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?

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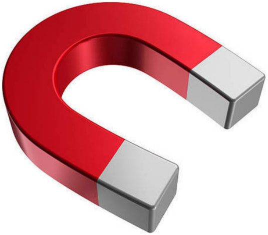

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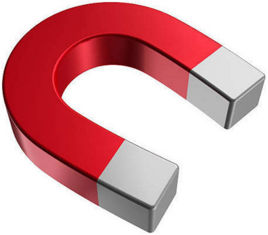

- System sizes: $100'000 \times 100'000$

Ising model II

Nearest neighbour interactions only!

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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

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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

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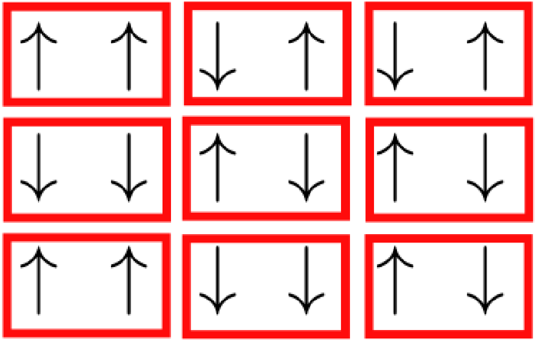

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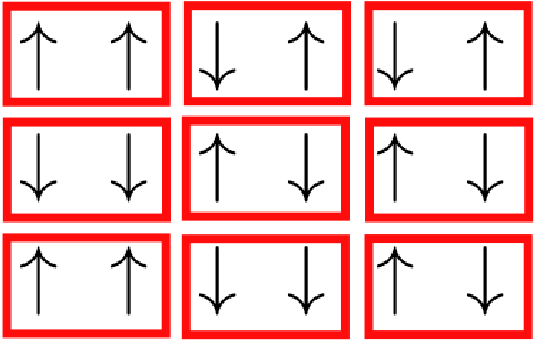

- $100'000 \times 100'000$ lattice: ≈ 1.2 GB

Single core CPU: Algorithm I

Type:	# opposed	ΔE caused by flip of $\uparrow$
$\begin{array}{ccc} & \uparrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{array}$	0	$+8J$
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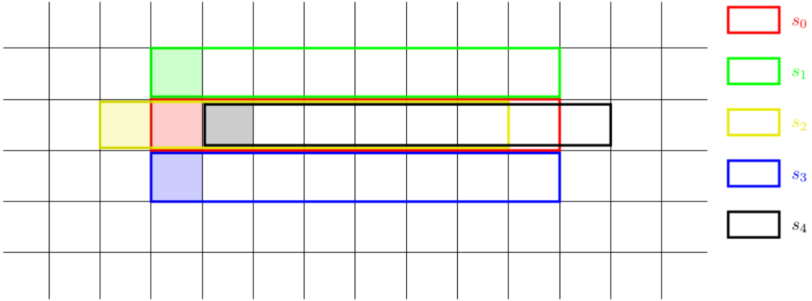
Count #opposed spins!

Single core CPU: Algorithm II



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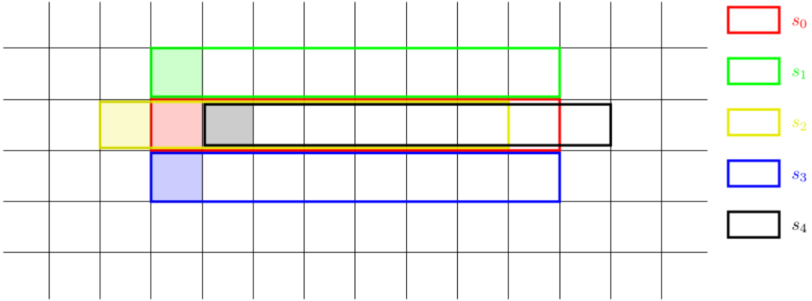

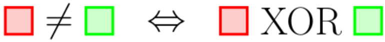

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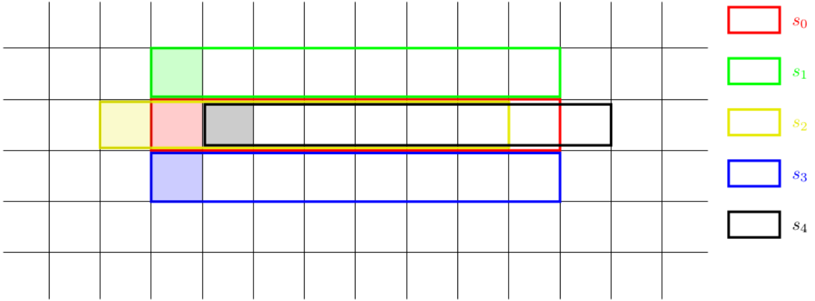

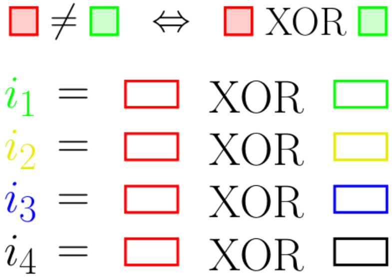

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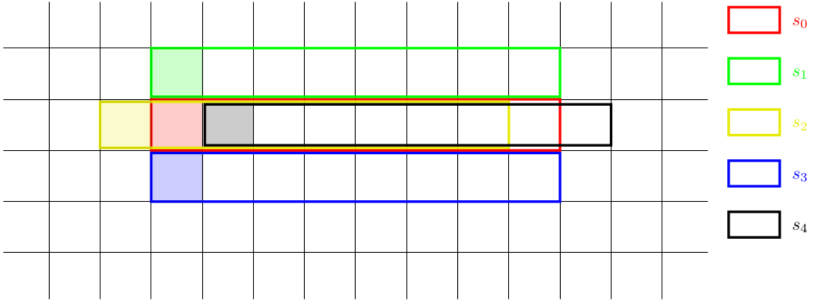

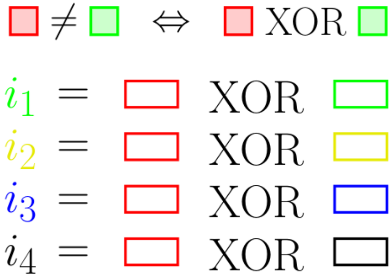

Combine with acceptance probability:

$$i_1 + i_2 + i_3 + i_4 + 2\exp_8 + \exp_4 \geq 2$$

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- Port CPU implementation

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    - big ($\approx$ 4 GB)
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Reduce # accesses to global memory!

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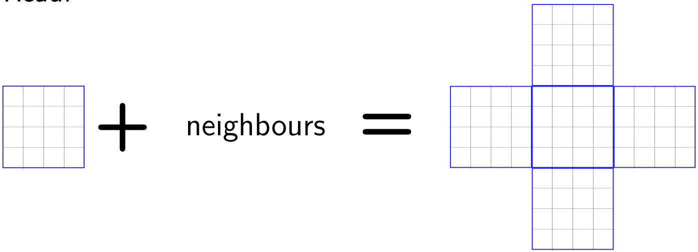

Single GPU implementation II

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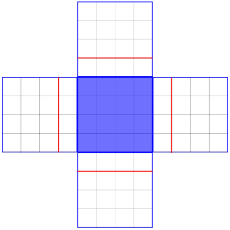
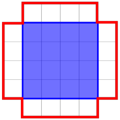


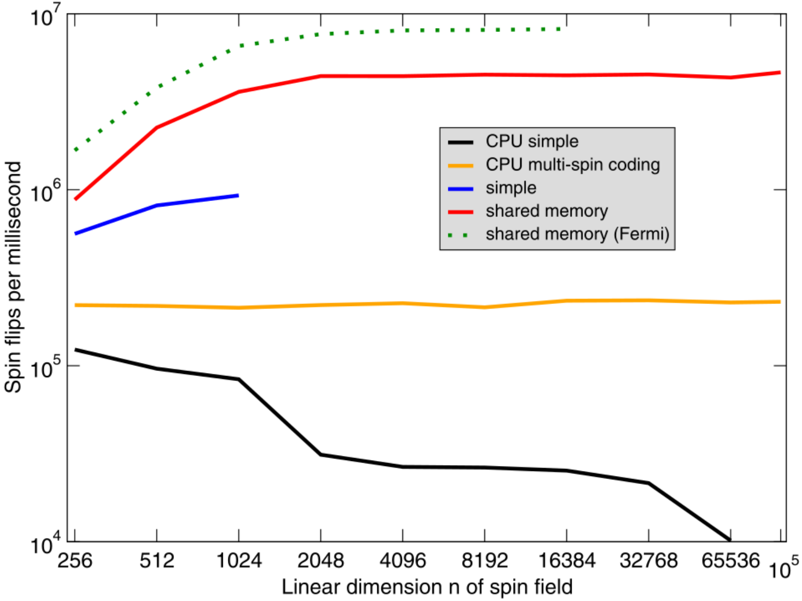
$\xrightarrow{5 \text{reads}}$

Shared memory:



$\Rightarrow$ 5 reads to flip entire metaspin!

Results: CPU vs. GPU



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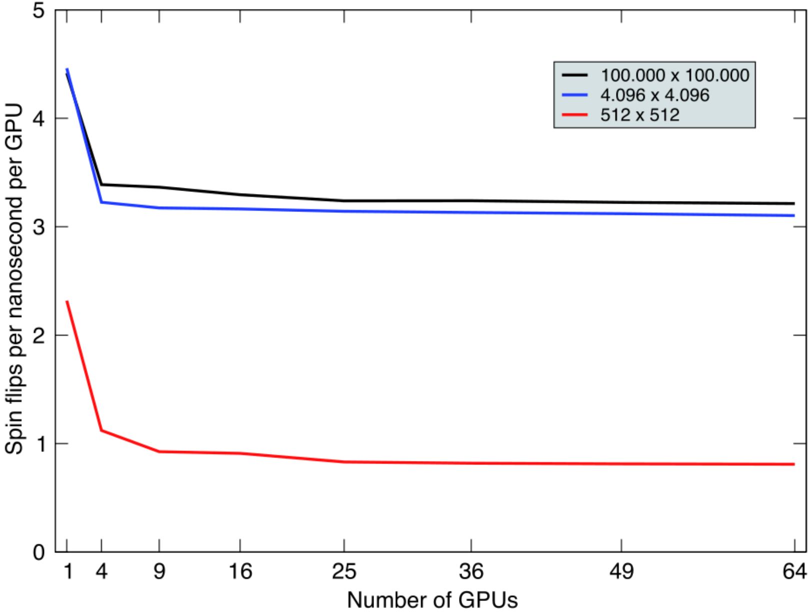
  5. Repeat or finish

Multi-GPU: Results



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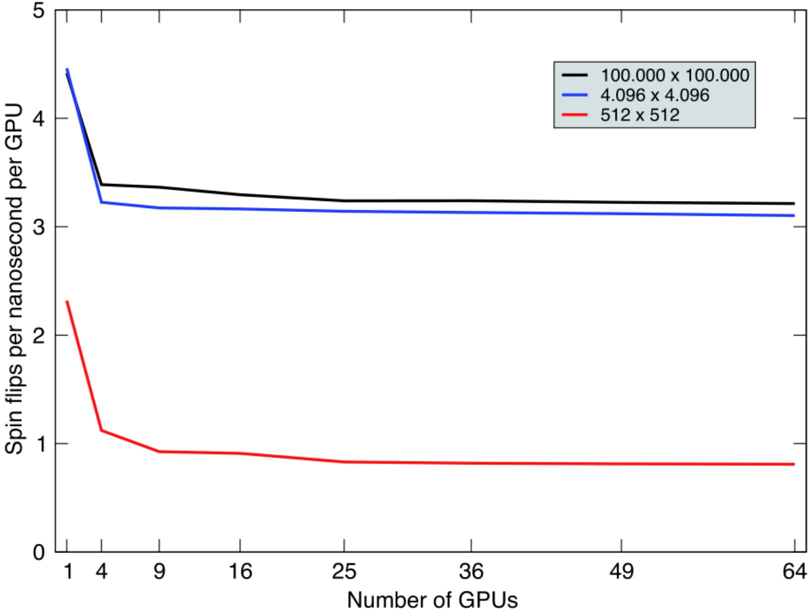

64 GPUs, $800'000 \times 800'000$: 3s

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Why this paper?!

Questions?