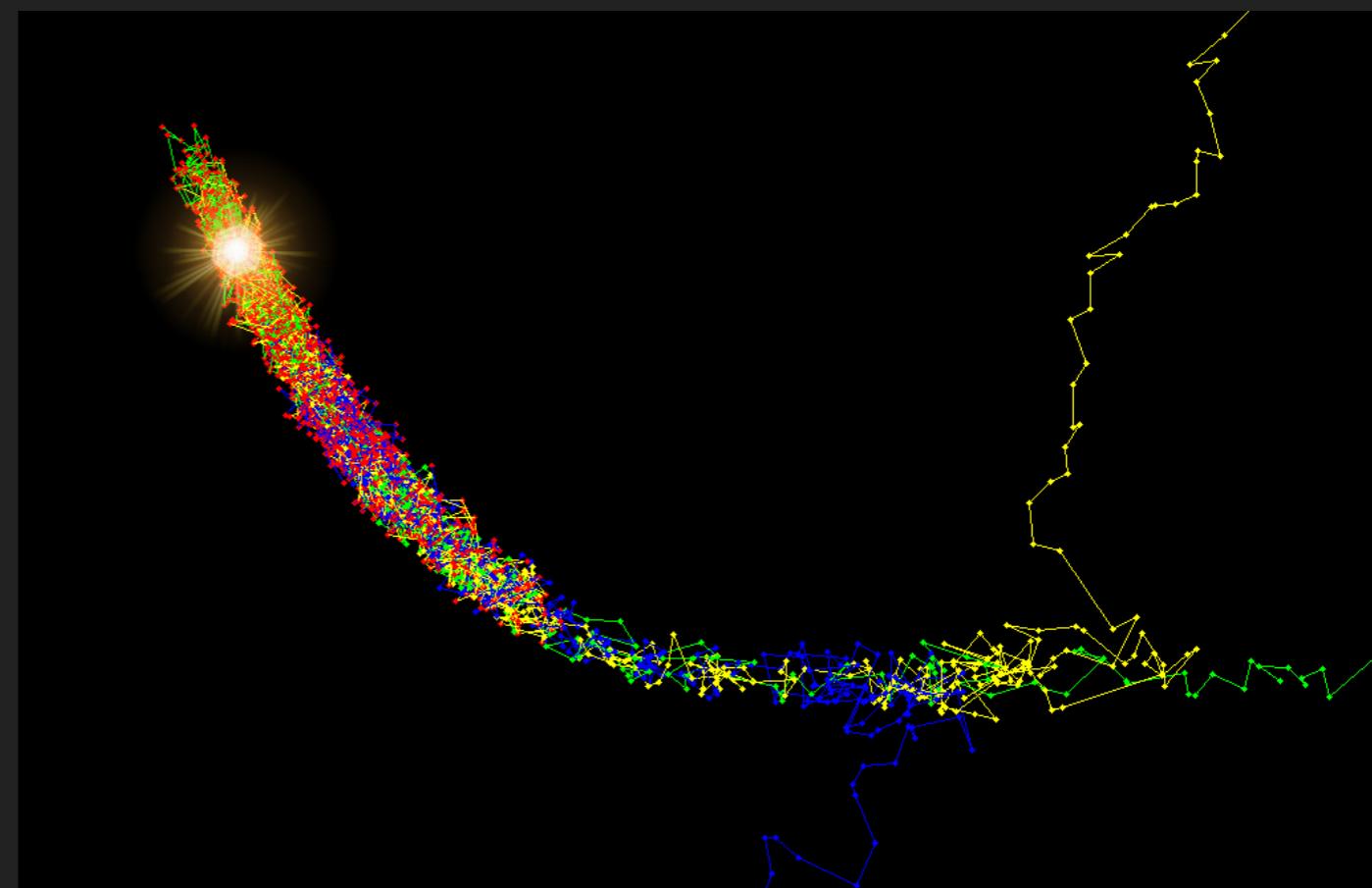
GRADIENT DESCENT



METROPOLIS-HASTINGS



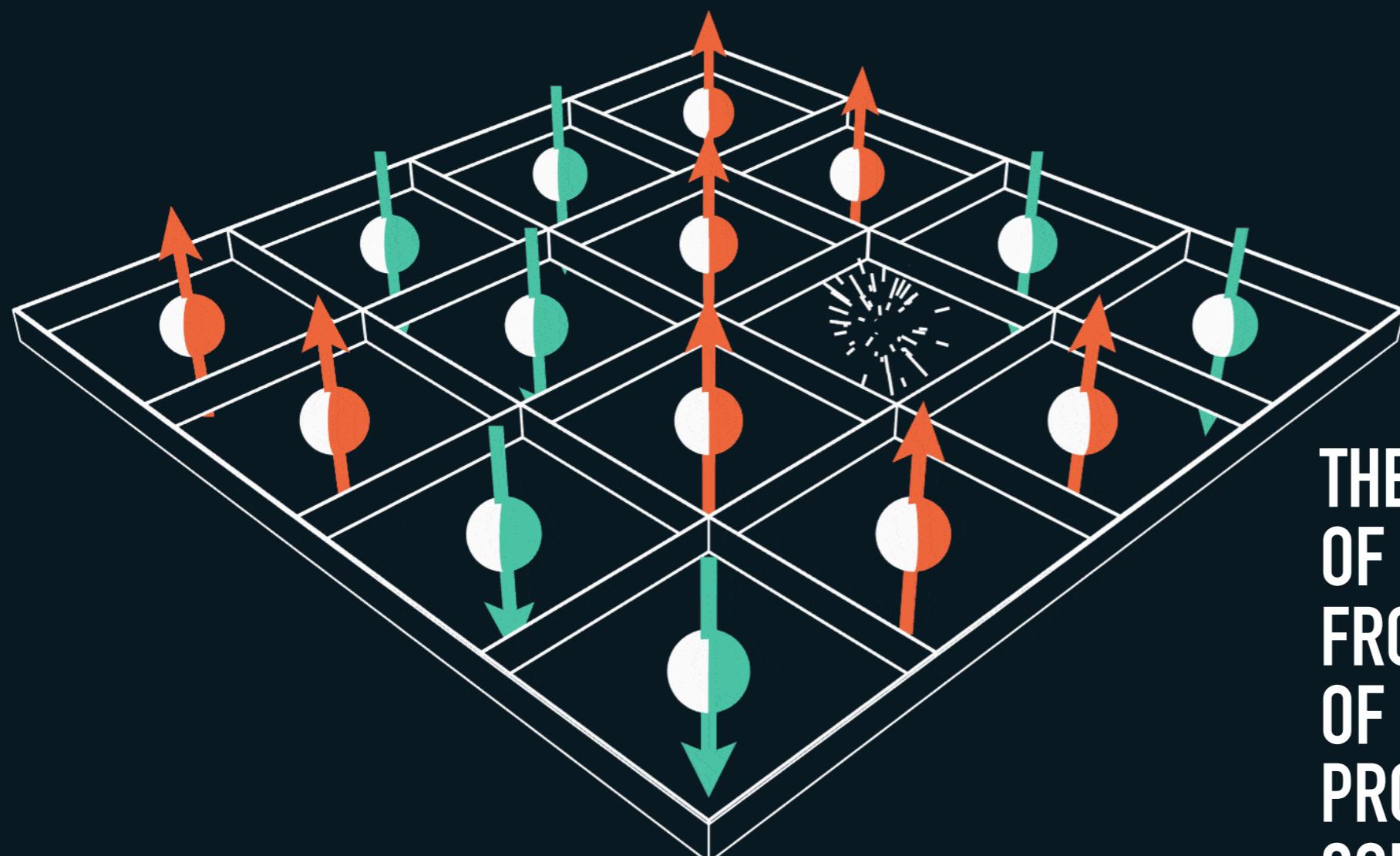
- ▶ Cryptography
- ▶ Fluids dynamics
- ▶ Swarm control
- ▶ Macro-Economics Analysis



The result of three Markov chains running on the 3D Rosenbrock function using the Metropolis-Hastings algorithm. The original uploader was Vasileios Zografos at English Wikipedia

NOW A LITTLE BIT
OF PHYSICS

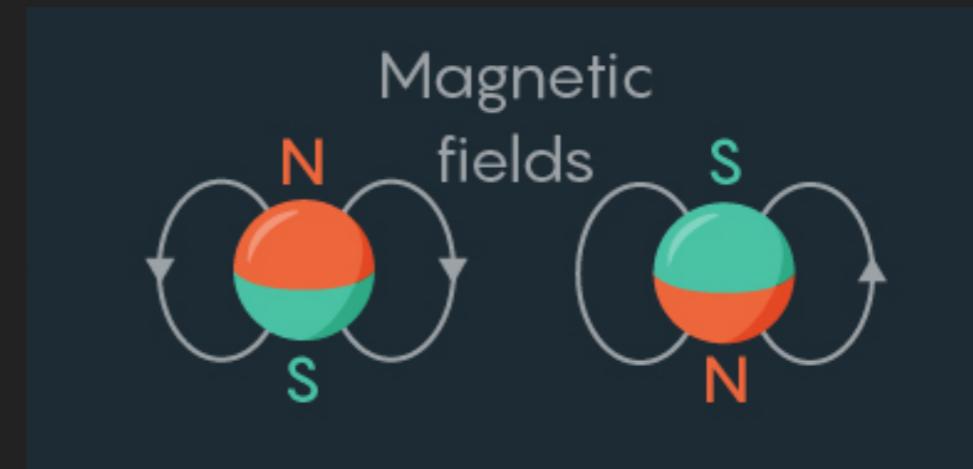
MAGNETS



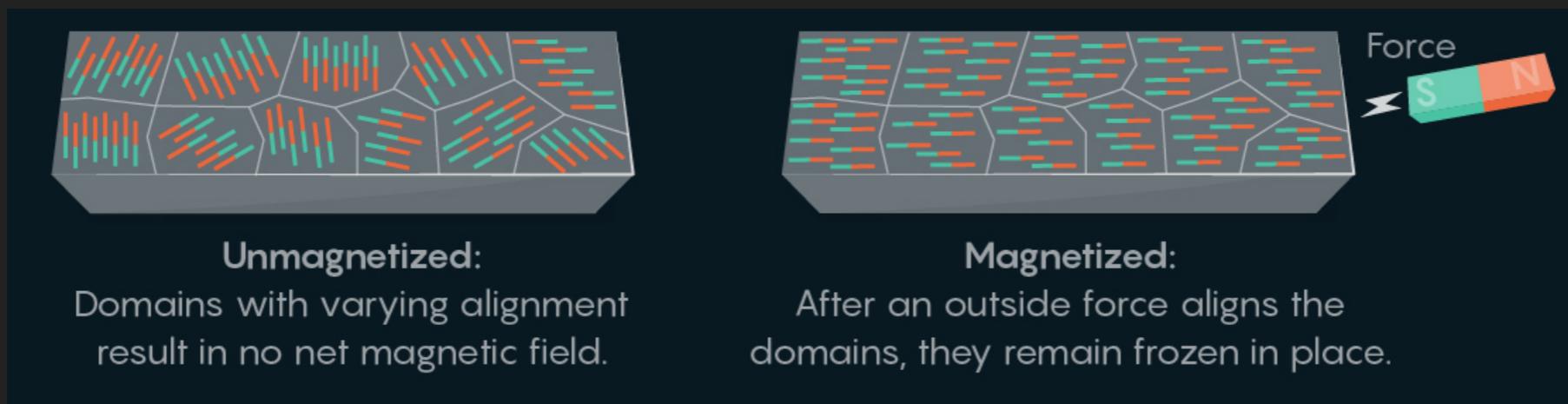
THE MAGNETIC PROPERTIES OF THE MATERIALS ARISES FROM ELECTRONS. THE SUM OF THE ELECTRONS PROPERTIES DESCRIBES COMPLETELY THE MAGNET

SPIN

11

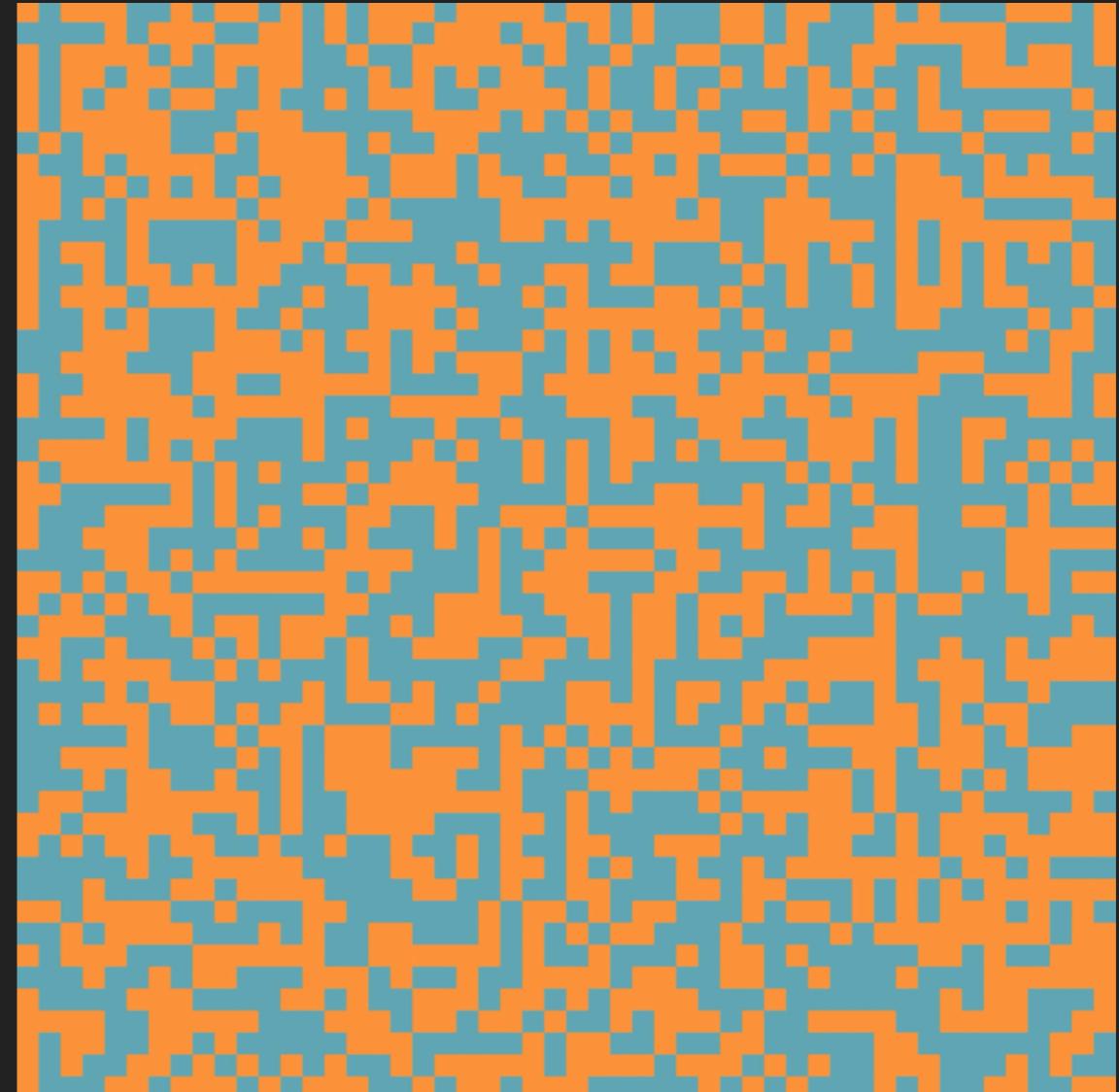


AS ELECTRONS HAVE CHARGE, AND THIS PROPERTY EXPLAINS ELECTRIC FIELDS.
THEY ALSO HAVE SPIN, AN INTRINSIC PROPERTY THAT EXPLAINS THE MAGNETIC FIELD



WE SIMULATE A
MAGNET AS AN
ARRAY OF SPINS.
EVERY TIME WE
INITIALIZE IT WE
MUST ASSURE A
RANDOM STATE

ORANGE IS SPIN UP AND BLUE IS SPIN DOWN



2D MODEL

```
SYSTEM = HBAR*2 * (0.5 - NP.RANDOM.RANDINT(0, 2,SIZE=[L, L, L]))
```

**BUT WHAT ABOUT
THE DYNAMICS ?**

MINIMIZE THE ENERGY

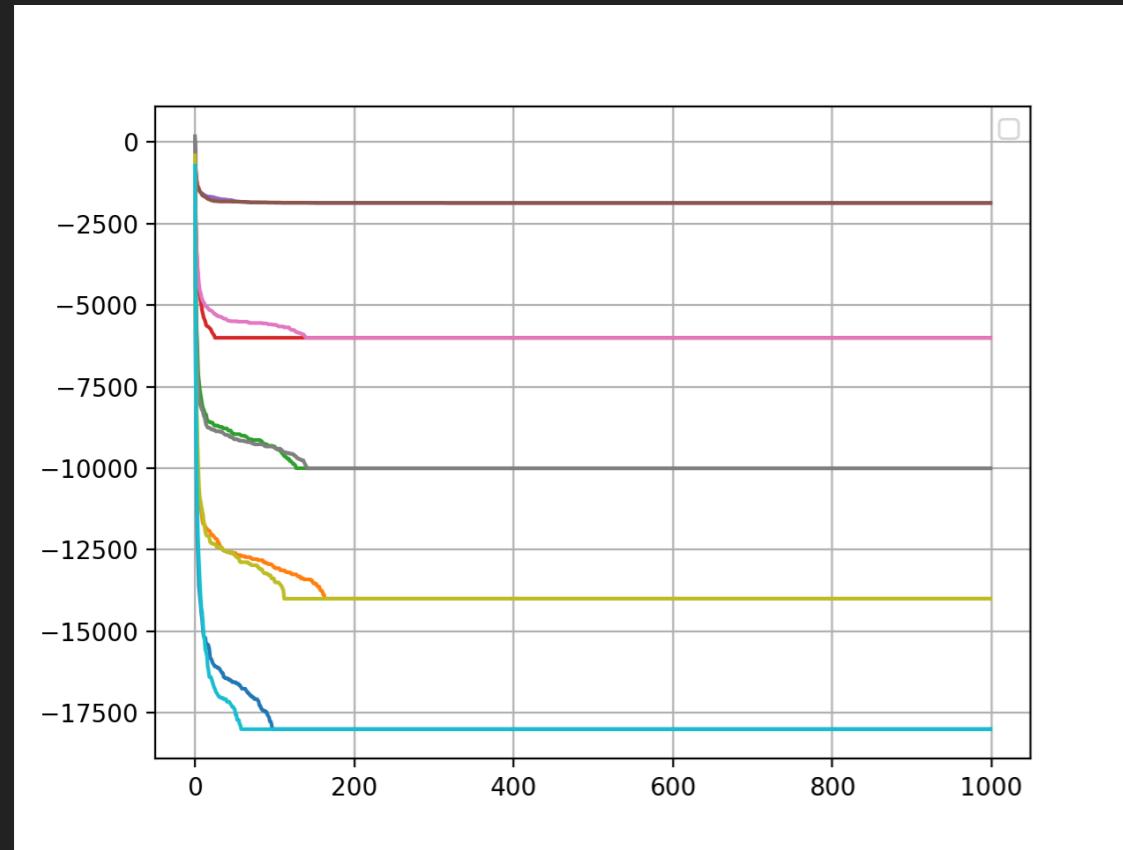
As the metropolis-hasting is a probabilistic method. We need to find a probability that help us to avoid a local minimum related to the minimization of the Energy

$$p_i = \frac{1}{Z} e^{-E_i/(K_B T)}$$

CANONICAL ENSEMBLE

MINIMIZATION OF ENERGY

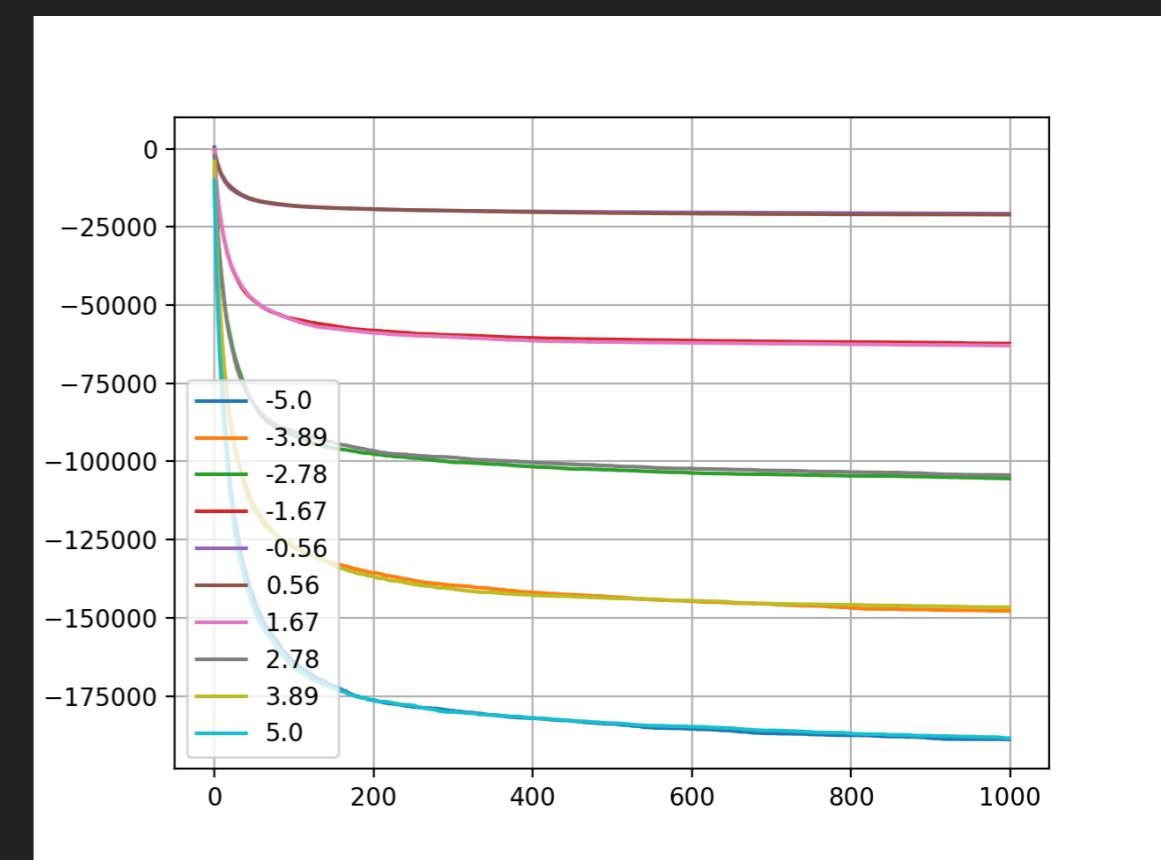
Energy



Iterations

 $M=30 \times 30$

Energy



Iterations

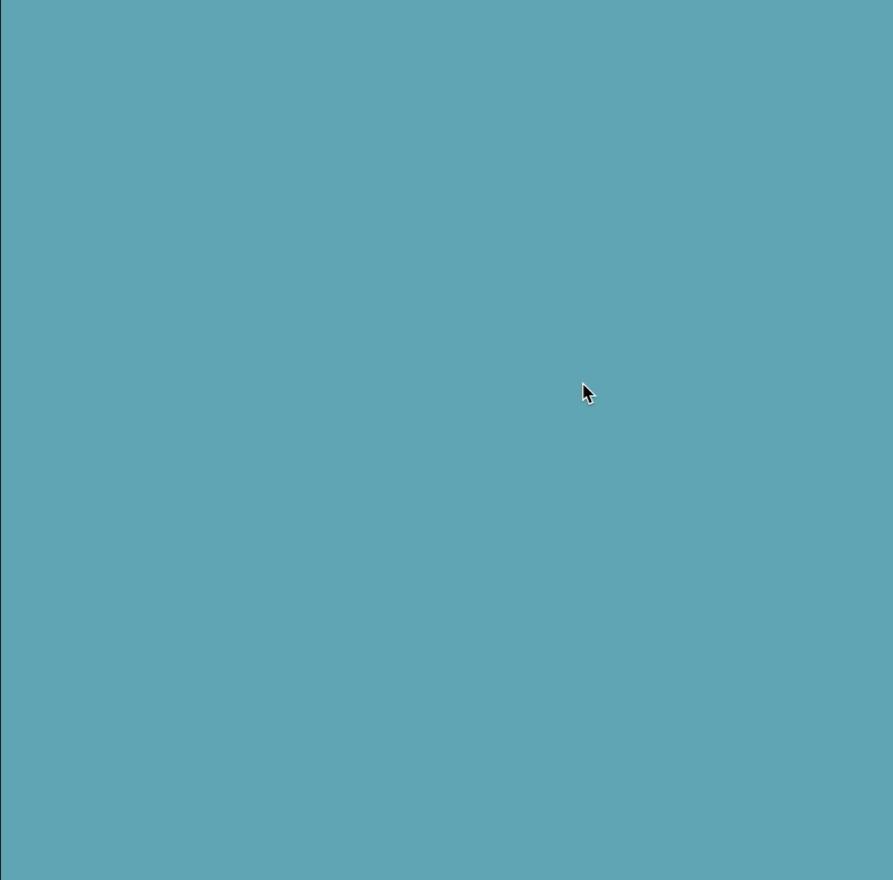
 $M=100 \times 100$

$$p_i = \frac{1}{Z} e^{-E_i/(K_B T)}$$

SO IF WE FIX THE ENERGY, ASSUMING IT'S ALREADY MINIMUM , WE CAN EXPECT THAT THE TEMPERATURE GIVE INFORMATION ABOUT THE MOST PROBABLE STATE OF THE SYSTEM

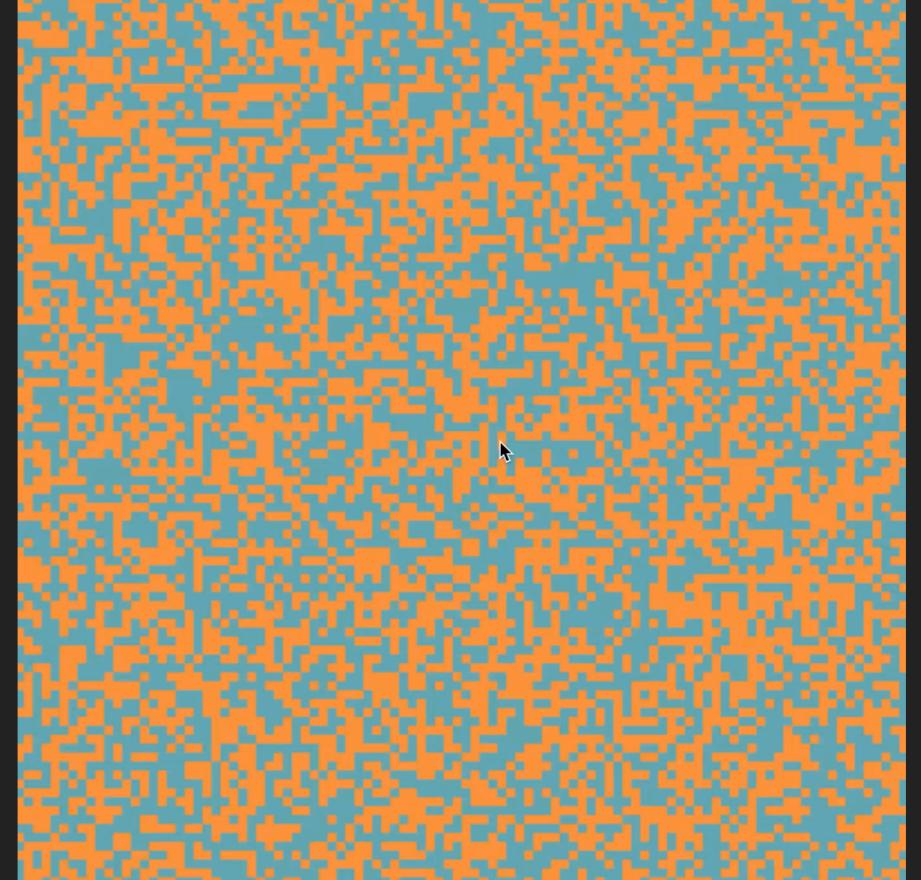
$$T \rightarrow 0 \Rightarrow p_i \approx 1$$

THERE IS ONE REALLY PROBABLE STATE



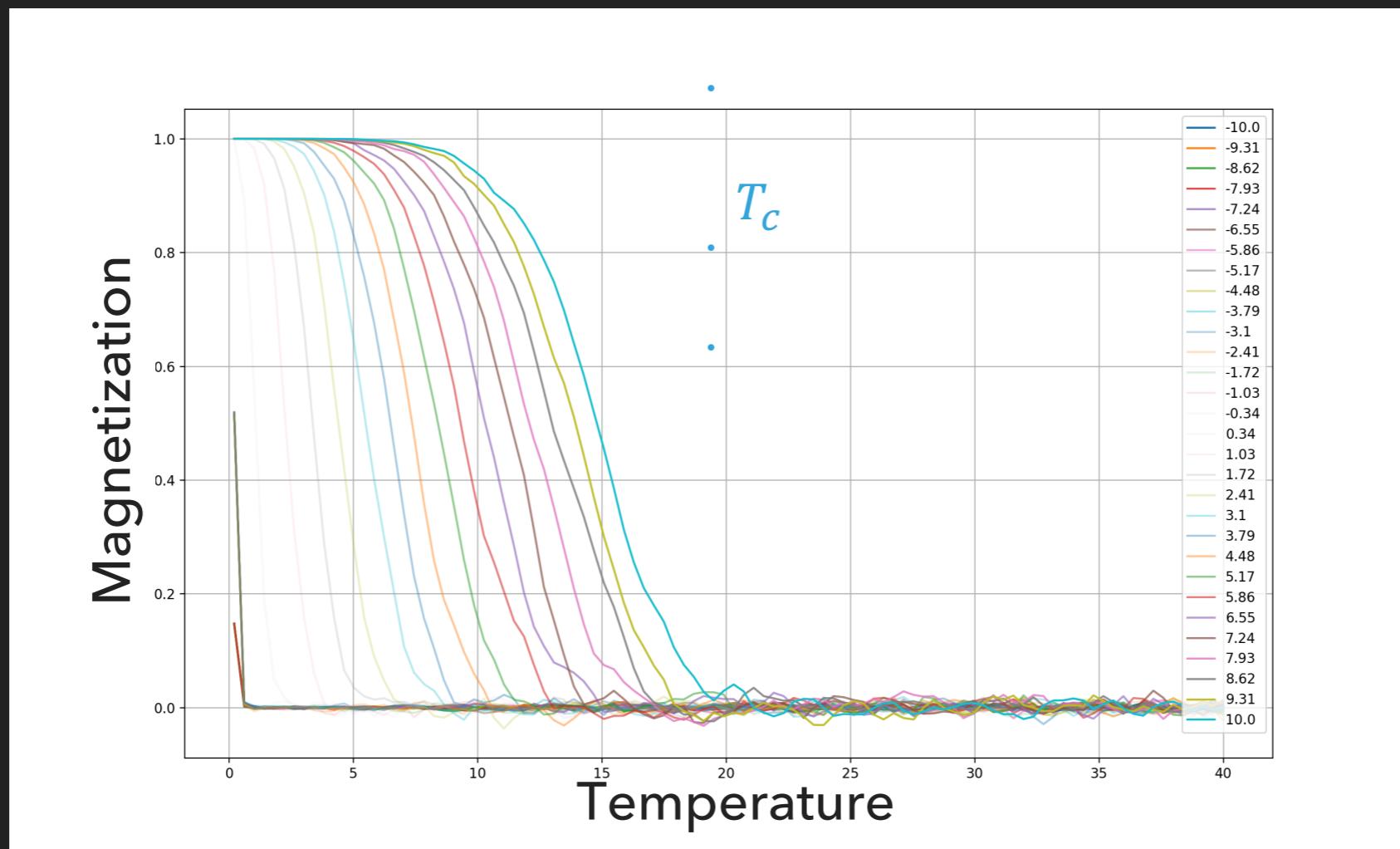
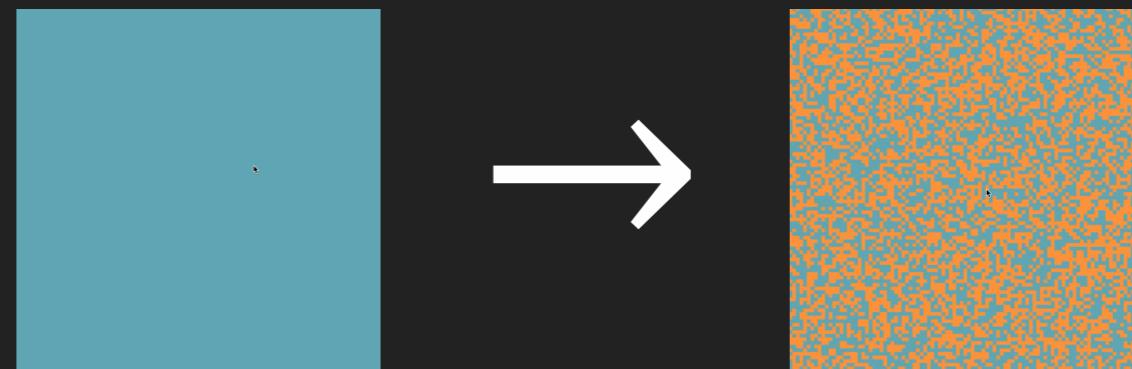
$$T \rightarrow \infty \Rightarrow p_i \approx 0$$

THERE ARE MANY PROBABLE MICRO-STATES



THE TEMPERATURE OF TRANSITION BETWEEN
THIS TWO STATES, IT'S CALLED THE CURIE
TEMPERATURE : T_c

17



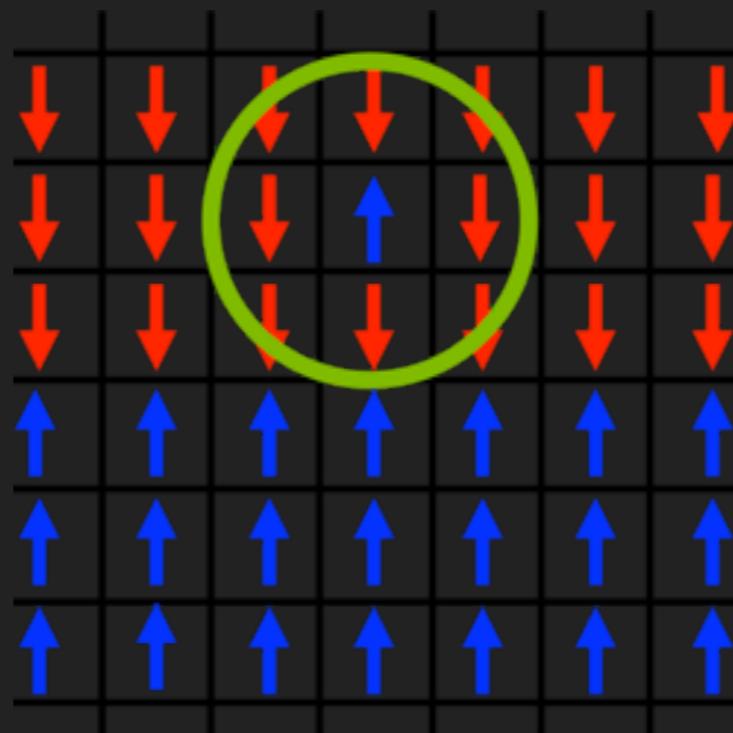
Transition of state, for different simulated systems

MEASURING THE ENERGY AND MAGNETIZATION

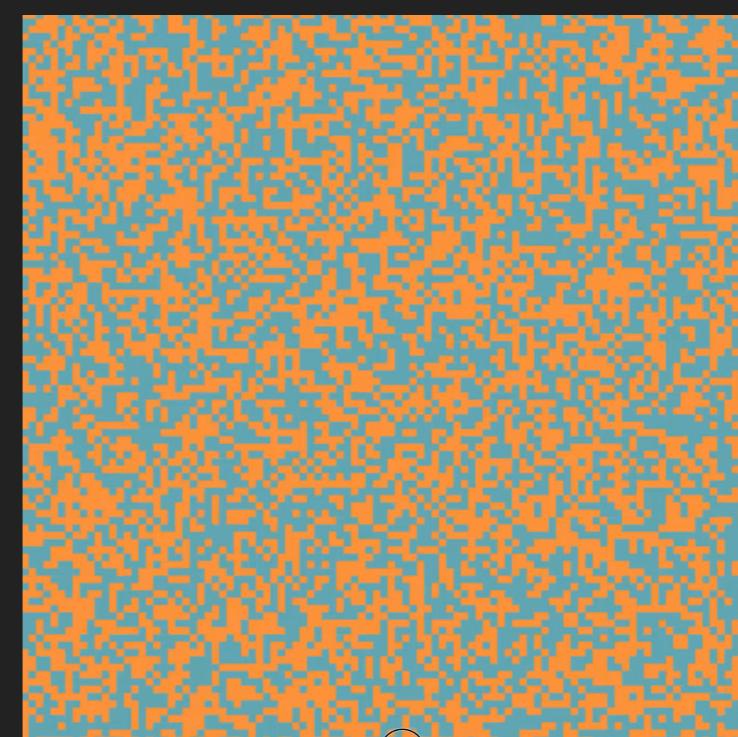
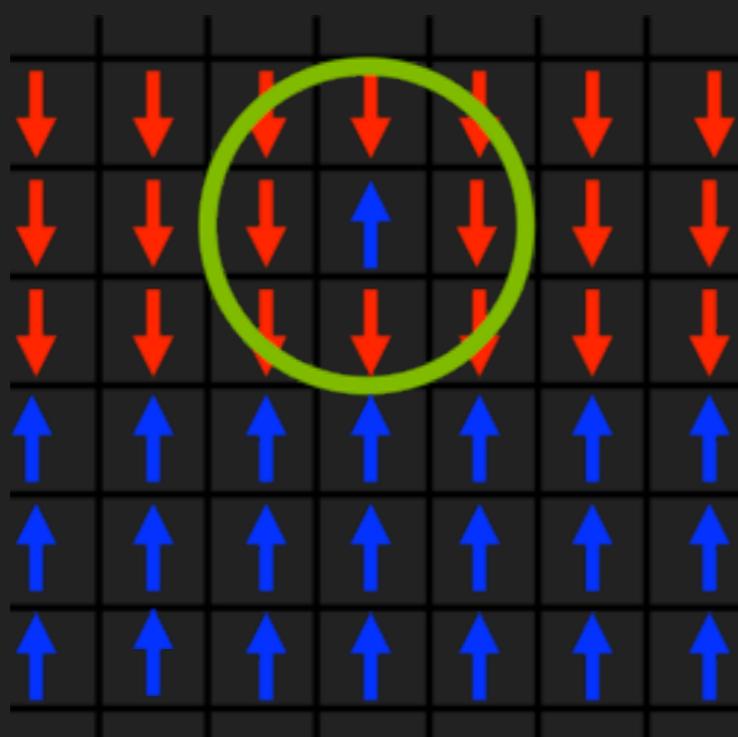
$$\mathcal{H}_i = s_{iz} \sum_j J_{ij} s_{jz}$$

WE CAN DESCRIBE THE DYNAMICS OF THE ENERGY USING THE ISING MODEL.

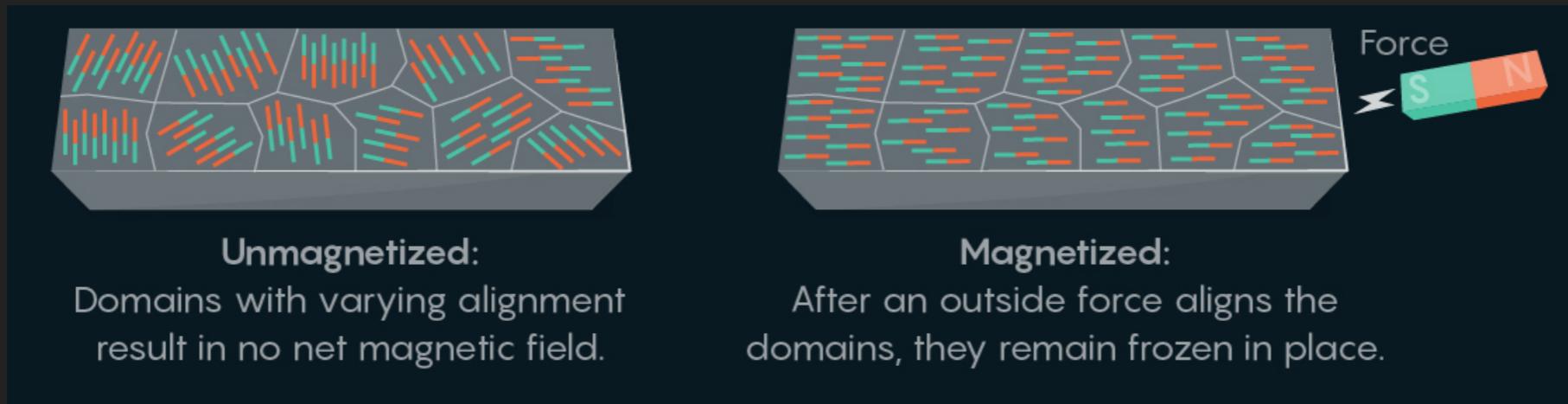
IT SAYS THAT IF $J_{ij} > 0$ SPINS TEND TO BE PARALLEL TO EACH OTHER,
BUT IF $J_{ij} < 0$ SPINS TEND TO BE ANTIPARALLEL



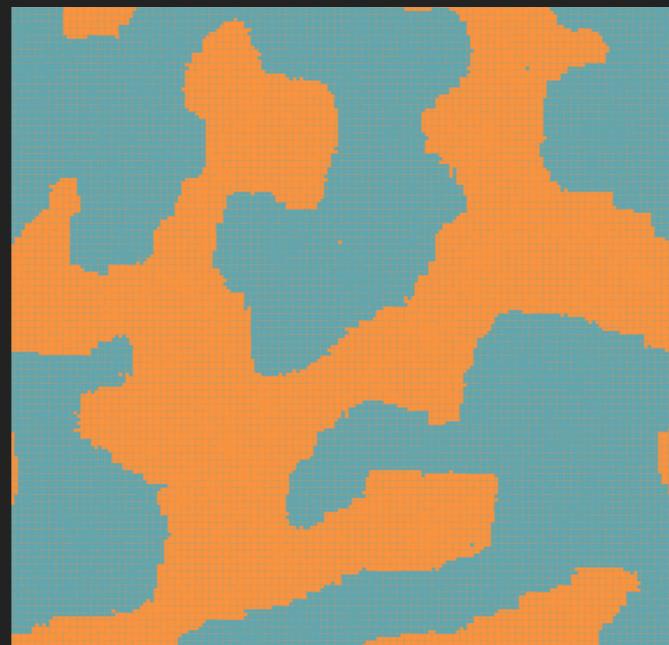
- ▶ Best we can do it's $\sim O(n)$
- ▶ But we can know if a flip in the system will reduce the energy and then update.
- ▶ Then update moment-Magnetization



- ▶ Write everything as a function
- ▶ Choose properly inputs and outputs
- ▶ Import jit
- ▶ Choose the Flags: nopython, nogil, parallel, fastmath



THANKS TO THE SIMULATION WE PREDICT THE FORMATION OF DOMAINS FOR TEMPERATURES IN THE RANGE OF THE TRANSITION OF STATE $0 < T < T_C$



Ernst Ising, Contribution to the Theory of Ferromagnetism. http://www.hsaugsburg.de/~harsch/anglica/Chronology/20thC/Ising/isi_fm00.html

WHAT IF THERE IS AN EXTERNAL MAGNETIC FIELD?

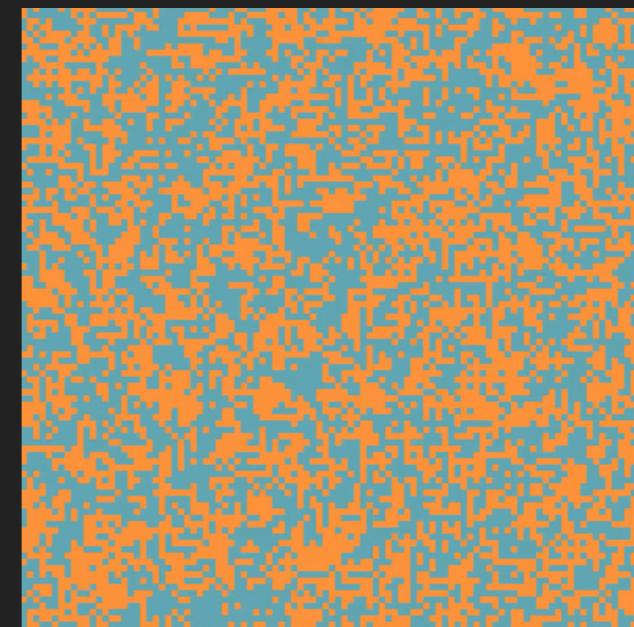
$$E_i \equiv \mathcal{H}_i = s_{iz} \sum_j J_{ij} s_{jz} \rightarrow \mathcal{H}_i = s_{iz} \sum_j J_{ij} s_{jz} + B s_{iz}$$

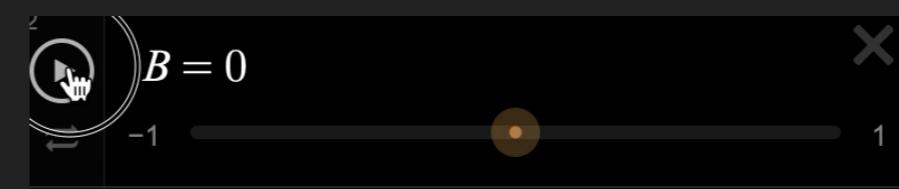
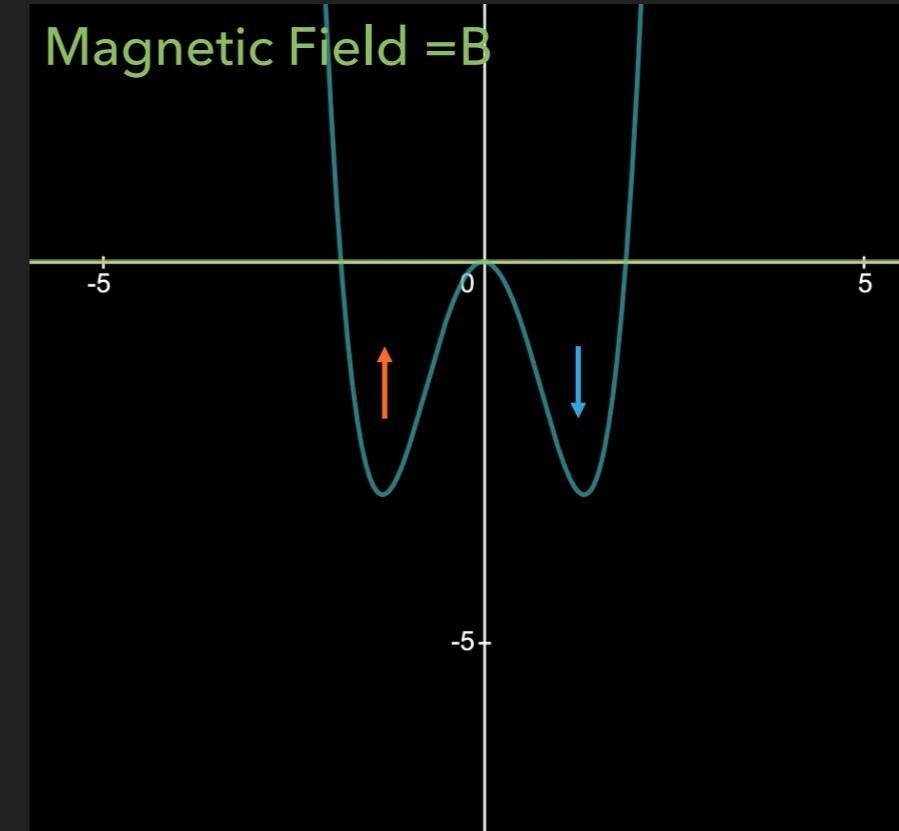
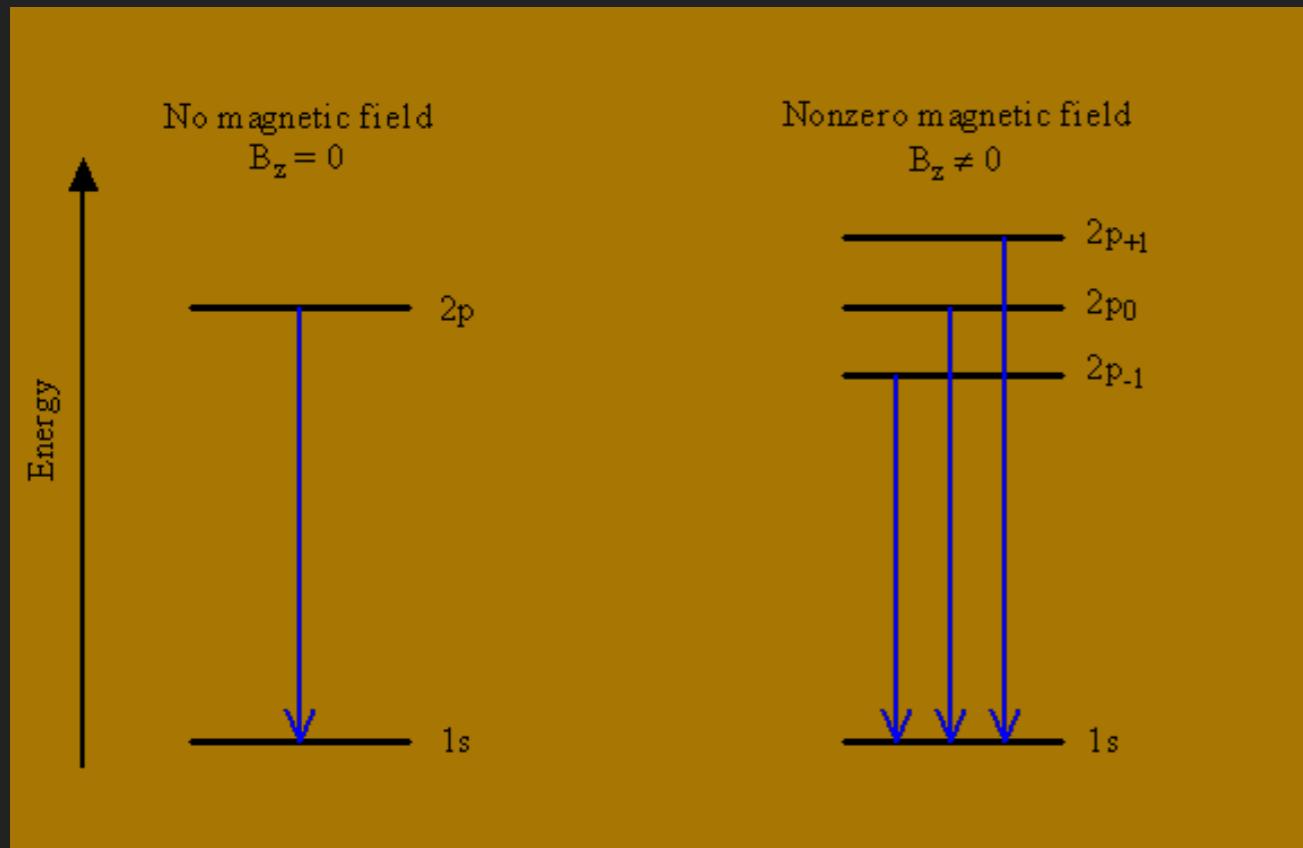
SPINS TENDS TO ALING TO THE FIELD

$T < T_c$



$T > T_c$

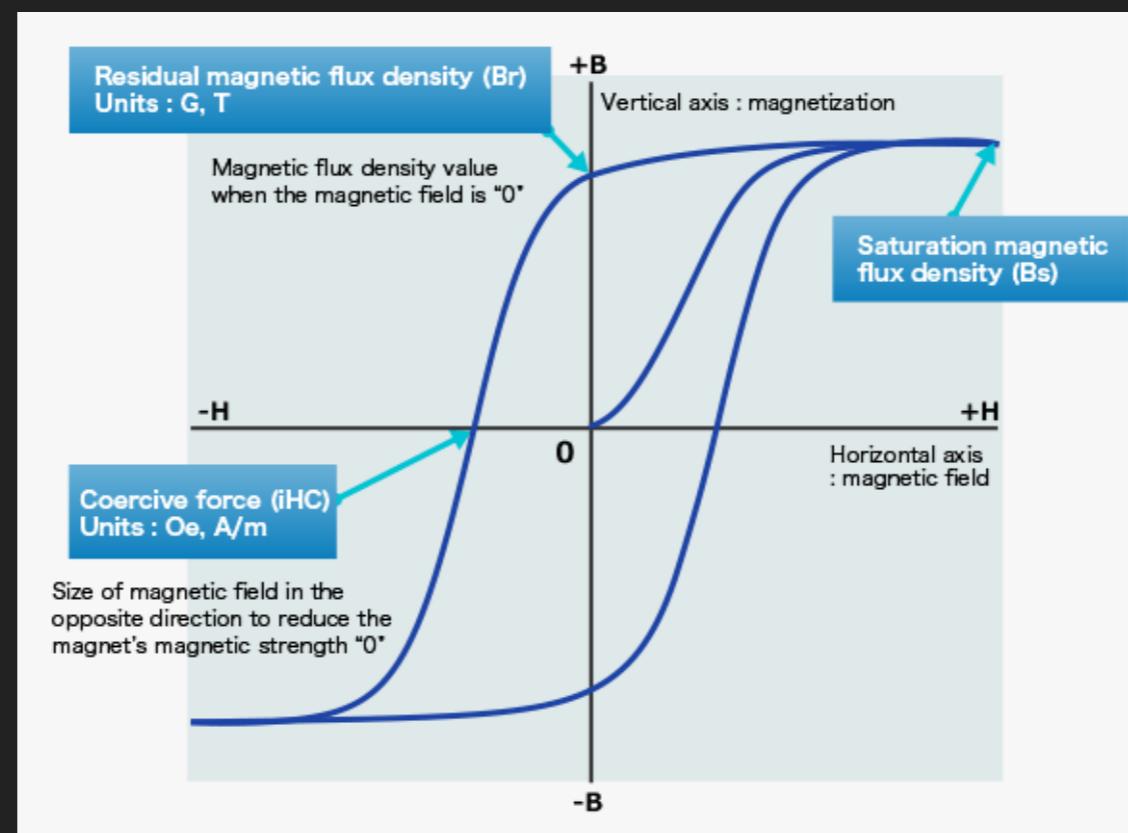


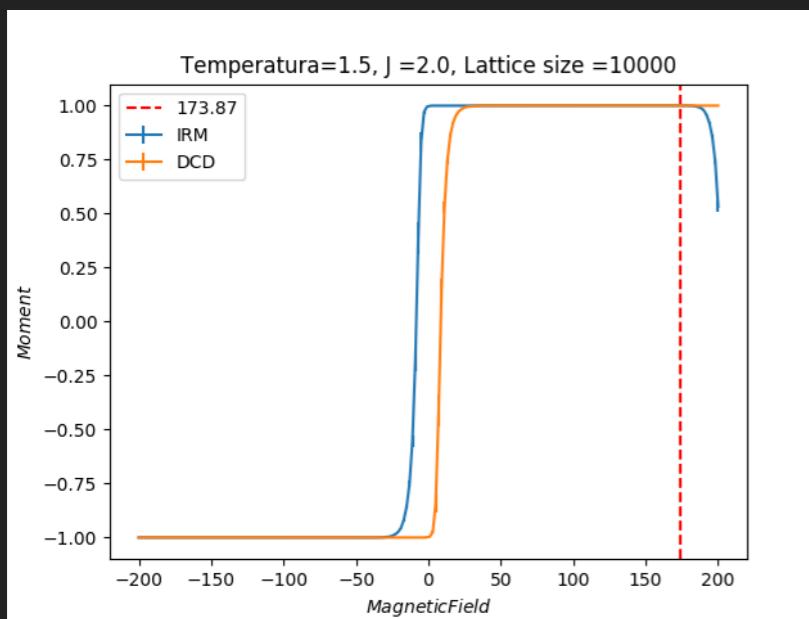
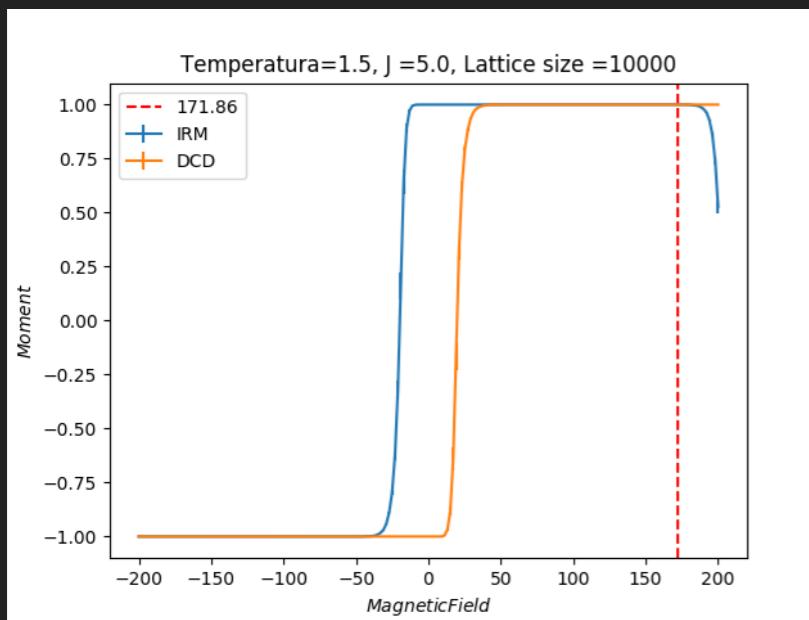
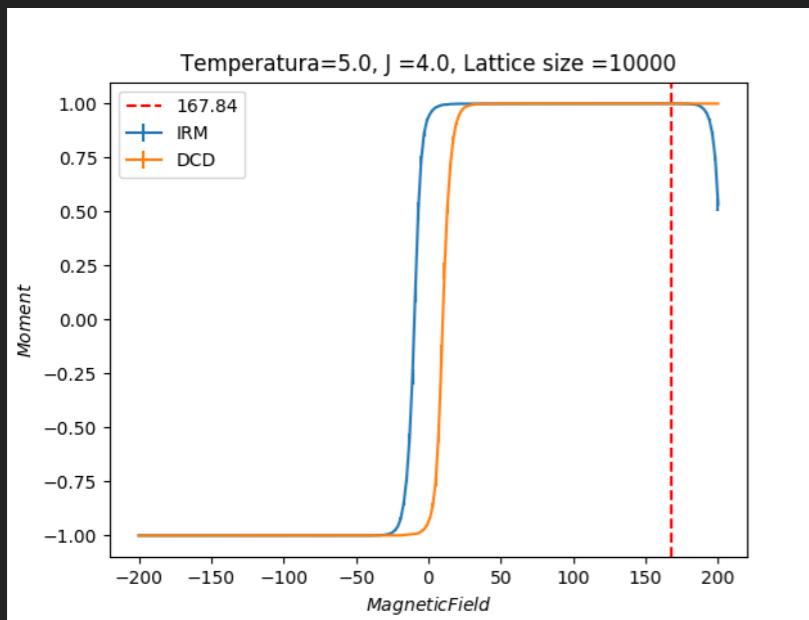


SPONTANEOUS SYMMETRY BREAKING

WHAT HAPPEN IF WE VARY THE FIELD, FROM²⁵ REALLY STRONG IN ONE DIRECTION, TO THE OTHER, AND MEASURE THE MAGNETIZATION?

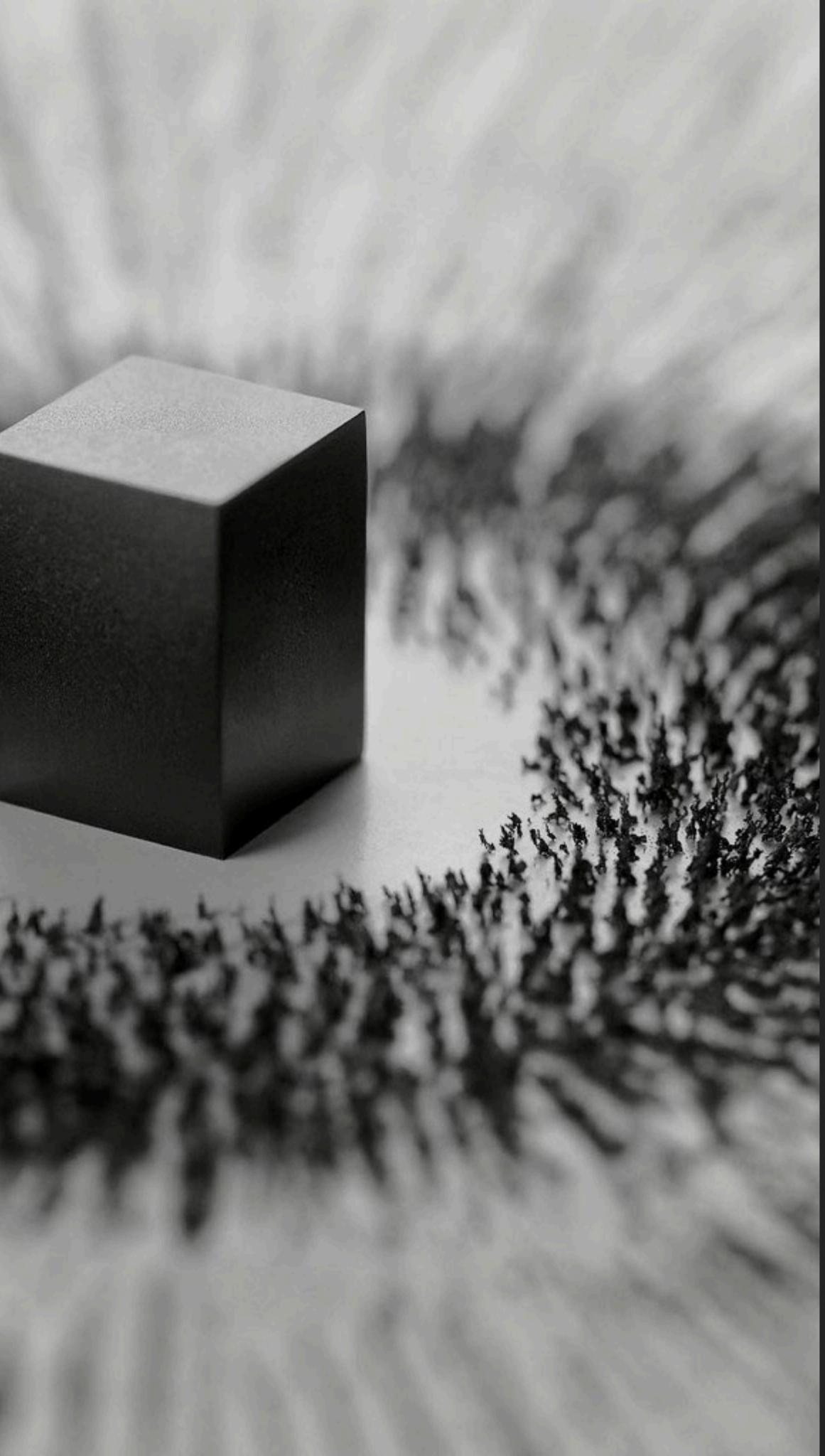
IT BEHAVES AS THE MAGNET HAS MEMORY. BECAUSE ,WE OBTAIN AN HYSTERESIS LOOP, IN OTHER WORDS IT DOES NOT RETURN BACK AT THE SAME PATH.





CAN WE REPRODUCE
THIS BEHAVIOR WITH
OUR SIMULATION?

YES, THE 2D ISING
MODEL HAS MEMORY.



BUT WHAT OTHER MEASURES CAN WE REPRODUCE WITH THIS MODEL AND THE METROPOLIS ALGORITHM?

ISOTHERMAL REMANENT
MAGNETIZATION

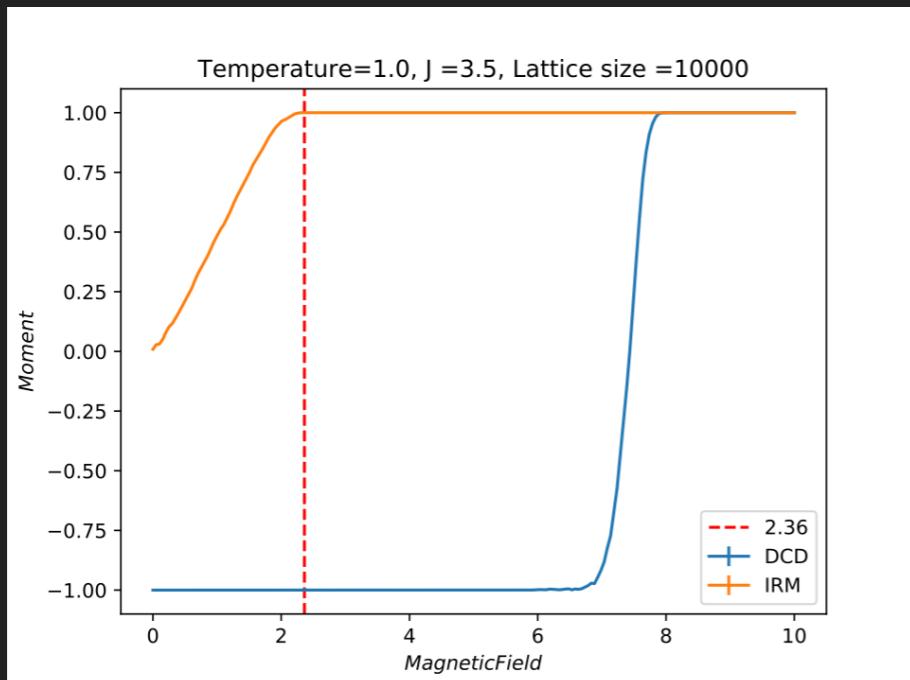
DIRECT CURRENT DEMAGNETIZATION

HEAT CAPACITY

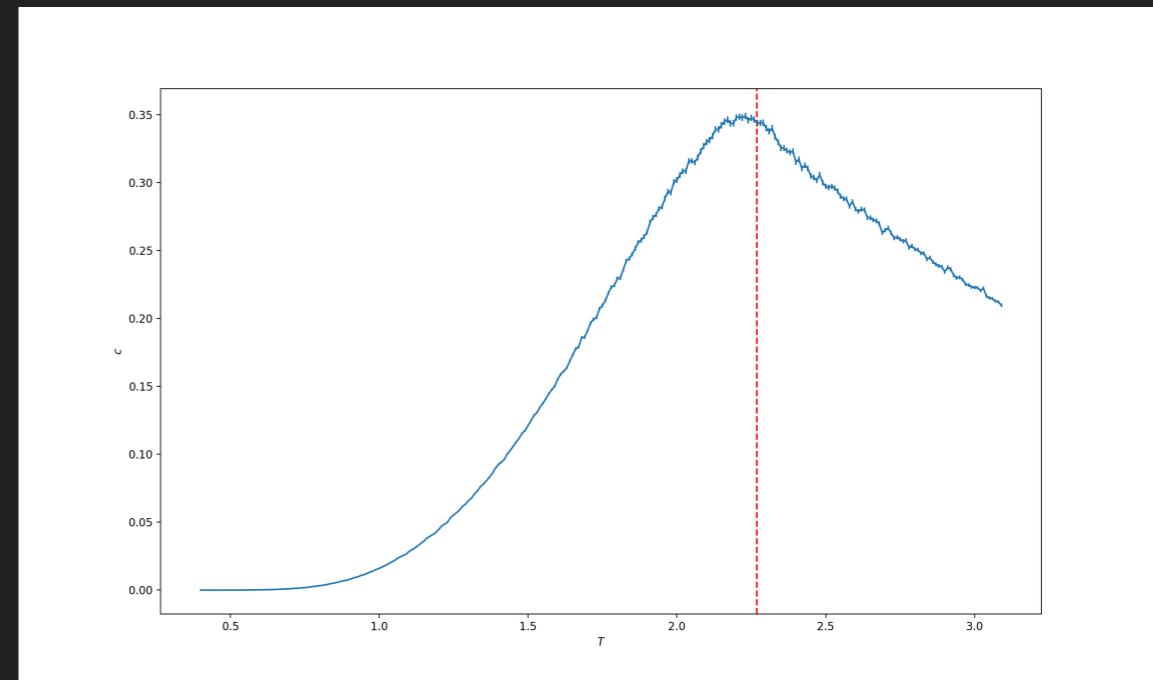
SUSCEPTIBILITY

ENERGY

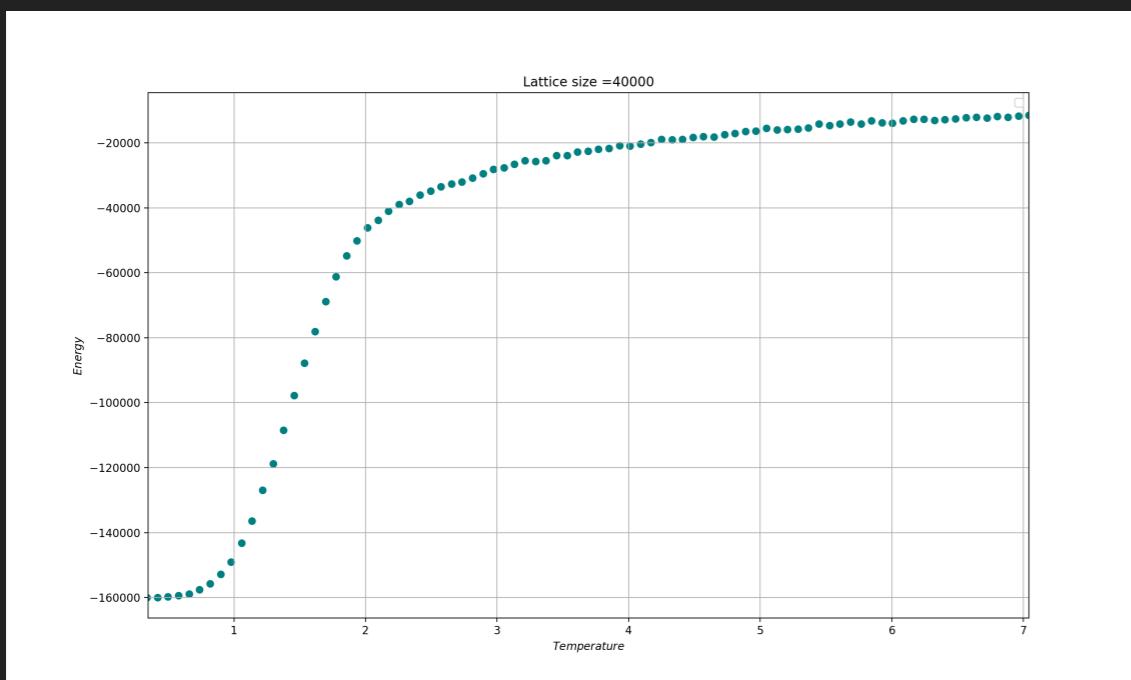
IRM AND DCD



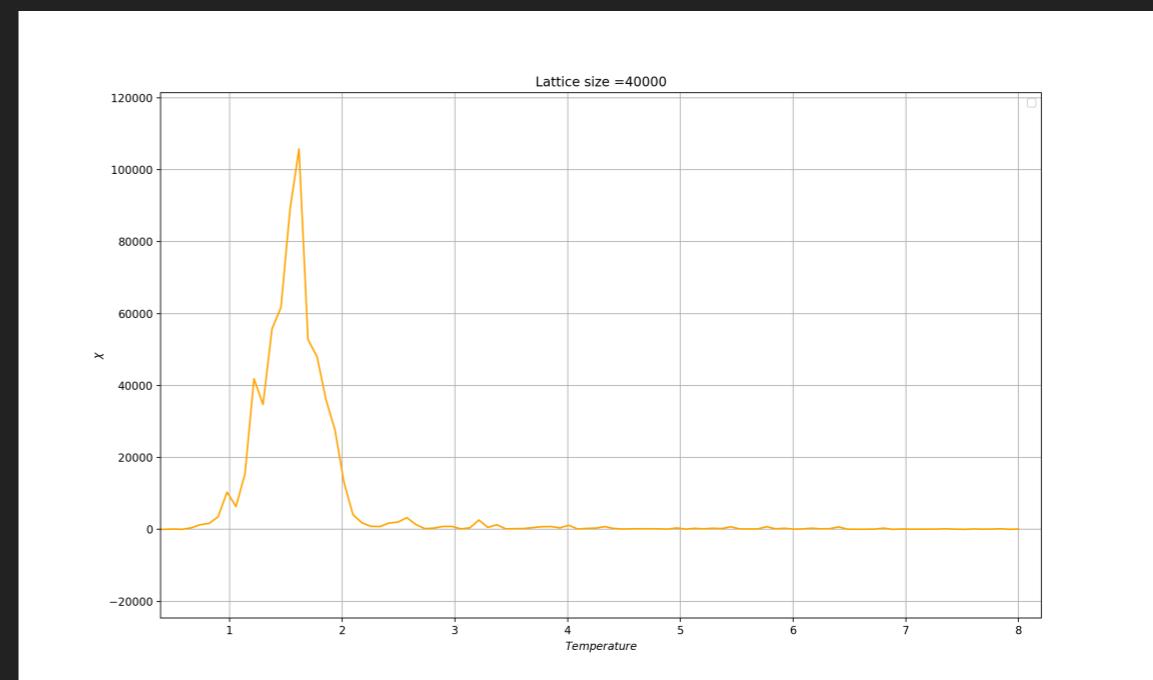
HEAT CAPACITY AS FUNCTION OF T



ENERGY AS FUNCTION OF T

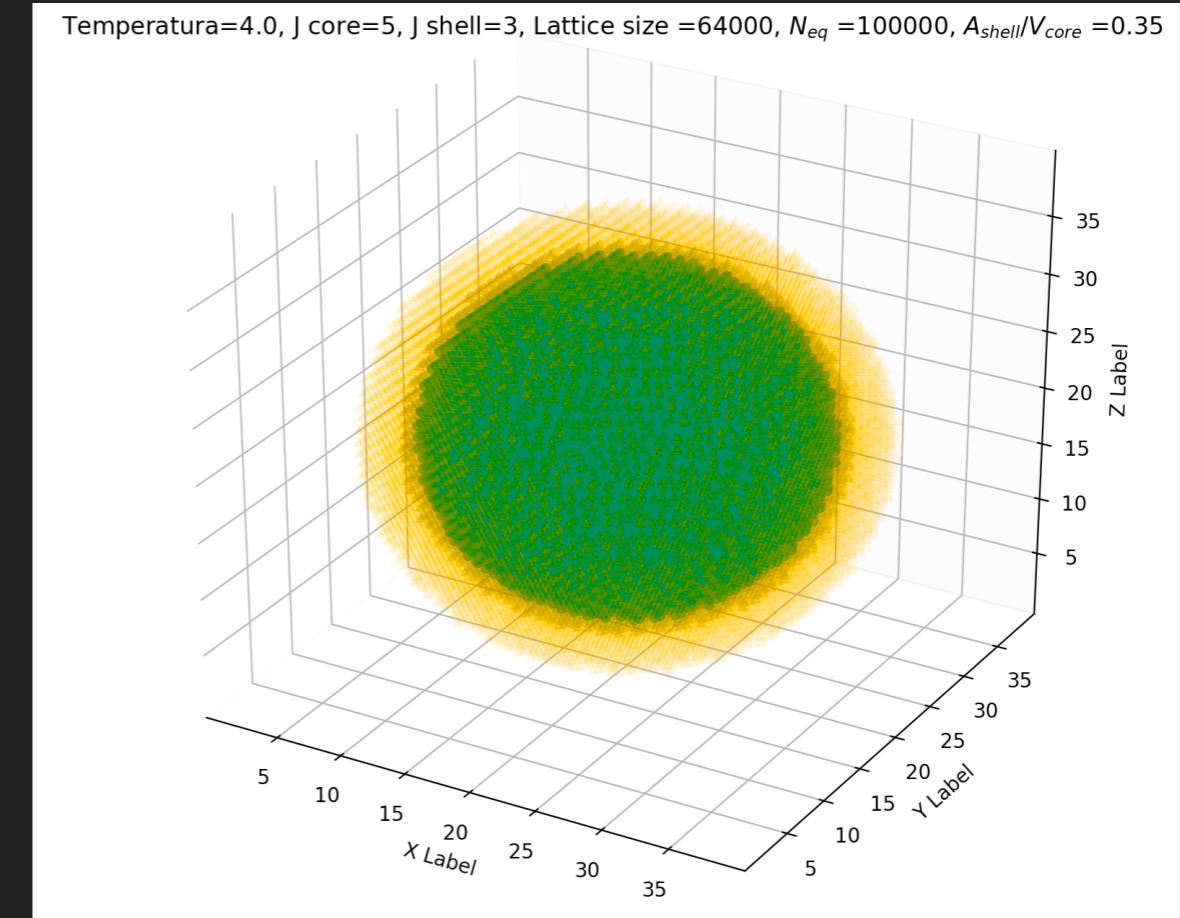


SUSCEPTIBILITY AS FUNCTION OF T



WHAT HAPPENS WHEN YOU MAKE A
MAGNET SMALLER?
BUT WE NEED TO GO ONE STEP
FURTHER.

WE SIMULATE A NANO-PARTICLE AS AN SPHERICAL ARRAY OF SPINS. WE ALSO COVER A CONFIGURATION CALLED CORE-SHELL

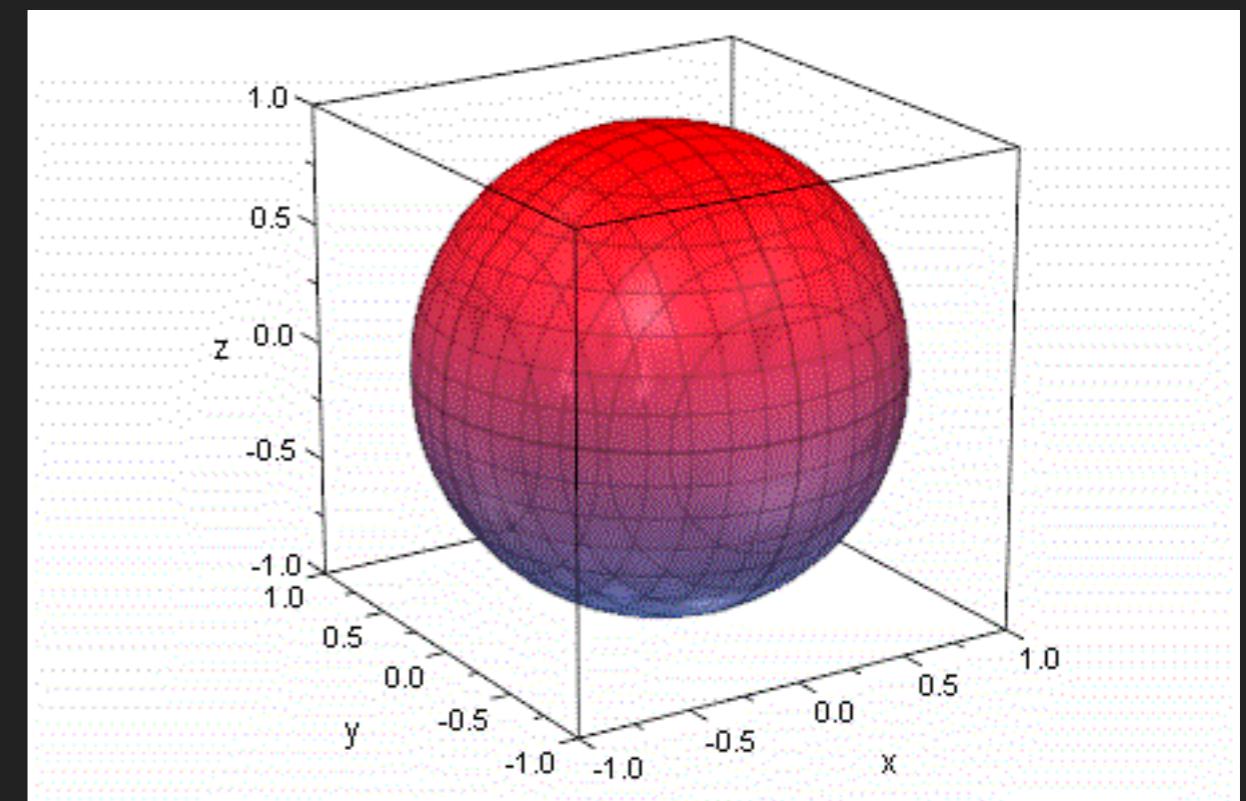
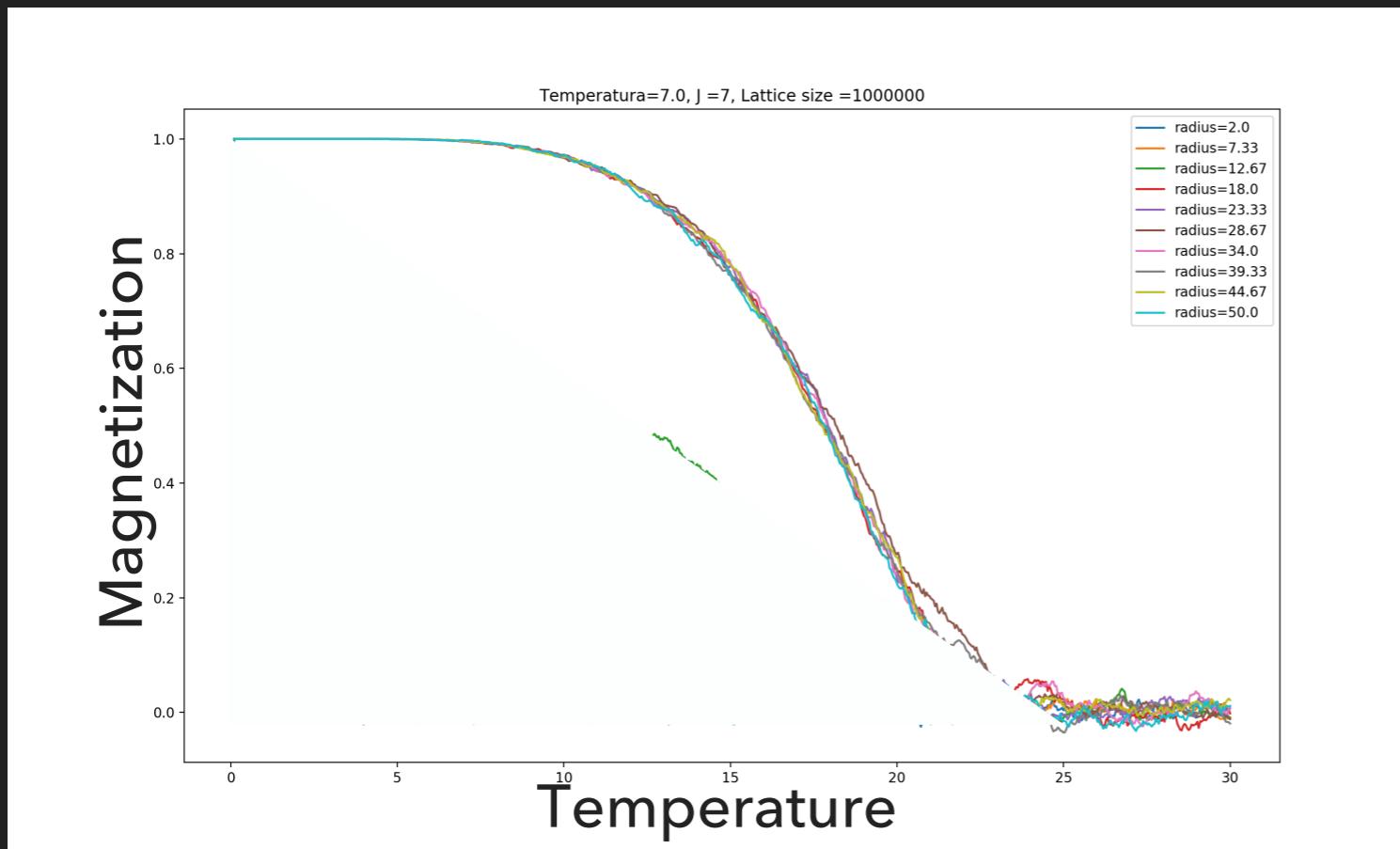


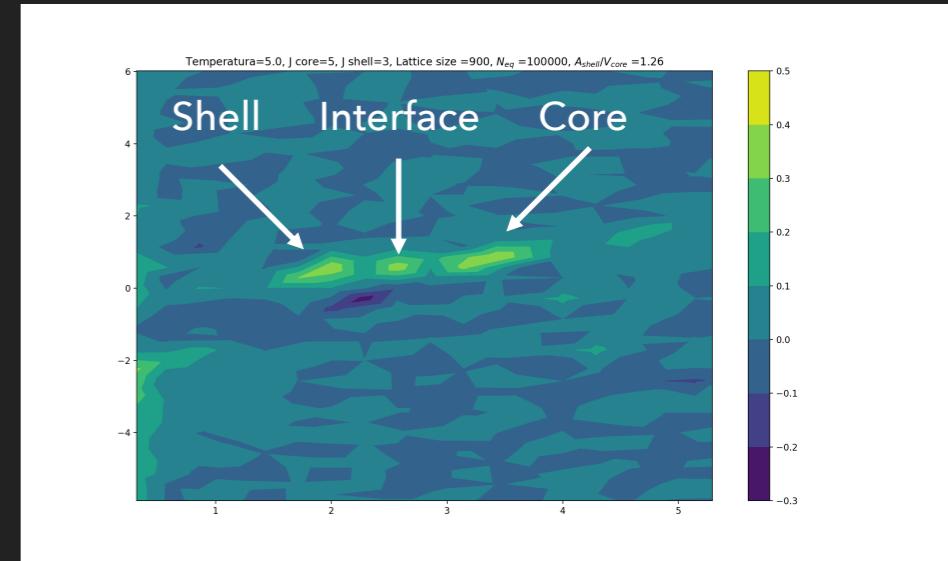
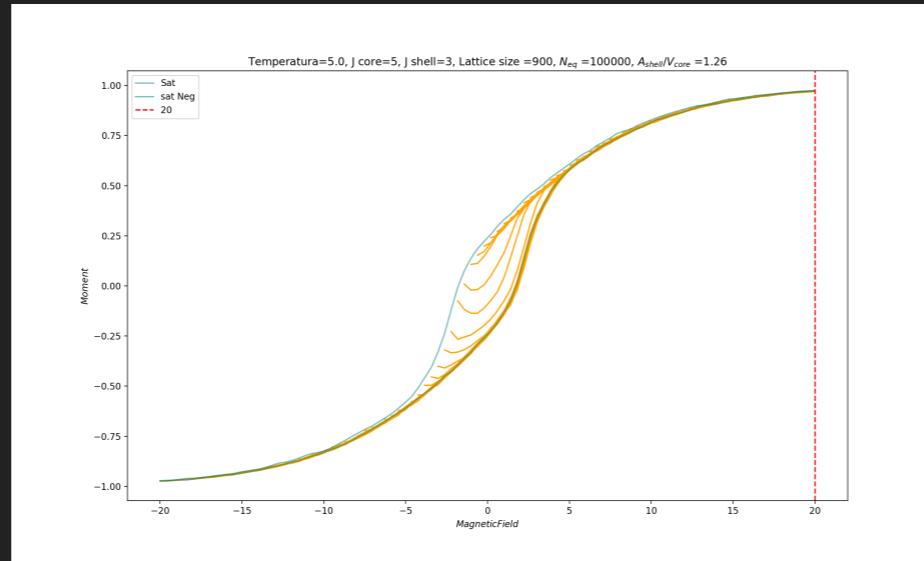
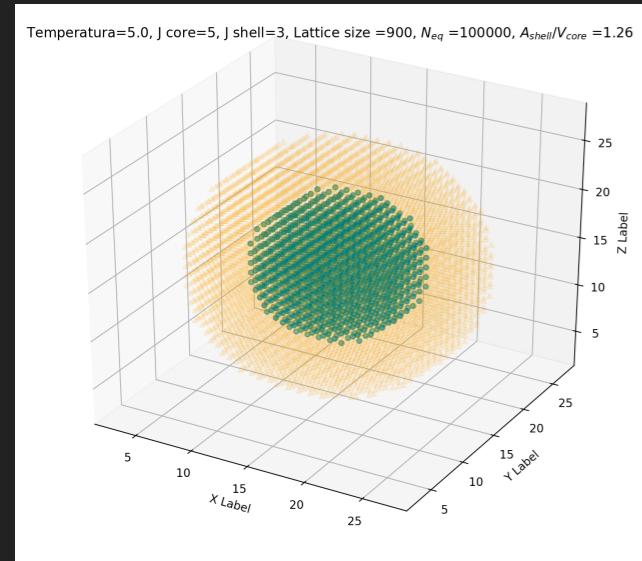
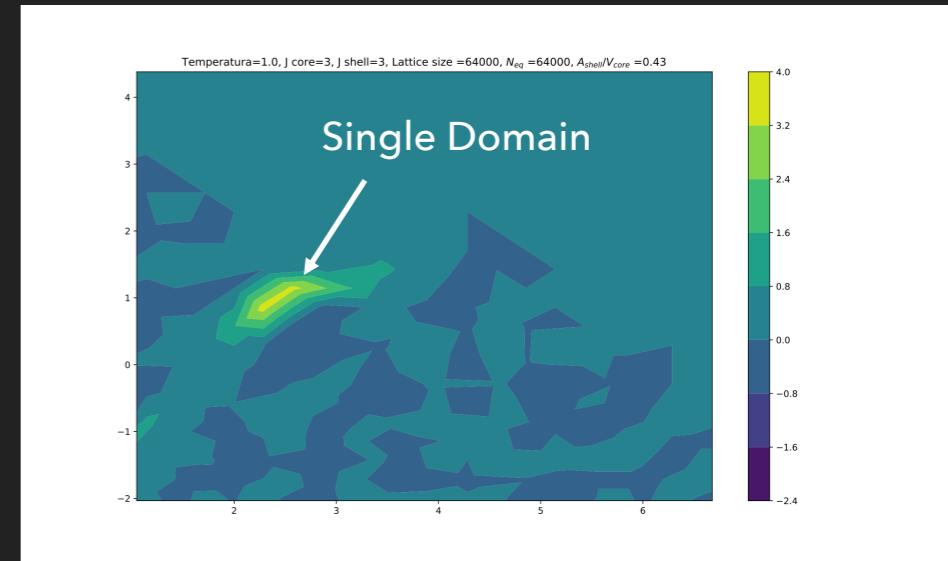
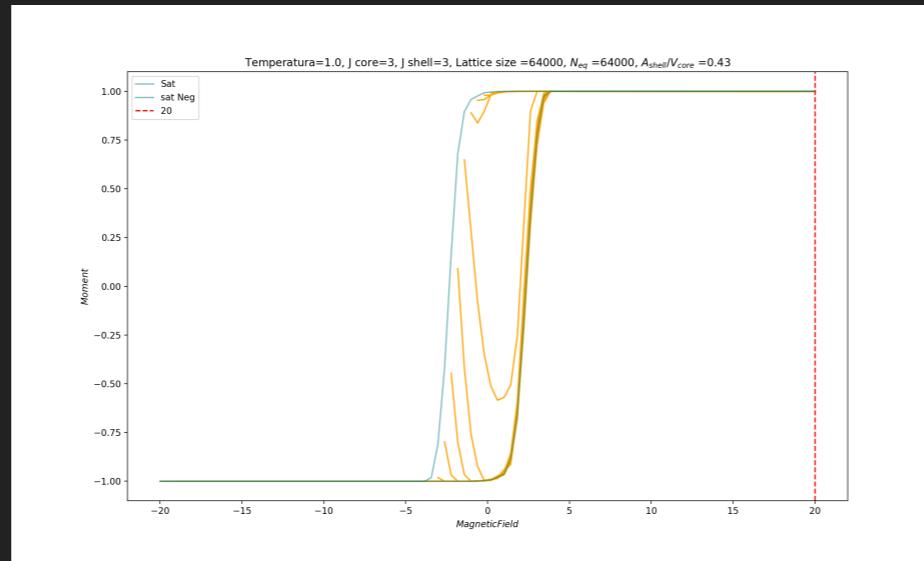
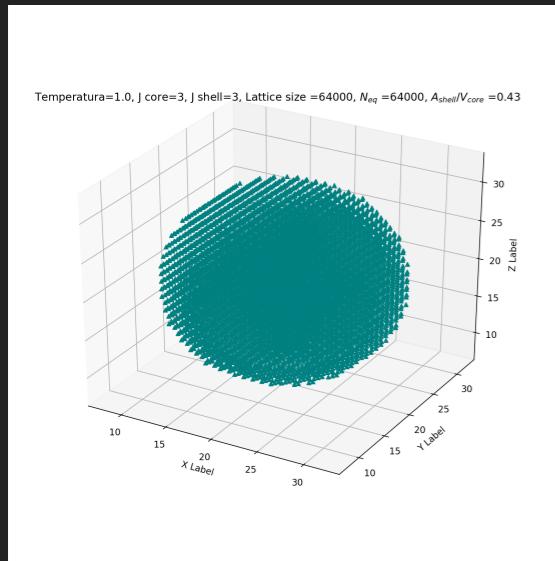
GREEN IS THE CORE, ORANGE THE INTERFACE AND YELLOW THE SHELL, EVERY DOMAIN HAS A DIFFERENT COUPLING CONSTANT

3D MODEL.



**WHIT THIS NEW MODEL
WE DISCOVER THAT:**





- ▶ Metropolis algorithm is an useful tool for optimization of non-convex problems, as it's the minimization of the energy of a system in the canonical ensemble
- ▶ The Ising model makes an important contribution to the explanation of the physical phenomena that involves magnetic materials.
- ▶ FORC diagrams shows the core, shell and interface domains.
- ▶ There is a limit on the size of the particles, at which the magnetic properties depends on the size.

- 1. INITIALIZATION:** CHOOSE INITIAL POINT x_0 AND AN ACCEPTANCE PROBABILITY DISTRIBUTION $g(x_i|x_{i-1})$.
- 2. GENERATE:** A CANDIDATE FOR THE NEXT SAMPLE $g(x_i|x_{i-1}) \rightarrow x_i'$
- 3. CALCULATE:** THE ACCEPTANCE RATIO $\alpha = \frac{f(x_i')}{f(x_{i-1})}$
- 4. ACCEPT OR REJECT:** GENERATE A RANDOM NUMBER $u \sim [0,1]$, IF $u \leq \alpha \Rightarrow x' = x_i$
ELIF $u > \alpha \Rightarrow x' = x_{i-1}$
- 5. REPEAT :** 2-3 UNTIL ACCOMPLISH CONDITION

1. INITIALIZATION: CREATE THE SYSTEM IN A RANDOM MICRO-STATE

2. GENERATE: CHOOSE A RANDOM ELEMENT OF THE SYSTEM WITH AN UNIFORM DISTRIBUTION S

3. CALCULATE: CHANGE THE STATE OF THE ELEMENT S , COMPUTE THE ENERGY AND CALCULATE $p_x = \frac{1}{Z} e^{-\frac{E_S}{K_b T}}$

4. ACCEPT OR REJECT: IF S REDUCE THE ENERGY ACCEPT THE NEW MICRO STATE. ELSE IF $u \sim [0,1]$. $u \leq p_x \Rightarrow \text{ACCEPT}$. ELSE REJECT.

5. REPEAT 2-3 UNTIL ENERGY CONVERGES.

- ▶ To Edwin Ramos for the guidance on the direction of the simulation, and the potential that it can have on the description of the physical phenomena.
- ▶ To Juan Gabriel Ramirez, for taking time to help me be prepare for this talk and being exigent in order to give a decent presentation
- ▶ To the nano-magnetism lab for the disposal of all the resources needed for the develop of this work

- ▶ 1. N. Metropolis; A.W. Rosenbluth; M.N. Rosenbluth; A.H. Teller & E. Teller (1953). "Equation of State Calculations by Fast Computing Machines". *Journal of Chemical Physics*. 21 (6): 1087-1092. [Bibcode:1953JChPh..21.1087M](#).
- ▶ 2. W. K. Hastings, Monte Carlo sampling methods using Markov chains and their applications, *Biometrika*, Volume 57, Issue 1, April 1970, Pages 97-109, <https://doi.org/10.1093/biomet/57.1.97>
- ▶ 3. [Ernst Ising, Contribution to the Theory of Ferromagnetism.](http://www.h-s-augsburg.de/~harsch/anglica/Chronology/20thC/Ising/isi_fm00.html) http://www.h-s-augsburg.de/~harsch/anglica/Chronology/20thC/Ising/isi_fm00.html
- ▶ 4. Heslop, D., Dekkers, M. J., Kruiver, P. P., & Van Oorschot, I. H. M. (2002). Analysis of isothermal remanent magnetization acquisition curves using the expectation-maximization algorithm. *Geophysical Journal International*, 148(1), 58-64.
- ▶ 5. Soares, J. M., Cabral, F. A. O., de Araújo, J. H., & Machado, F. L. A. (2011). Exchange-spring behavior in nanopowders of CoFe₂O₄-CoFe₂. *Applied Physics Letters*, 98(7), 072502.