Classical spin models: From local simulations to cluster algorithms 2/2

Simulations of quantum many-body systems - part 1

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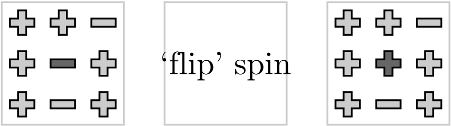
Local Monte Carlo algorithm
Metropolis & Heatbath, Half-order
Cluster algorithms
Spin glasses
liquids as spin glasses; spin glasses as liquids

Paris

Metropolis Monte Carlo (schema)



a (move) b

- satisfies detailed balance
- …as in Alg. `markov-disks` …

Local Monte Carlo (algorithm)

procedure `markov-ising`
input $\{\sigma_1, \ldots, \sigma_N\}, E$
$k \leftarrow \texttt{Nran}\,(1, N)$
$h \leftarrow \sum_n \sigma_{\mathrm{Nbr}(n,k)}$
$\Delta E \leftarrow 2h \cdot \sigma_k$
$\Upsilon \leftarrow \exp\,[-\beta \Delta E]$
if $(\texttt{ran}\,(0,1) < \Upsilon)$ **then**

$$\begin{cases} \sigma_k \leftarrow -\sigma_k \\ E \leftarrow E + \Delta E \end{cases}$$

output $\{\sigma_1, \ldots, \sigma_N\}, E$

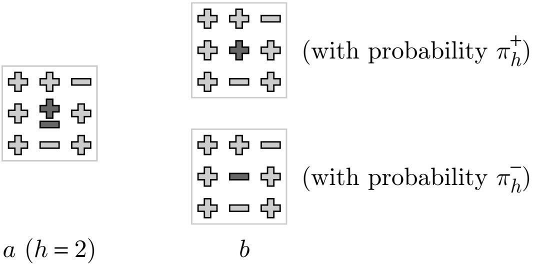
- Metropolis algorithm...

Local Monte Carlo (example)

- Using fluctuation formulas for energy and specific heat (6×6 lattice without periodic boundary conditions)

run	$\langle E/N \rangle$	c_V
1	-1.74562	0.6942
2	-1.74617	0.6915
3	-1.74648	0.6865
4	-1.75017	0.6729
5	-1.74587	0.6898

Heat bath Monte Carlo (schema)



- simplest example of an a priori probability applied to subsystem
- roughly equivalent to Metropolis algorithm

Heat bath Monte Carlo (theory)

- $$\pi_h^+ = \frac{e^{-\beta E^+}}{e^{-\beta E^+} + e^{-\beta E^-}} = \frac{1}{1 + e^{-2\beta h}}$$
  $$\pi_h^- = \frac{e^{-\beta E^-}}{e^{-\beta E^+} + e^{-\beta E^-}} = \frac{1}{1 + e^{+2\beta h}}$$

Heat bath Monte Carlo (algorithm)

procedure `heat-bath-ising`
input $\{\sigma_1, \ldots, \sigma_N\}, E$
$k \leftarrow \texttt{Nran}\,(1, N)$
$\Upsilon \leftarrow \texttt{ran}\,(0, 1)$
$h \leftarrow \sum_n \sigma_{\mathrm{Nbr}(n,k)}$
$\sigma' \leftarrow \sigma_k$
if $(\Upsilon < \pi_h^+)$ **then**
  $\{\ \sigma_k \leftarrow 1$
else
  $\{\ \sigma_k \leftarrow -1$
if $(\sigma' \neq \sigma_k)$ $E \leftarrow E - 2\sigma_k \cdot h$
output $\{\sigma_1, \ldots, \sigma_N\}$
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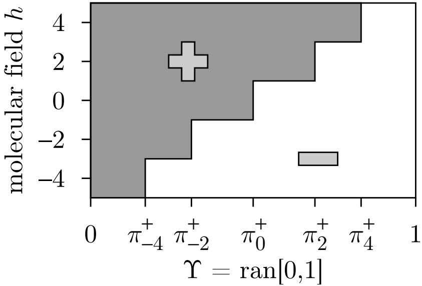
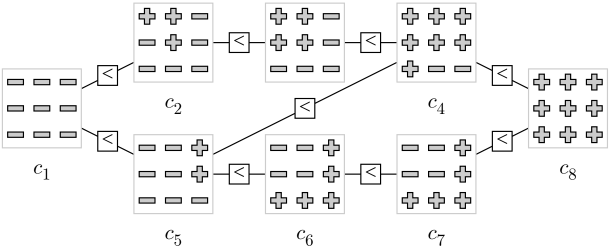
- Molecular field-random number diagram



- Together with half-order ...

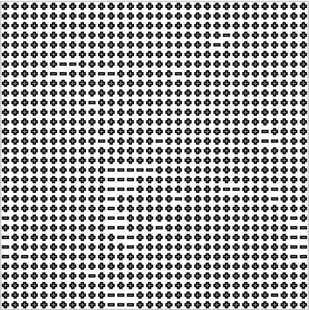
Heat bath Monte Carlo (half-order)

- Half order in the Ising model

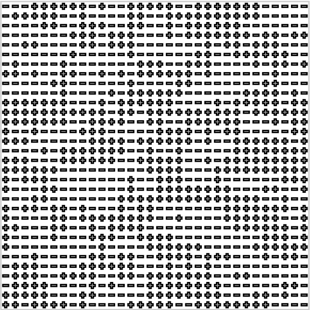


- Yields powerful exact sampling algorithm

Typical configurations of Ising model

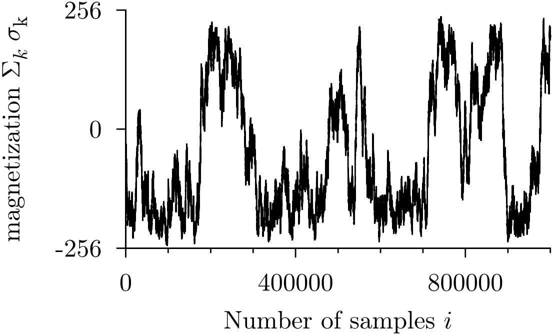


low T ($\beta = 0.5$)



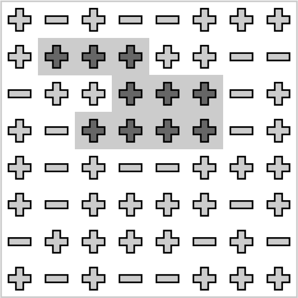
high T ($\beta = 0.3$)

Slowness of local Monte Carlo approaches



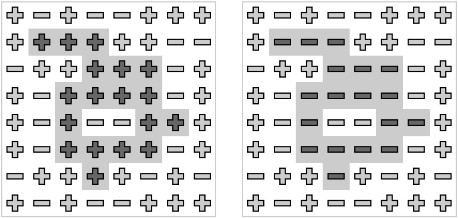
- The throwing-range issue. . .

Moving many spins at a time: Cluster algorithms



- add all sites of same spin: bad idea
- Add neighbors with probability p

Cluster algorithms–A priori probabilities



a $\qquad$ b

$$\{\text{cluster } a\}: \quad \begin{bmatrix} \text{int} & \text{ext} & \# \\ + & - & n_1(16) \\ + & + & n_2(14) \end{bmatrix} \qquad E|_{\partial\mathcal{C}} = n_1 - n_2$$

$$\{\text{cluster } b\}: \quad \begin{bmatrix} \text{int} & \text{ext} & \# \\ - & - & n_1(16) \\ - & + & n_2(14) \end{bmatrix} \qquad E|_{\partial\mathcal{C}} = -n_1 + n_2$$

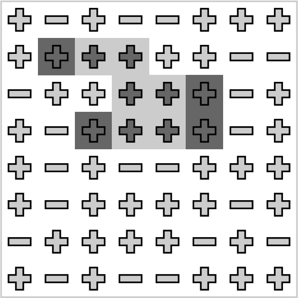
Stopping probabilities and energies

- accepting new link with probability p ...
- rejecting n links with proba $(1-p)^n$
- gives:

$$\mathcal{P}(a \to b) = \min\left(1, \frac{\mathrm{e}^{-\beta[n_2-n_1]}(1-p)^{n_1}}{\mathrm{e}^{-\beta[n_1-n_2]}(1-p)^{n_2}}\right)$$

- special value $p = 1 - \mathrm{e}^{-2\beta}$

Setting up a cluster algorithms



- ten cluster sites
- four “pocket” sites

Ising clusters (algorithm)

procedure `cluster-ising`
input $\{\sigma_1, \ldots, \sigma_N\}$
$j \leftarrow \texttt{Nran}\,(1, N)$
$\mathcal{C} \leftarrow \{j\}$
$\mathcal{P} \leftarrow \{j\}$
while $(\mathcal{P} \neq \emptyset)$ **do**

$$\left\{\begin{array}{l}
k \leftarrow \text{any element of } \mathcal{P} \\
\textbf{for } \forall\ l \notin \mathcal{C} \text{ with } l \text{ neighbor of } \ k,\ \sigma_l = \sigma_k \textbf{ do} \\
\quad \left\{\begin{array}{l}
\textbf{if } (\texttt{ran}\,(0,1) < p) \textbf{ then} \\
\quad \left\{\begin{array}{l}
\mathcal{P} \leftarrow \mathcal{P} \cup \{l\} \\
\mathcal{C} \leftarrow \mathcal{C} \cup \{l\}
\end{array}\right.
\end{array}\right. \\
\mathcal{P} \leftarrow \mathcal{P} \setminus \{k\}
\end{array}\right.$$

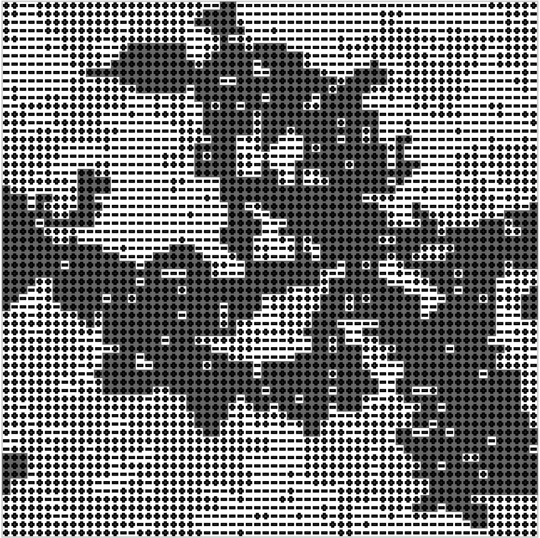
for $\forall k \in \mathcal{C}$ **do**

$$\left\{\ \sigma_k \leftarrow -\sigma_k\right.$$

output $\{\sigma_1, \ldots, \sigma_N\}$

- NB: $p = 1 - \mathrm{e}^{-2\beta}$

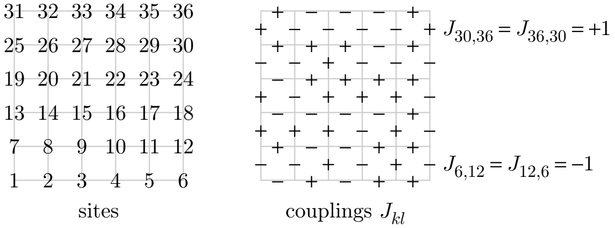
Ising clusters (example)



- NB: single move

Frustrated Ising model

- rarely, things work out as well...
- Example: two-dimensional spin-glass



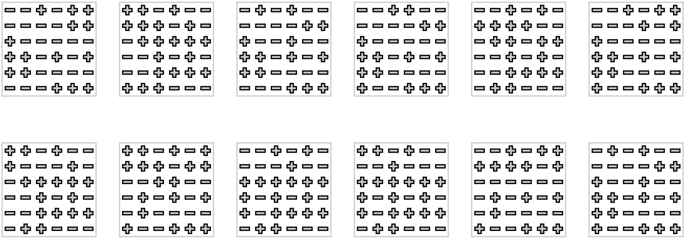
- Gray-code enumeration as before. . .

Enumeration (results)

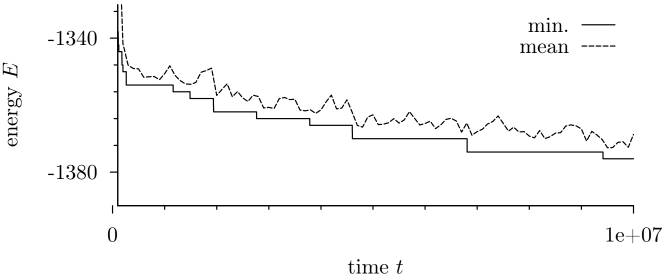
- density of states by Gray-code enumeration

E	$\mathcal{N}(E) = \mathcal{N}(-E)$
0	6969787392
−2	6754672256
⋮	⋮
−34	59456
−36	6912
−38	672

Some of the 672 groundstates . . .



- leads to slowdown of simulations...



- (energy vs time of 32×32 Ising model at $\beta = 2$).
- hopeless, but much easier than $3 - d$ spinglass.

Cluster simulation of frustrated spin glass

procedure `cluster-spin-glass`
input $\{J_{kl}\}$
input $\{\sigma_1, \ldots, \sigma_N\}$
$\vdots$
while $(\mathcal{P} \neq \emptyset)$ **do**

$$\left\{ \begin{array}{l} i \leftarrow \text{any element of } \mathcal{P} \\ \textbf{for } \forall\ j \notin \mathcal{C} \text{ with } j \text{ neighbor of } \ i, \sigma_i J_{ij} \sigma_j > 0 \textbf{ do} \\ \vdots \end{array} \right.$$

$\vdots$

- also very slow
- bad coupling to slow variable ...

procedure `combinatorial-ising`

input $\{u_\rightarrow, u_\uparrow, u_\leftarrow, u_\downarrow\}$ (4×4 matrices)

$\{U(j,j')\} \leftarrow \{0,\ldots,0\}$

for $k = 1,\ldots,N$ **do**

  for $n = 1,\ldots,4$ **do**

    $j \leftarrow 4 \cdot (k-1) + n$

    for $n' = 1,\ldots,4$ **do**

      $k' \leftarrow \mathrm{Nbr}(1,k)$

      if $(k' \neq 0)$ **then**

        $j' \leftarrow 4 \cdot (k'-1) + n'$

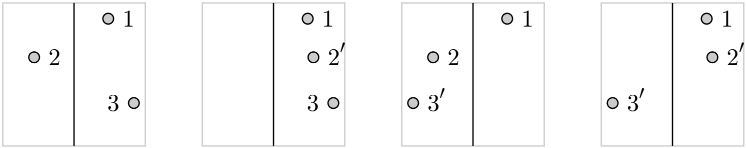
        $U(j,j') \leftarrow J_{j,j'} u_\rightarrow(n,n')$

      $\ldots$

output $\{U(j,j')\}$

- Saul–Kardar algorithm, hot topic in $2-d$ spin glasses

Liquids as Ising spin glasses



$E_{12} + E_{13} + E_{23}$ $\quad E'_{12} + E_{13} + E'_{23}$ $\quad E_{12} + E'_{13} + E'_{23}$ $\quad E'_{12} + E'_{13} + E_{23}$

- Liquids $\equiv$ Spin-glasses!! (Liu-Luijten)
- with

$$J_{ij} = \frac{1}{2}(E_{ij} + E'_{ij})$$