SWAP algorithm for lattice spin models

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We adapted the SWAP molecular dynamics algorithm for use in lattice Ising spin models. We dressed the spins with a randomly distributed length and we alternated long-range spin exchanges with conventional single spin flip Monte Carlo updates, both accepted with a stochastic rule which respects detailed balance. We show that this algorithm, when applied to the bidimensional Edwards-Anderson model, speeds up significantly the relaxation at low temperatures and manages to find ground states with high efficiency and little computational cost. The exploration of spin models should help in understanding why SWAP accelerates the evolution of particle systems and shed light on relations between dynamics and free-energy landscapes.

1 SWAP algorithms

For poly-disperse particle system | **For a spin lattice system**

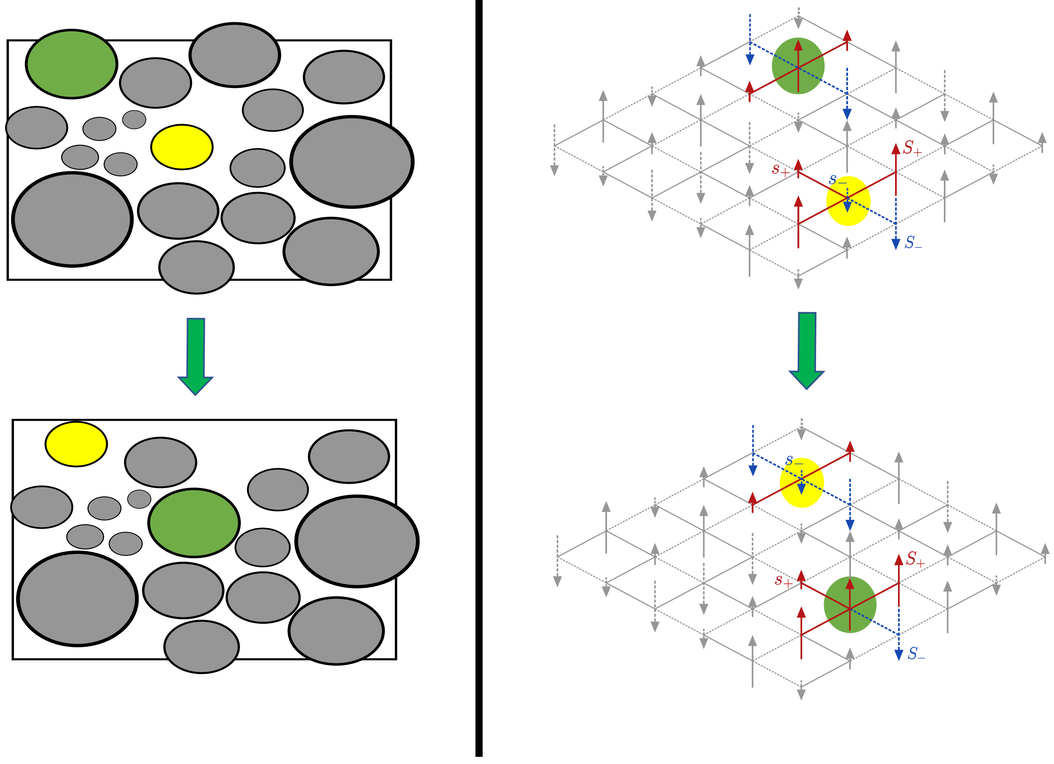

Figure 1: Pictorial representation of microscopic non-local SWAP moves for both types of systems.

2 "Poly-disperse" model for spins, the Δ-Model

We studied the Hamiltonian

$$H = -\sum_{\langle ij \rangle} J_{ij}\tau_i\sigma_i\tau_j\sigma_j \ , \tag{1}$$

with

$$\sigma_i \in \{-1,+1\}, \quad \tau_i \in [1-\Delta/2, 1+\Delta/2] \quad \text{and} \quad 0 \leq \Delta \leq 2 \ ,$$

and J_{ij} are unitary and bimodal distributed, i.e.

$$p(J_{ij}) = \frac{1}{2}\delta(J_{ij}-1) + \frac{1}{2}\delta(J_{ij}+1) \ . \tag{2}$$

This problem can be recast as

$$H = -\sum_{\langle ij \rangle} \mathcal{J}_{ij}\sigma_i\sigma_j \ , \quad \text{with} \quad \mathcal{J}_{ij} = J_{ij}\tau_i\tau_j \ . \tag{3}$$

Thus, we still deal with an Ising spin model, but with effective couplings $\mathcal{J}_{ij}$ that exhibit spatial correlation through the τ_i variables.

3 SWAP Monte Carlo dynamics

We simulate the Δ-Model in finite size systems, particularly in $2d$ square lattices with linear dimension L and periodic boundary conditions.

The attempted dynamical moves are determined by a Bernoulli process with probability p_{swap}

$$\left\{ \begin{array}{ll} \text{with } p_{\text{swap}} & \mapsto N \text{ (non-local) exchange attempts} \\ & (\sigma_i,\tau_i) \leftrightarrow (\sigma_j,\tau_j) \ , \\ \text{with } 1-p_{\text{swap}} & \mapsto N \text{ single spin flip attempts} \\ & \sigma_i \to -\sigma_i \ . \end{array} \right\}$$

Each microscopic move is accepted with Metropolis acceptance probability $p_{acc} = \min\{1, \exp(-\beta\Delta E)\}$. Depending on the nature of the moves, our effective couplings $\mathcal{J}_{ij}$ may be either **annealed** or **quenched**.

4 Temperature quench

From an infinite temperature configuration, we perform a SWAP evolution for a temperature quench at $T = 0$. After a time $t_{\max}$, the dynamics freeze. We call the converged effective couplings $\mathcal{J}^*_{ij}$ $(= \mathcal{J}_{ij}(t_{\max}))$. Using the McSparse solver, we found the respective ground states, $\{\sigma_i^{GS}\}$.

$$q(t) = \frac{1}{N}\sum_{i=1}^{N} \sigma_i^{GS}\sigma_i(t) \tag{4}$$

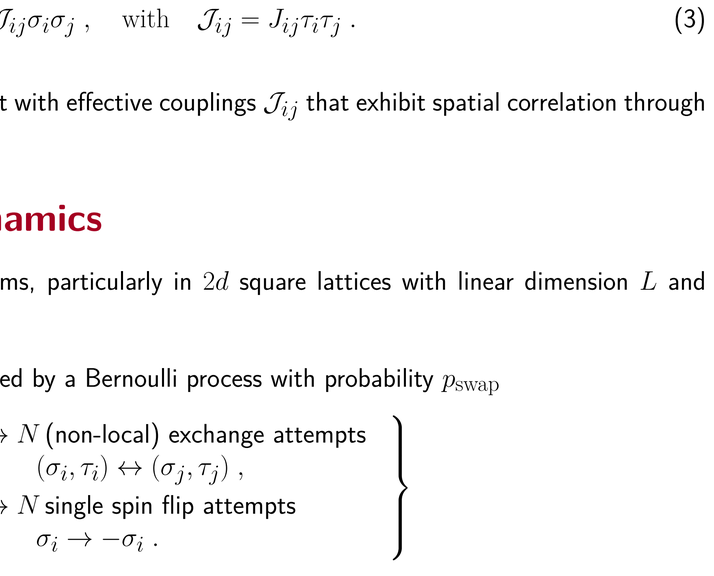

Figure 2: Snapshots of the overlap between the ground state found and the dynamic configuration $s_i = \sigma_i\tau_i$. Parameters: $L = 32$, $\Delta = 1.5$. The light bullets and triangles are located at frustrated plaquettes ($f_P = \prod_{\langle ij \rangle \in P} \mathcal{J}_{ij}$ such that $f_P < 0$) with local frustration f_P being greater or smaller than one-half in magnitude, respectively.

5 Temperature annealing

With the same initial conditions, we perform a SWAP evolution again, this time annealing the temperature from $T_0 = 1.0$ towards $T = 0$ according to the protocol

$$T(t) = T_0\left(1 - \frac{t}{t_f}\right)^2 \ . \tag{5}$$

We also define the resulting couplings as $\mathcal{J}^*_{ij}$ $(= \mathcal{J}_{ij}(t_f))$.

6 Ground state identification

We run both procedures several times ($N_r = 100$), changing the sample of J_{ij}, $\{\tau_i\}$, and $\{\sigma_i(t=0)\}$ at each iteration. We compare the resulting σ-configurations with the ground states by measuring

$$\mathcal{P}_0(t) = \frac{1}{N_r}\sum_{\alpha=1}^{N_r} \delta_{|q_\alpha(t)|,1} \ , \tag{6}$$

then setting $\mathcal{P}_0^\infty = \mathcal{P}_0(t_{\max})$ for the quench, $\mathcal{P}_0^\infty = \mathcal{P}_0(t_f)$ for the annealing.

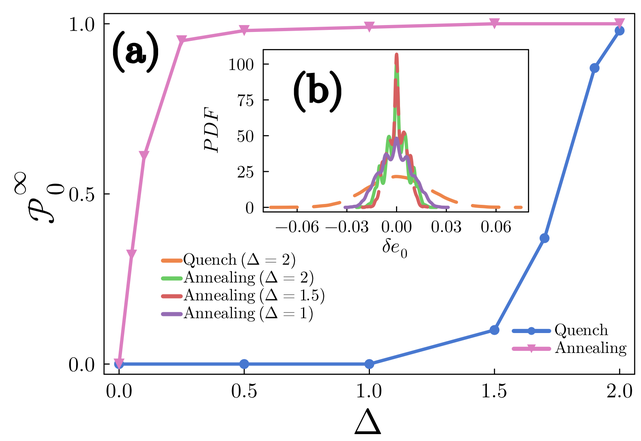

Figure 3: **(a)** Asymptotic probability of reaching a ground state. Parameters: $L = 32$, $t_{\max} \approx 10^4$, $t_f \approx 10^7$. Inset **(b)** Probability distributions of the ground state energy density differences, over 10^3 σ-initial conditions.

7 Equilibrium relaxation time

For a quench at non-vanishing temperatures ($T \neq 0$), we investigate the characteristic relaxation time, defined as τ_α, and compare it with:

(I) Purely single spin flip dynamics ($p_{\text{swap}} = 0$) with the converged $J^*_{ij} = J_{ij}(t_f)$.

(II) Evolution with spin exchanges just between nearest neighbors.

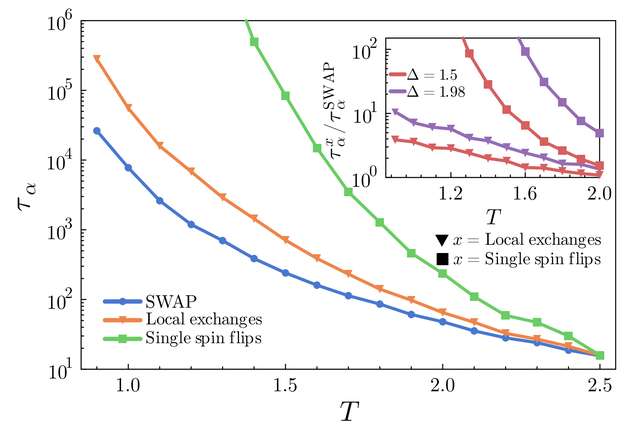

Figure 4: Characteristic relaxation time, τ_α for SWAP method, and the dynamics defined in **(I)** and **(II)** with $\Delta = 1.5$. In the inset, comparison of the two relaxation times, for **(I)** and **(II)** with respect to SWAP.

8 Conclusions

- We devised a disorder annealing that samples $2d$ Edwards-Anderson ground states with little computational cost ($\approx 10^2$ faster than with parallel tempering), and that preserves the symmetry of the distribution.
- We explored the effect of SWAP moves in models that lack dynamical facilitation, shedding a light to the inner workings of the algorithm.

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