Multi-GPU accelerated multi-spin Monte Carlo simulations of the 2D Ising model

$$\begin{array}{ccccc} \uparrow & \downarrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \downarrow & \downarrow \\ \uparrow & \uparrow & \downarrow & \uparrow & \downarrow \\ \uparrow & \downarrow & \uparrow & \uparrow & \downarrow \end{array} \quad +$$

$=$

What was done?

- **Ising model**

$$H = -J \sum_{<i,j>} S_i S_j$$

- **Metropolis algorithm:**
  Efficient sampling

$$p_a = e^{-\frac{E}{k_B T}}$$

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How does it scale? Is it worth the effort?

Ising model I

- Formula:

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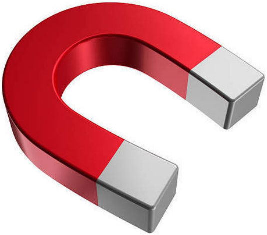

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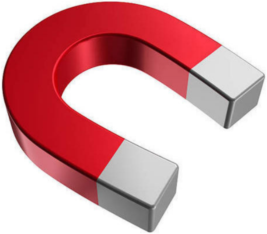

- System sizes: $100'000 \times 100'000$

Ising model II

Nearest neighbour interactions only!

$$H = -J \sum_{<i,j>} S_i S_j$$

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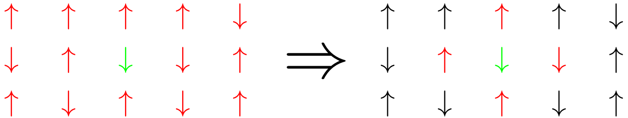

$$\begin{array}{ccccc} \uparrow & \uparrow & \uparrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \end{array} \Longrightarrow \begin{array}{ccccc} \uparrow & \uparrow & \uparrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \end{array}$$

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Calculation of energy: $\mathcal{O}\left(n^2\right) \Rightarrow \mathcal{O}\left(n\right)$

Metropolis algorithm

- **Goal:** Sample phase space

$$\begin{matrix} \uparrow & \downarrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \downarrow & \downarrow \\ \uparrow & \uparrow & \downarrow & \uparrow & \downarrow \\ \uparrow & \downarrow & \uparrow & \uparrow & \downarrow \end{matrix} \quad \overset{!}{\sim} \quad e^{-\frac{E}{k_B T}}$$

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- **Algorithm:**

Metropolis algorithm

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  1.) Propose new state: Random spin flips!

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  2.) Accept the new configuration: $p_a = e^{-\frac{\Delta E}{k_B T}}$

Single core CPU: Data structure

- Multi-spin coding: 1 spin $\widehat{=}$ 1 bit

Single core CPU: Data structure

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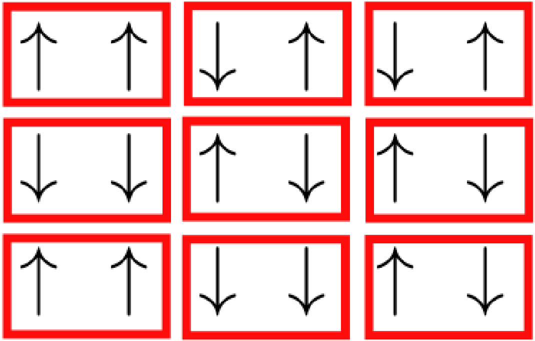

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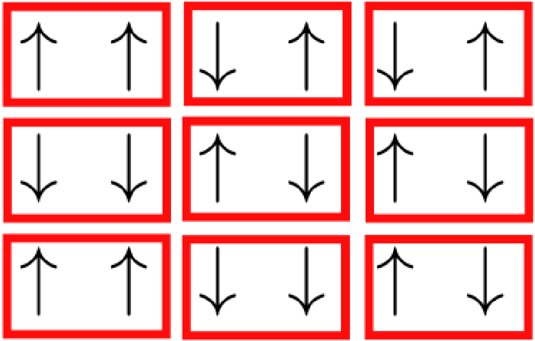

- 100’000 × 100’000 lattice: $\approx$ 1.2 GB

Single core CPU: Algorithm I

Type:	**# opposed**	**ΔE caused by flip of ↑**
$\begin{array}{ccc} & \uparrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{array}$	0	$+8J$
$\begin{array}{ccc} & \downarrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{array}$	1	$+4J$
$\begin{array}{ccc} & \downarrow & \\ \uparrow & \uparrow & \downarrow \\ & \uparrow & \end{array}$	2	0
$\begin{array}{ccc} & \downarrow & \\ \downarrow & \uparrow & \downarrow \\ & \uparrow & \end{array}$	3	$-4J$
$\begin{array}{ccc} & \downarrow & \\ \downarrow & \uparrow & \downarrow \\ & \downarrow & \end{array}$	4	$-8J$

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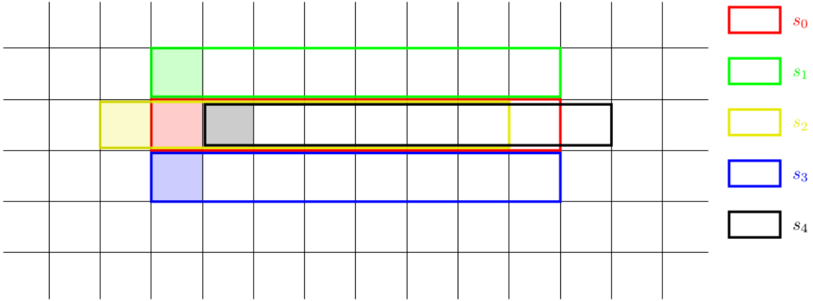
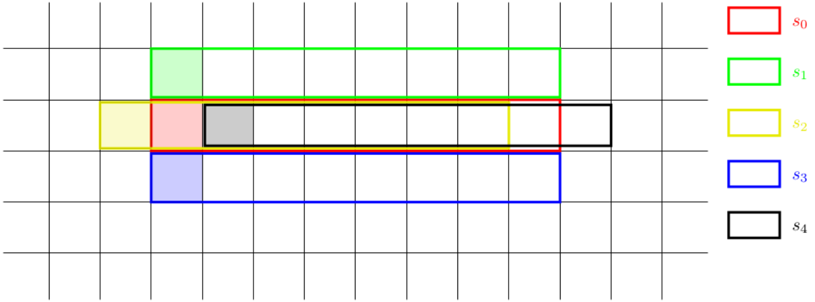
Count #opposed spins!

Single core CPU: Algorithm II

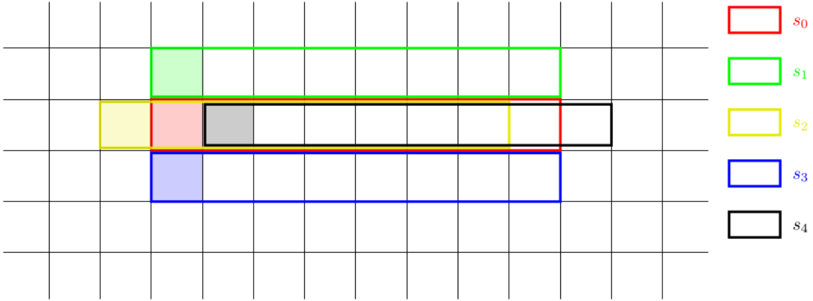


Single core CPU: Algorithm II



🟥 ≠ 🟩 ⇔ 🟥 XOR 🟩

Single core CPU: Algorithm II



🟥 ≠ 🟩 ⇔ 🟥 XOR 🟩

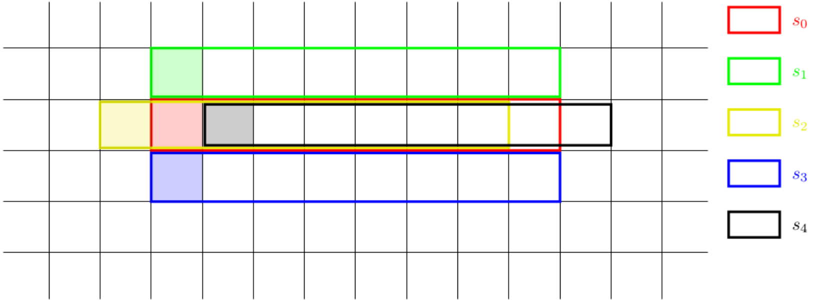
i_1 = 🟥 XOR 🟩

i_2 = 🟥 XOR 🟨

i_3 = 🟥 XOR 🟦

i_4 = 🟥 XOR ▭

Single core CPU: Algorithm II



🟥 $\neq$ 🟩 $\Leftrightarrow$ 🟥 XOR 🟩

i_1 = 🟥 XOR 🟩

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i_3 = 🟥 XOR 🟦

i_4 = 🟥 XOR ⬛

Combine with acceptance probability:

$i_1 + i_2 + i_3 + i_4 + 2\mathrm{exp}_8 + \mathrm{exp}_4 \geq 2$

Single GPU implementation I

- Port CPU implementation

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  ☹ Bad performance!

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    - big (≈ 4 GB)
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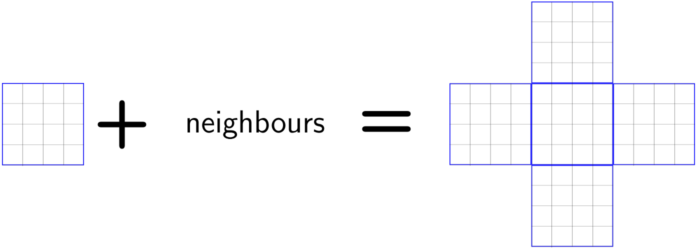
Reduce # accesses to global memory!

Single GPU implementation II

- Metaspins (4×4)
  $\rightarrow$ 1 metaspin $\widehat{=}$ 2 bytes = 1 unsigned short int
  $\rightarrow$ only 1 read per metaspin

Single GPU implementation II

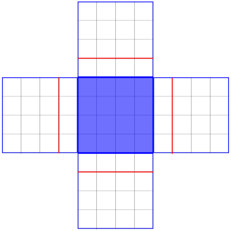
- Metaspins (4 × 4)
  → 1 metaspin $\widehat{=}$ 2 bytes = 1 unsigned short int
  → only 1 read per metaspin
- Read:



+ neighbours =

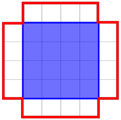
Single GPU implementation II

Global memory:



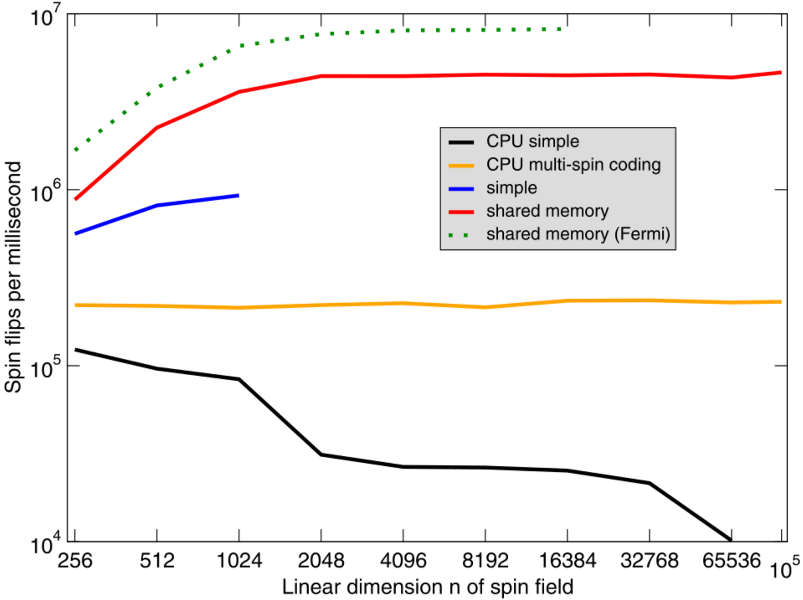
$\xrightarrow{5reads}$

Shared memory:



⇒ 5 reads to flip entire metaspin!

Results: CPU vs. GPU



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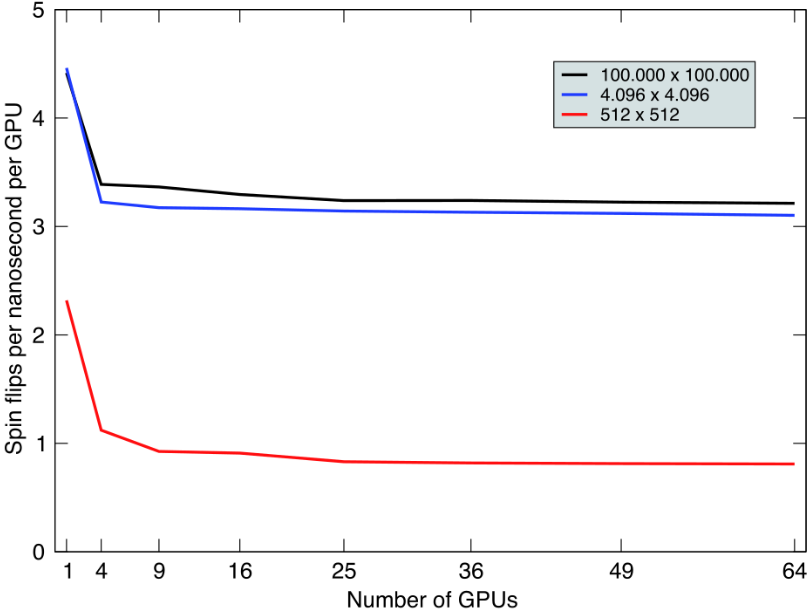
  5. Repeat or finish

Multi-GPU: Results



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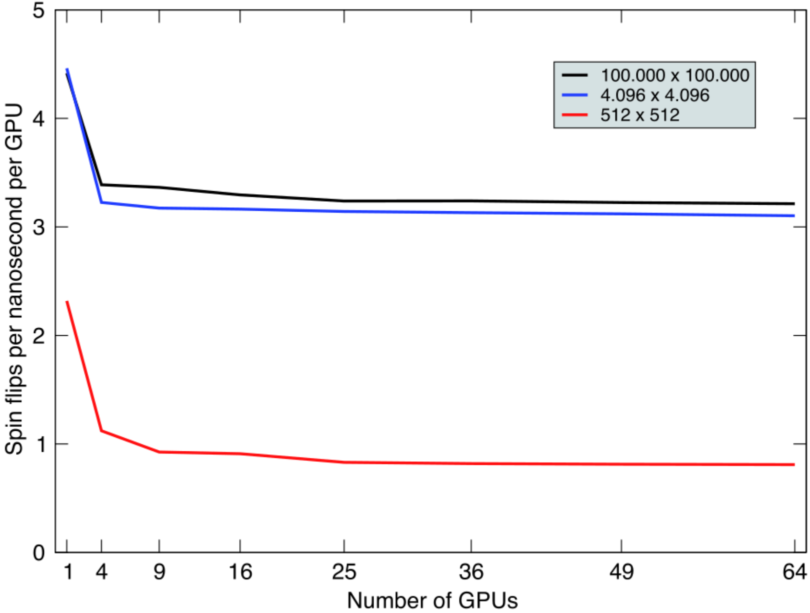

64 GPUs, $800'000 \times 800'000$: 3s

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Why this paper?!