Coupling from the Past for Statistical Mechanics Models

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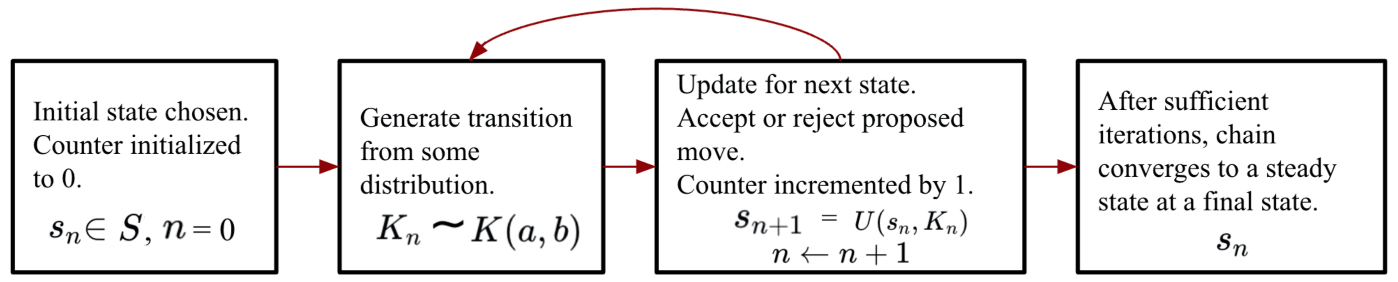
Markov Chain Monte Carlo (MCMC)

Markov Chain - Process of **stochastic** transitions from one state to another.
- Each transition is **memoryless.**

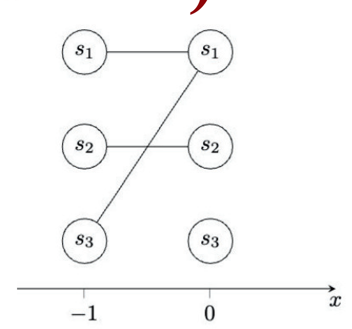
Problems
1. **Distribution discrepancies:** Not sampling from the exact distribution desired. $\tilde{\pi}^{(n)} \neq \pi$
2. **Upper bound on transition steps:** Difficult to find the upper bound of N (steps taken). $|\tilde{\pi}^{(n)} - \pi| < \epsilon$



Typical MCMC Algorithm Process.

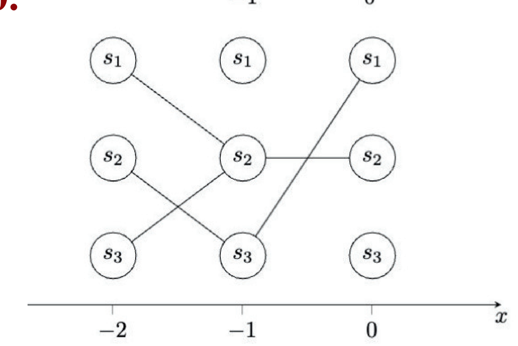
Coupling From the Past (CFTP)

Perfect Sampling **(Propp & Wilson, 1996)**

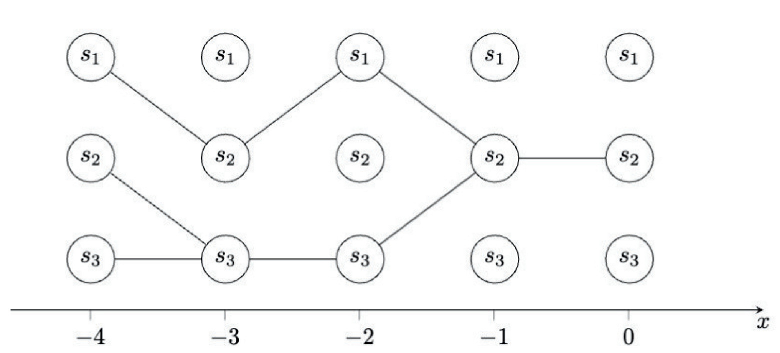


Properties - Multiple instances of the same chain.
Seeing where chains eventually **coalesce**.
- Chains from finite time in the **past to 0.**

Solutions



1. Starting the chain at -∞, we get the same final states and now in **equilibrium**, giving a **perfect sample**.
2. The algorithm stops when chains coalesce so finding an appropriate N is not a problem anymore.



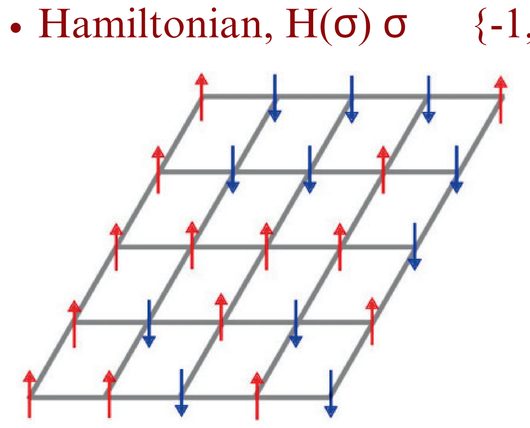
Steps Further in the Past till **Coupling**.

The Ising Model

Let **G = (V, E)** be a graph.

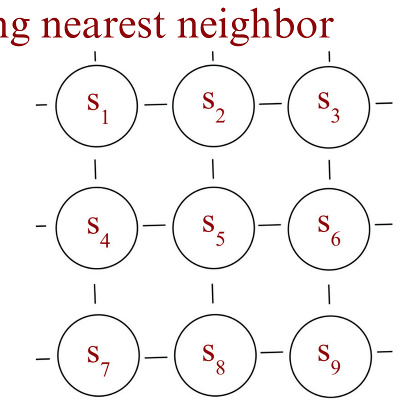
Randomly assign **-1's** and **+1's** to the **vertices** of G representing **dipoles** in a **ferromagnetic material**.

Probability distributions depend on:
- Inverse temperature, β ≥ 0
- Hamiltonian, H(σ) σ {-1, 1}



Lattice of **magnetic dipole** moments, each either spin up (+1) or down (-1).

Energy (Hamiltonian)
Using nearest neighbor



$$H(\sigma) = -\sum_{\langle i,j\rangle \in E} \sigma(i)\sigma(j)$$

$$= -s_1s_2 - s_2s_3 - s_3s_1$$
$$- s_4s_5 - s_5s_6 - s_6s_4$$
$$- s_7s_8 - s_8s_9 - s_9s_7$$
$$- s_1s_4 - s_2s_5 - s_3s_6$$
$$- s_4s_7 - s_5s_8 - s_6s_9$$
$$- s_7s_1 - s_8s_2 - s_9s_3$$

The Ising Model

Phase Transition Phenomena
Low temperatures (high β), spontaneous magnetization.
High temperatures (low β), magnetization is entirely lost.

Onsager Critical Value:

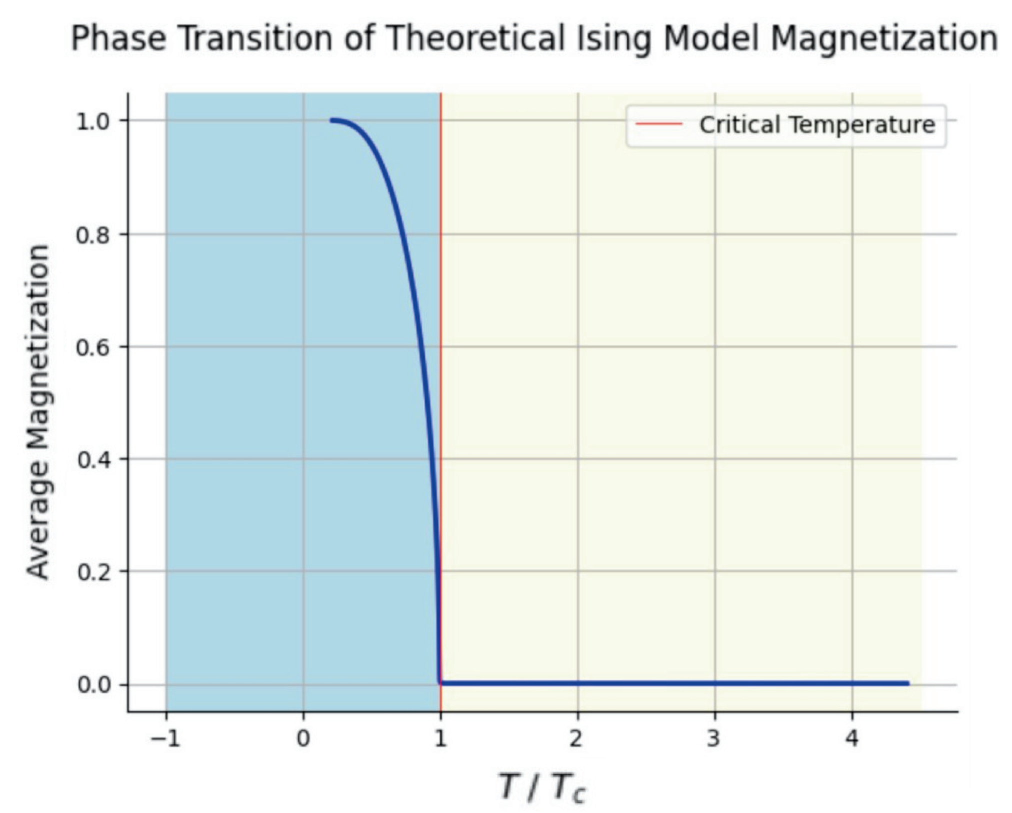
$$\beta_c = \frac{1}{2}log(1+\sqrt{2}) \approx 0.441$$

Theoretical Average Magnetization Iteration Scheme:

$$s_{i+1} = \tanh\{\frac{T_c}{T}(\frac{H}{H_c} + s_i)\}$$

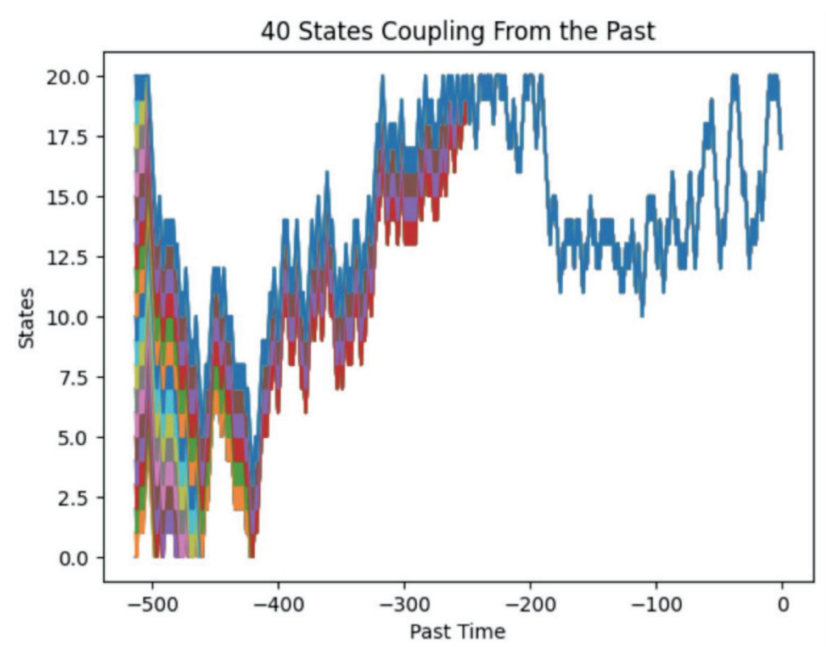
$$s_{i+1} = \tanh\{\frac{T_c}{T}s_i\}$$

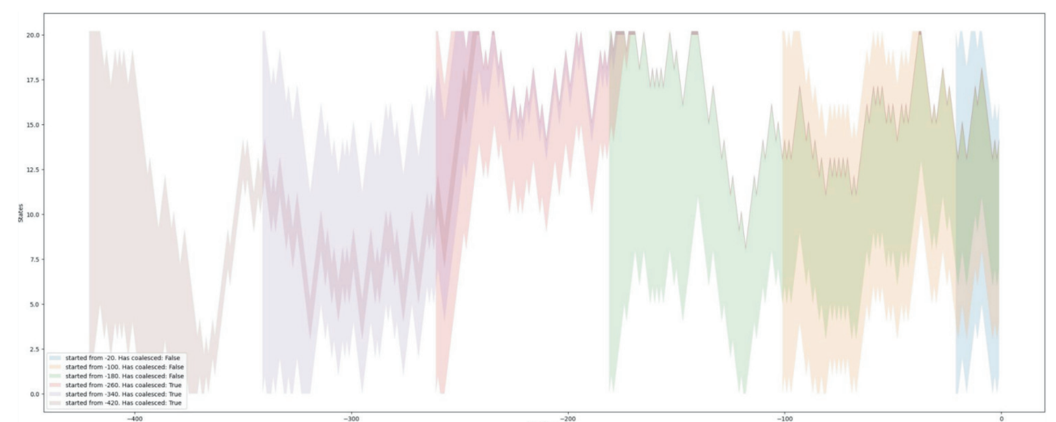
Neglecting External Magnetic Field



Implementation - Simple Applications

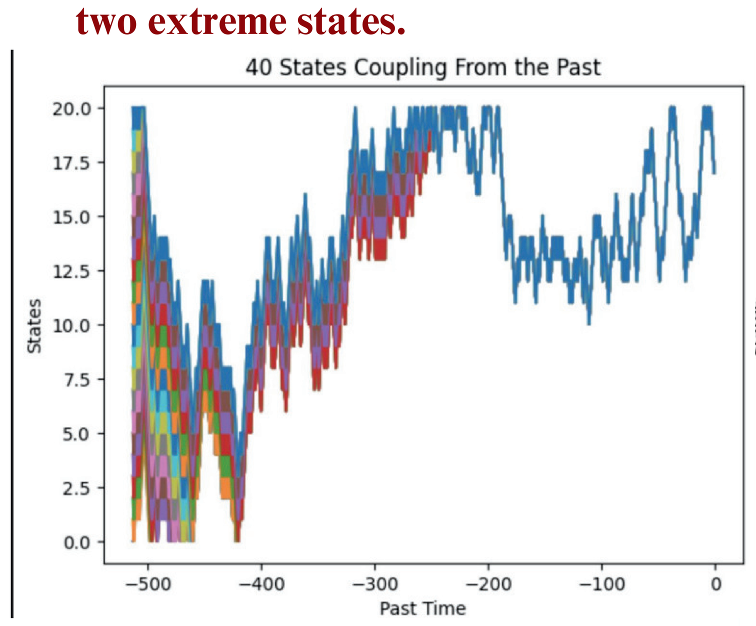
Simpler Applications of CFTP

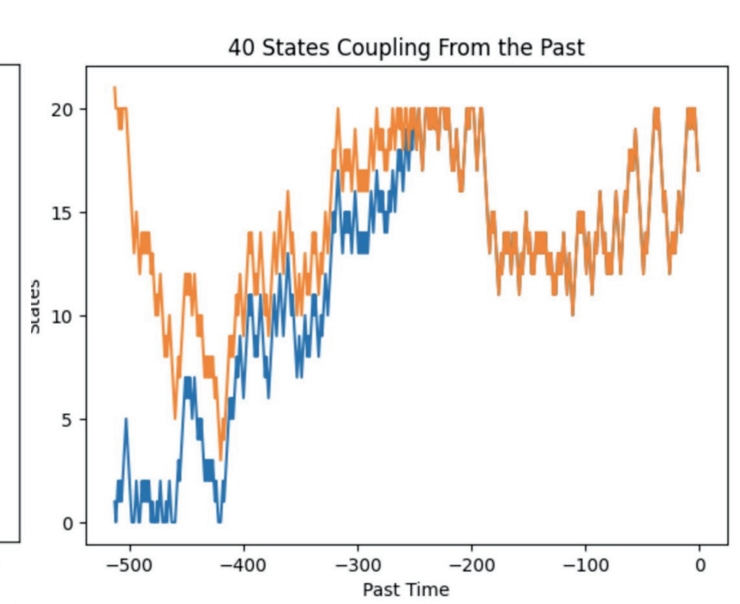




Once we reach a starting point **far enough** that all states coalesce (pink, starting at -260), taking further steps in the past produces **the same result** (violet and brown starting at -340 and -420, respectively).

Monotone CFTP - Sandwiching
- Running k separate instances of a chain becomes **practically difficult** as k reaches **large values**.
- For Markov chains obeying **monotonicity properties**, sandwiching applies CFTP focusing only on the **two extreme states.**





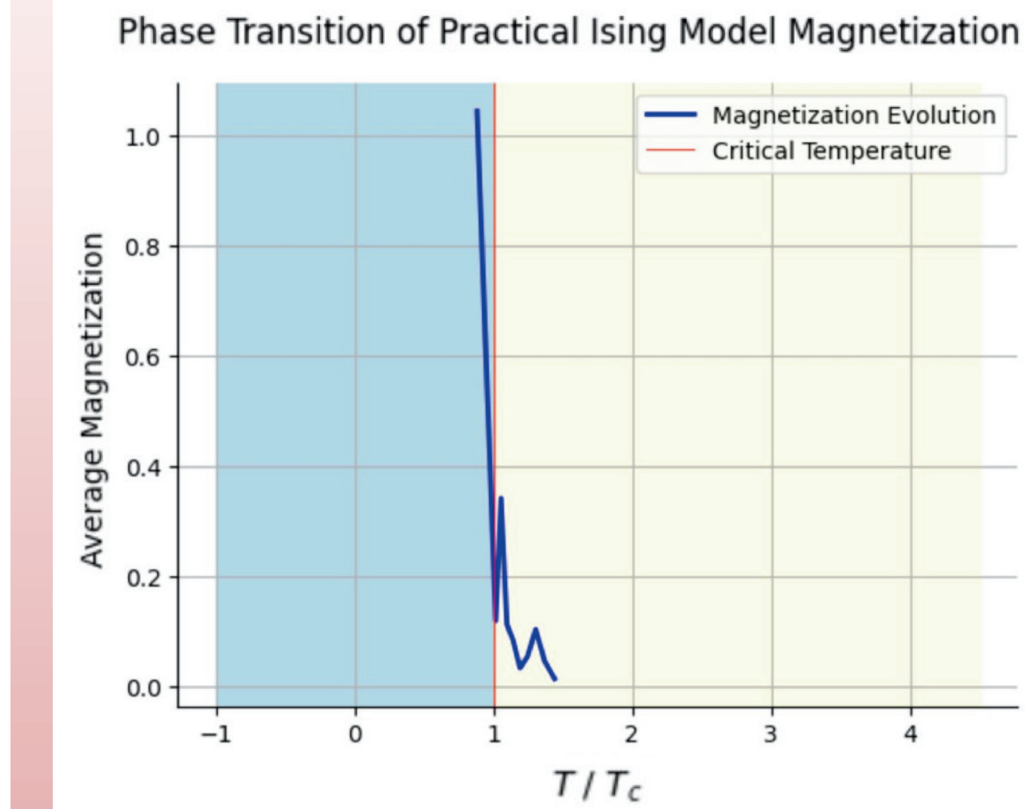
Two Extreme States
For a 3x3 lattice: 512 possible states. Monotonicity suggests that the two bounding states are: all states spin up (+1), and all states spin down (-1).

Update Function
Accept or reject a spin (state) change.

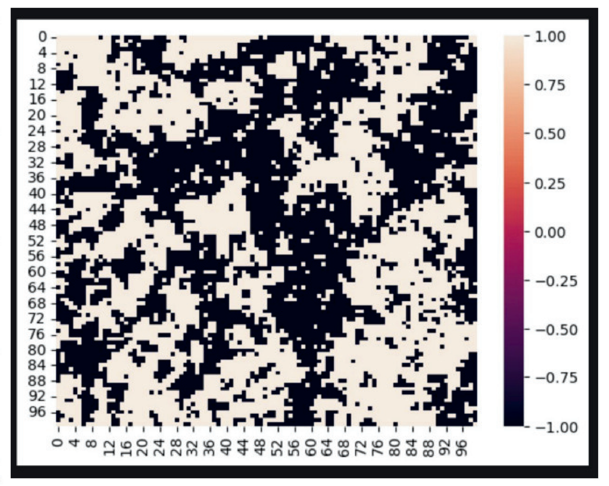
- Choose $v \in_R V$, $s \in_R \{+1, -1\}$ and $r \in_R [0, 1]$.
- Let $X'(v) = s$ and $X'(w) = X_t(w)$, $w \neq v$.
- Set $$X_{t+1} = \begin{cases} X' & \text{if } r \leq \min\{1, e^{-\beta H(X')}/e^{-\beta H(X_t)}\} \\ X_t & \text{otherwise} \end{cases}$$

Vigoda 2003

Implementation - The Ising Model



Phase transition phenomena of **practical ising model** using the **CFTP algorithm.**



β = 0.4
Our simulation of CFTP for a 100x100 lattice at β = 0.4, close to the critical temperature

Optimization

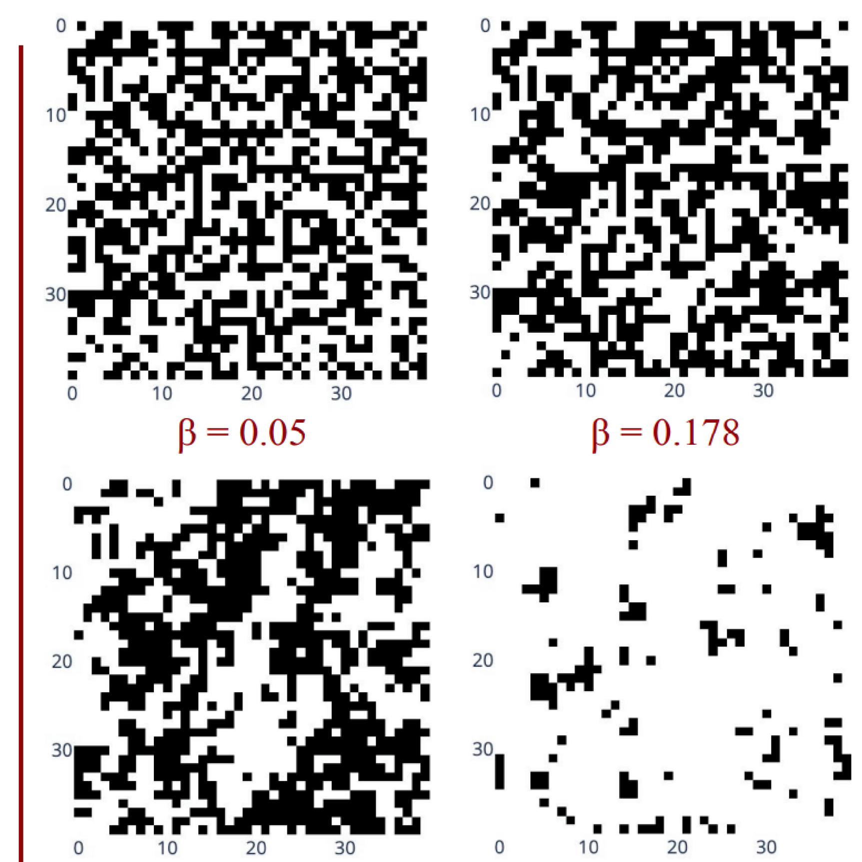
Numba:
Using **Numba** before each time-consuming function significantly sped up processing, but adjustments were needed - Unsupported Python features.

Update Test Simplification:
Only 1 vertex is changing, so a sum over 4 edges only is required instead of a total re-calculation

$$H(X_t) - H(X') = \sum_{\omega,\omega'}(X_t(\omega)X_t(\omega') - X'(\omega)X'(\omega'))$$
$$= X_t(\omega)X_t(\omega^N) - X'(\omega)X'(\omega^N)$$
$$+X_t(\omega)X_t(\omega^E) - X'(\omega)X'(\omega^e)$$
$$+X_t(\omega)X_t(\omega^S) - X'(\omega)X'(\omega^S)$$
$$+X_t(\omega)X_t(\omega^W) - X'(\omega)X'(\omega^W)$$

Single line calculation instead of multi-line iterations

$$= X_t(\omega^N)(X_t(\omega) - S)$$
$$+X_t(\omega^E)(X_t(\omega) - S)$$
$$+X_t(\omega^S)(X_t(\omega) - S)$$
$$+X_t(\omega^W)(X_t(\omega) - S)$$



β = 0.05 β = 0.178
β = 0.354 β = 0.45

Progression of 40x40 lattice at different β

Acknowledgments & References

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