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

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How does it scale? Is it worth the effort?

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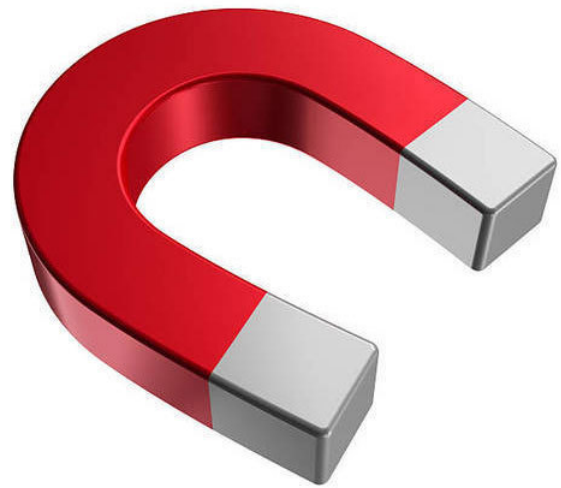
$$\begin{array}{cccccc} \uparrow & \downarrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \downarrow & \downarrow \\ \uparrow & \uparrow & \downarrow & \uparrow & \downarrow \\ \uparrow & \downarrow & \uparrow & \uparrow & \downarrow \end{array} \quad \widehat{=}$$



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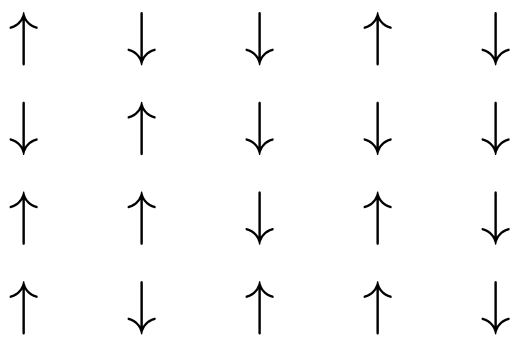

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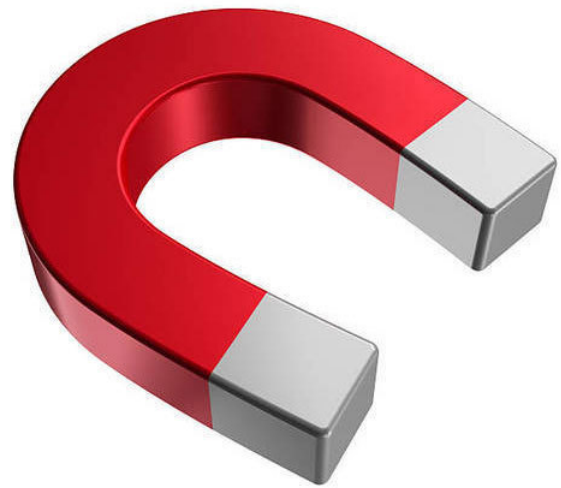

- System sizes: $100'000 \times 100'000$

Ising model II

Nearest neighbour interactions only!

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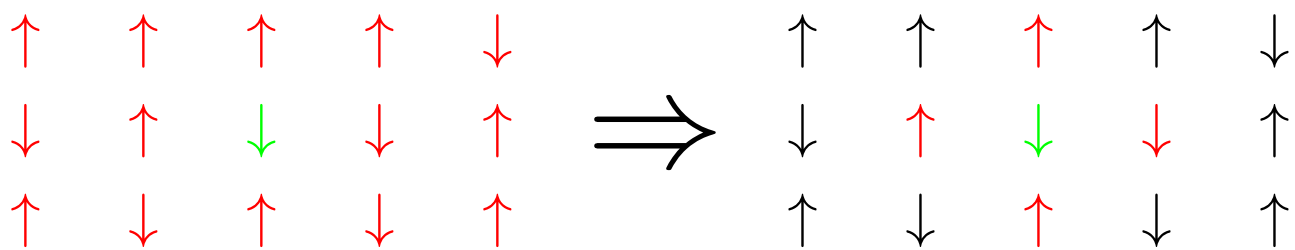

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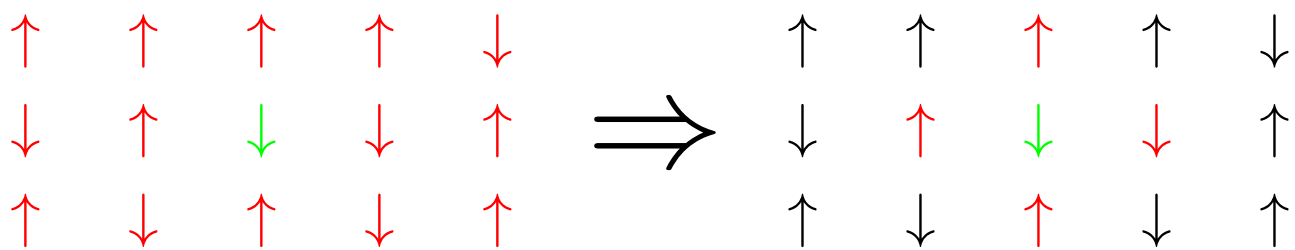
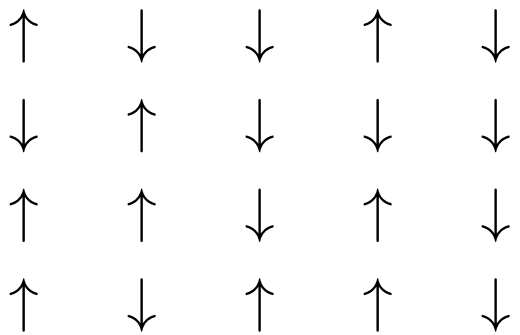


Calculation of energy: $\mathcal{O}\left(n^2\right) \Rightarrow \mathcal{O}\left(n\right)$

Metropolis algorithm

- **Goal:** Sample phase space



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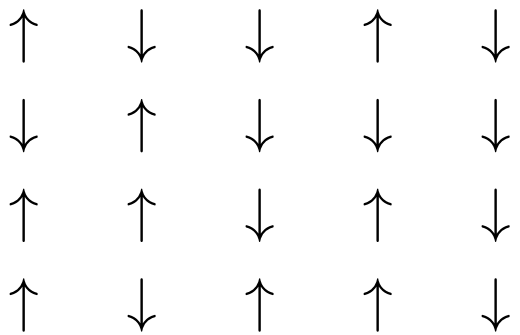

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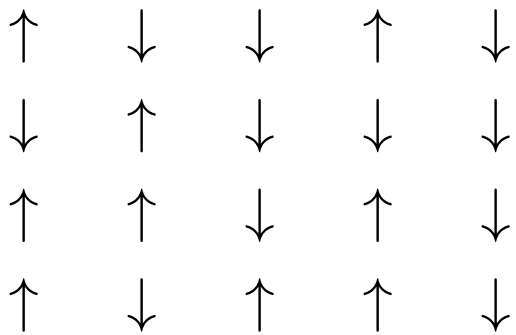

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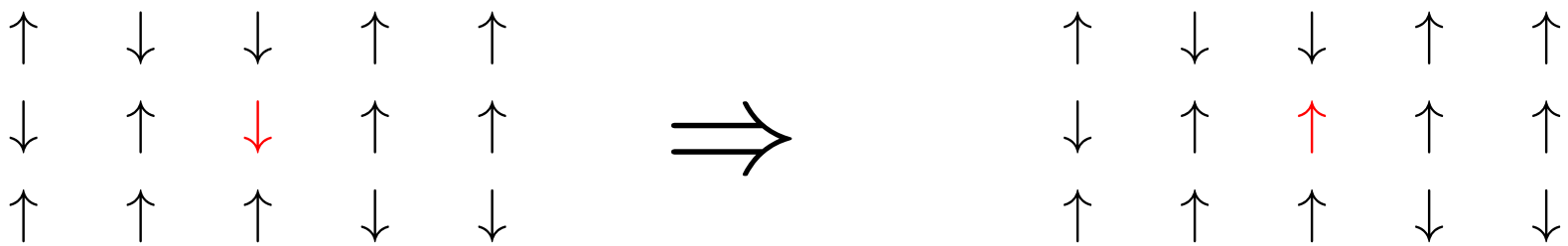
  1.) Propose new state: Random spin flips!



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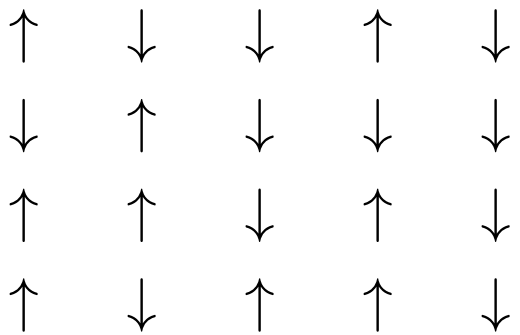

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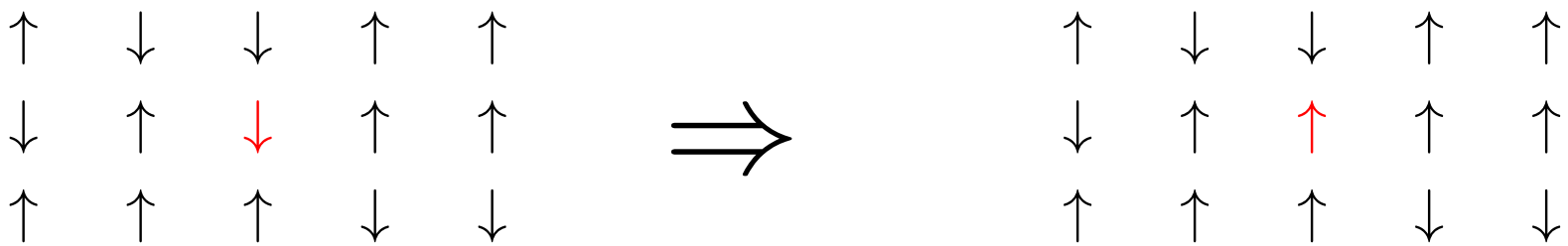

  2.) Accept the new configuration: $p_a = e^{-\frac{\Delta E}{k_B T}}$

Single core CPU: Data structure

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

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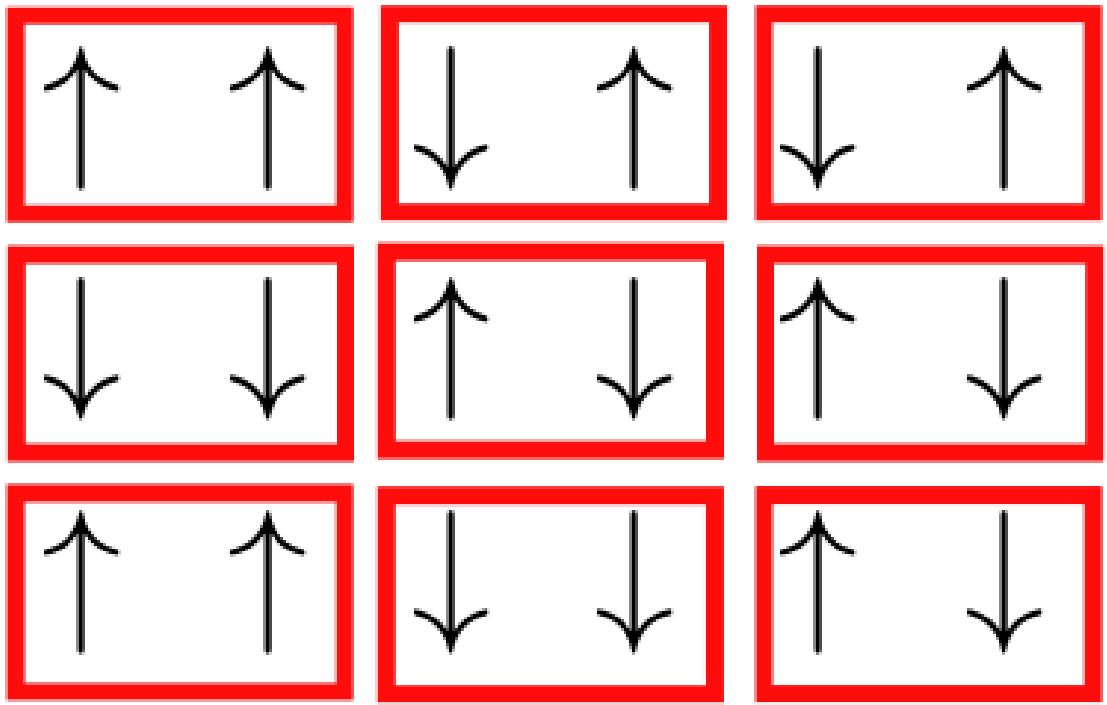

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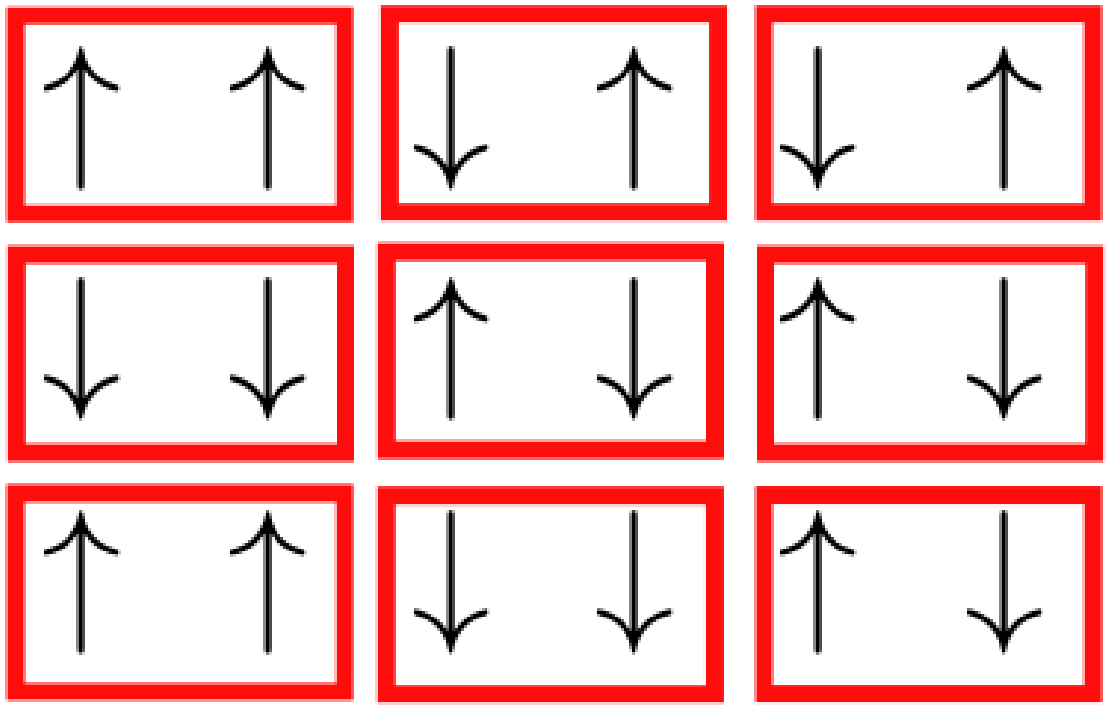
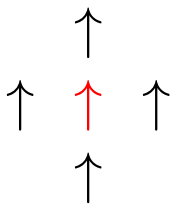
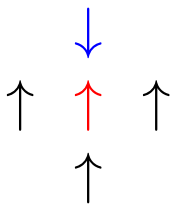
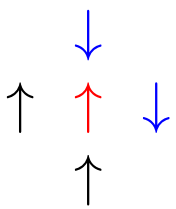
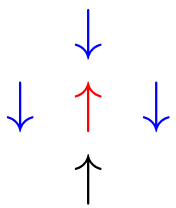
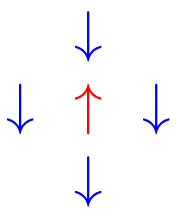


- 100'000 $\times$ 100'000 lattice: $\approx$ 1.2 GB

Single core CPU: Algorithm I

Type:	# opposed	ΔE caused by flip of $\uparrow$
	0	$+8J$
	1	$+4J$
	2	0
	3	$-4J$
	4	$-8J$

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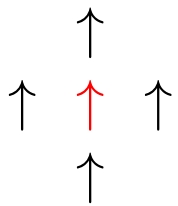
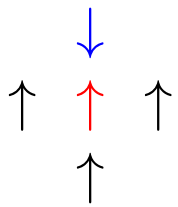
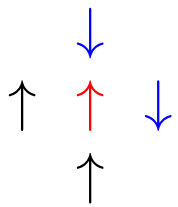
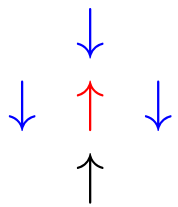
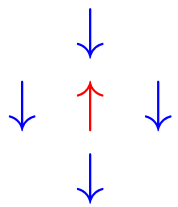
	0	$+8J$
	1	$+4J$
	2	0
	3	$-4J$
	4	$-8J$

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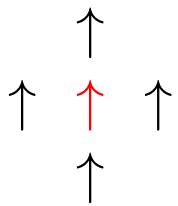
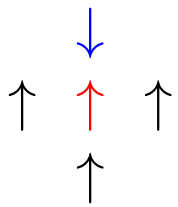
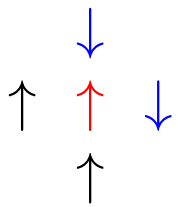
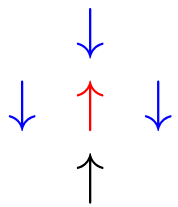
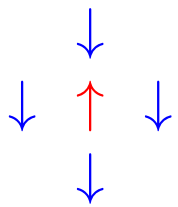
	0	$+8J$
	1	$+4J$
	2	0
	3	$-4J$
	4	$-8J$

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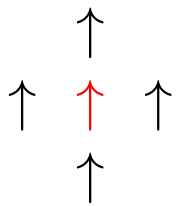
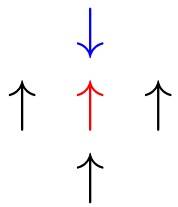
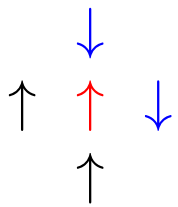
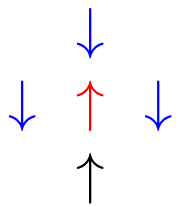
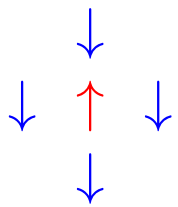
	0	$+8J$
	1	$+4J$
	2	0
	3	$-4J$
	4	$-8J$

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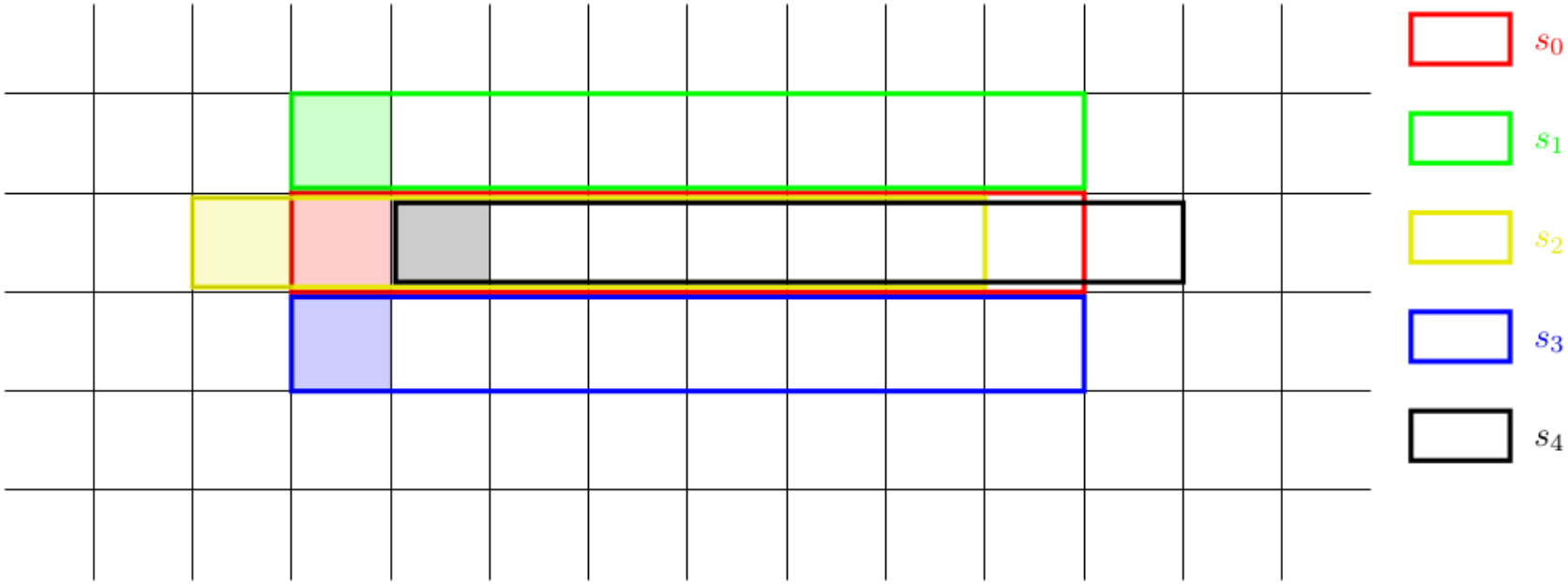
Count #opposed spins!

Single core CPU: Algorithm II



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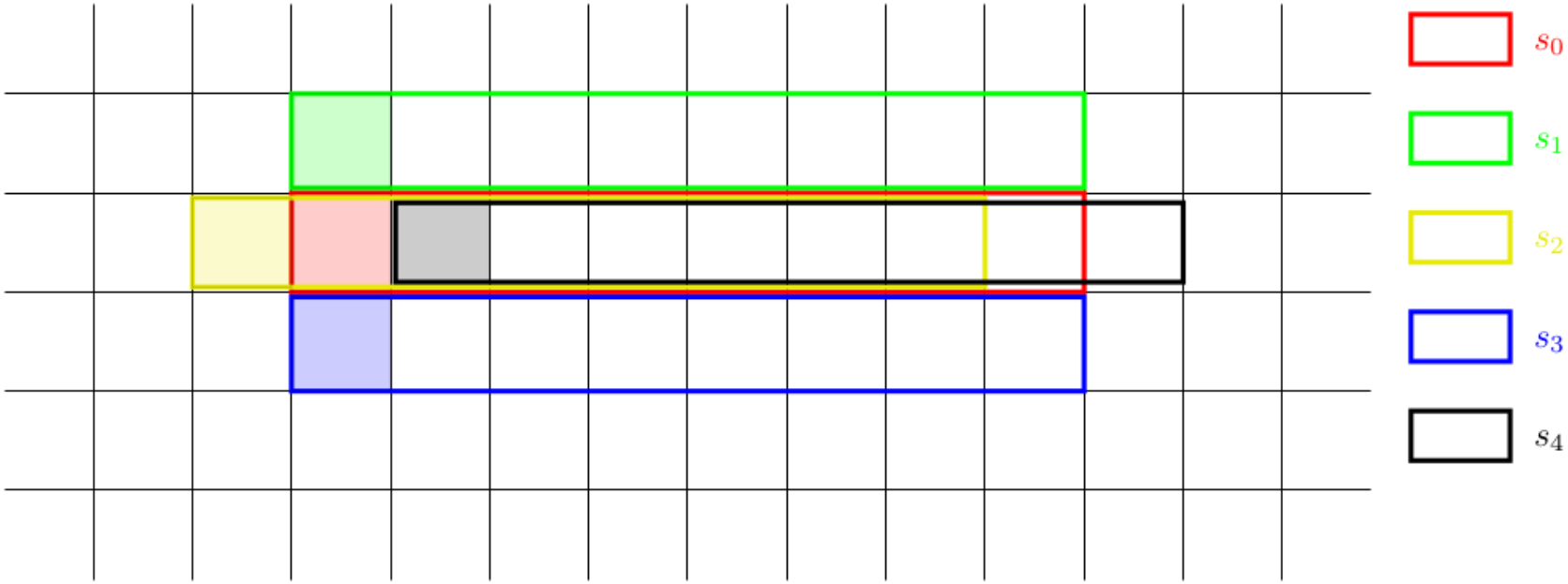

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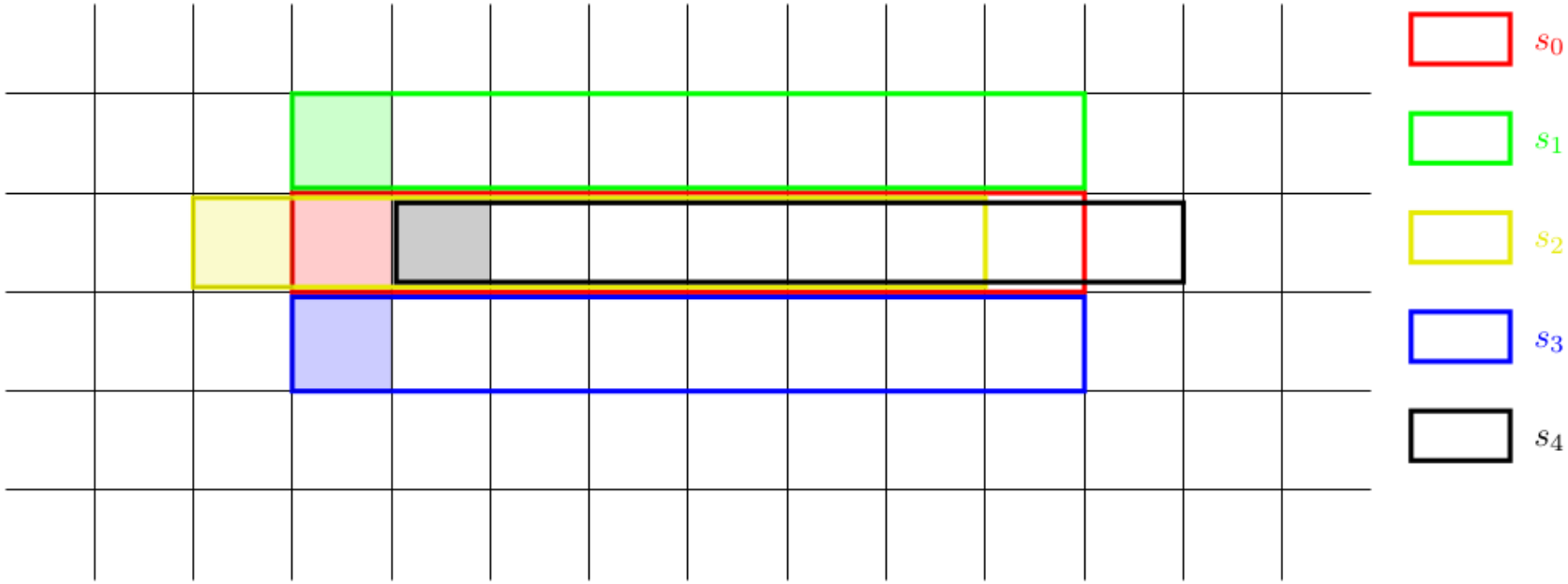

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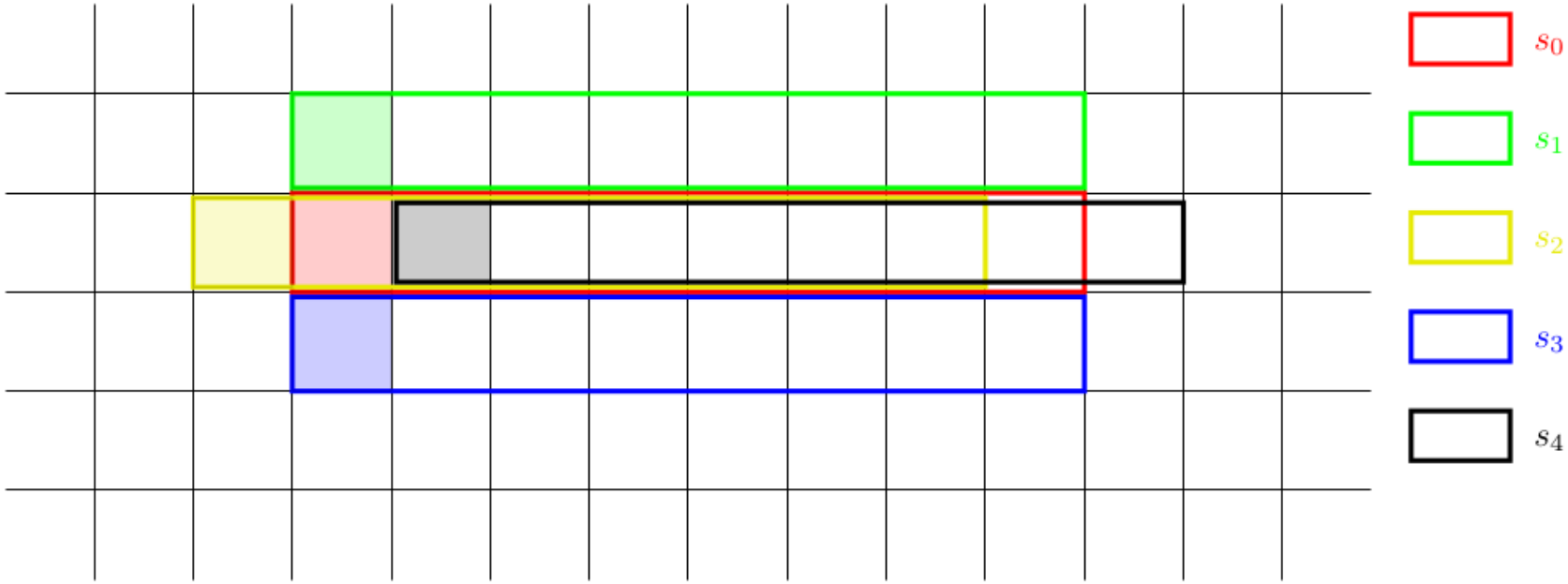

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Combine with acceptance probability:

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

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- Port CPU implementation

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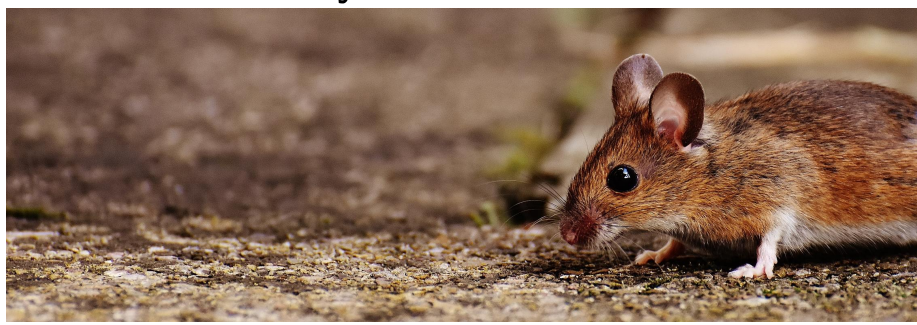

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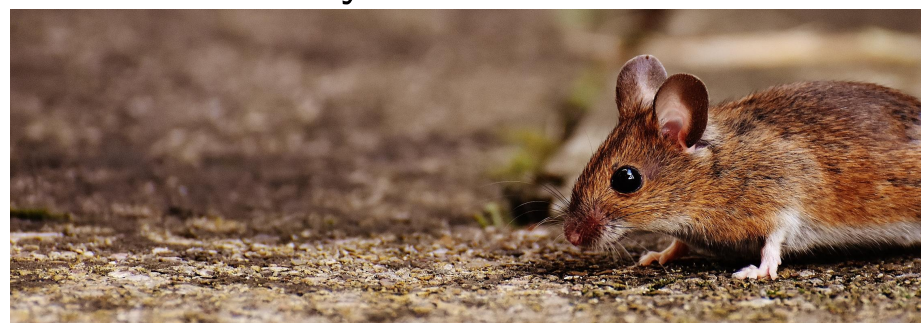

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Reduce # accesses to global memory!

Single GPU implementation II

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  $\rightarrow$ 1 metaspin $\widehat{=}$ 2 bytes $=$ 1 unsigned short int
  $\rightarrow$ only 1 read per metaspin

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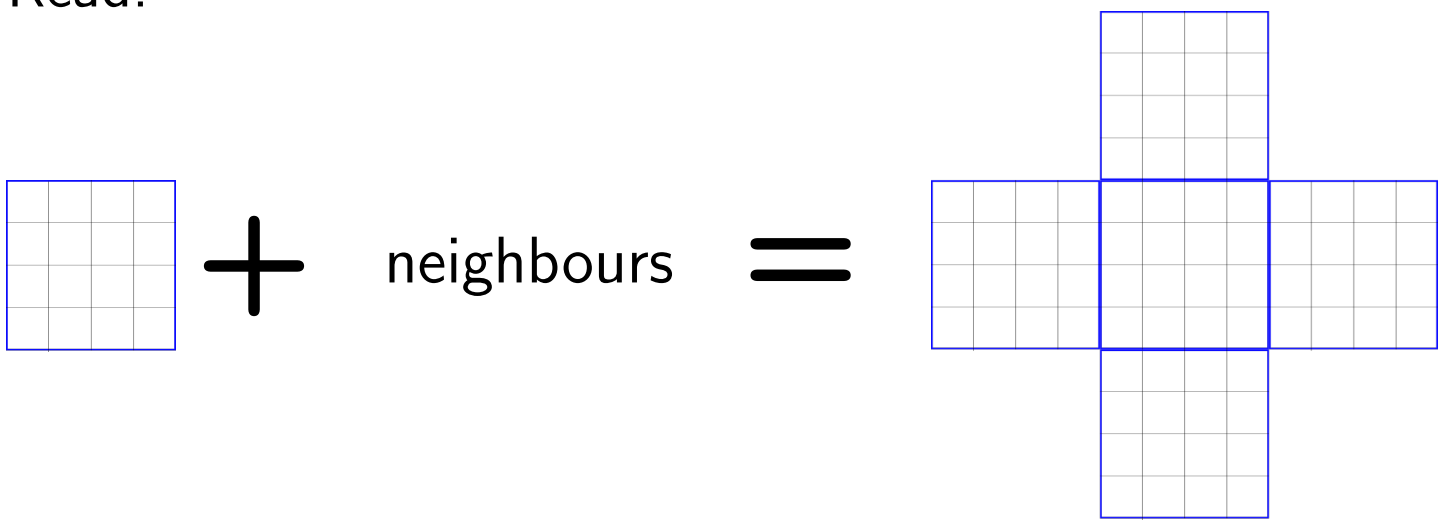
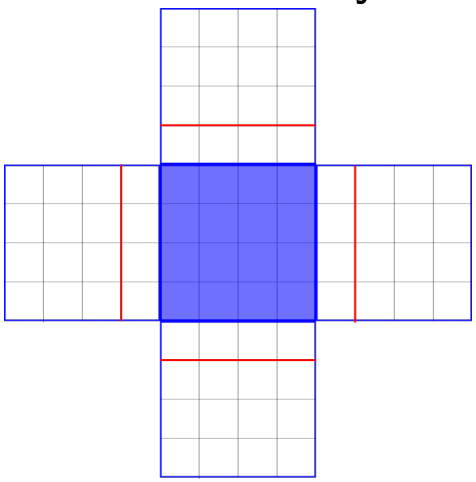
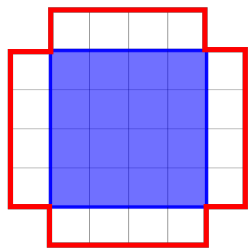


Single GPU implementation II

Global memory:



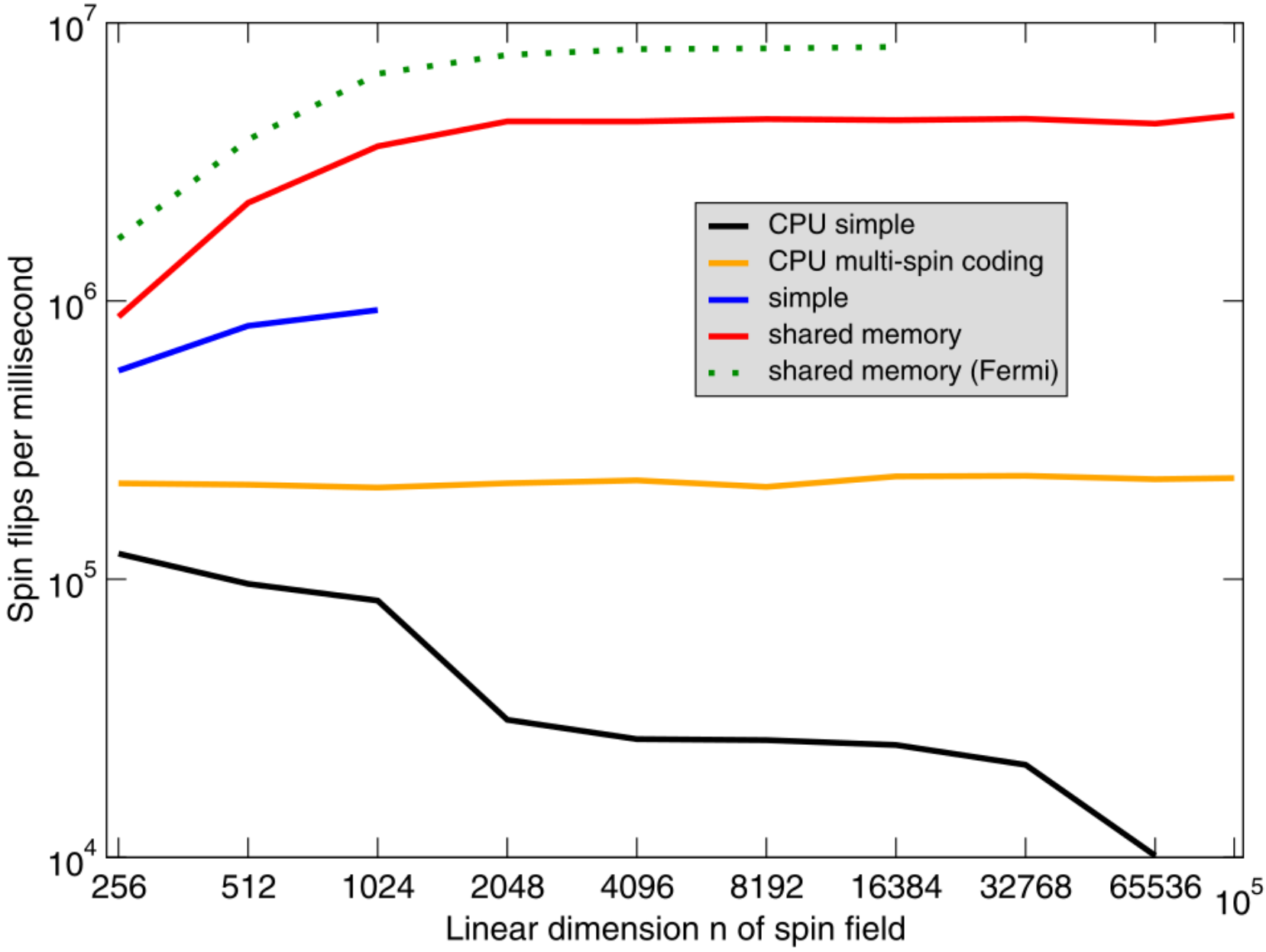
5reads



Shared memory:

$\Rightarrow$ 5 reads to flip entire metaspin!

Results: CPU vs. GPU



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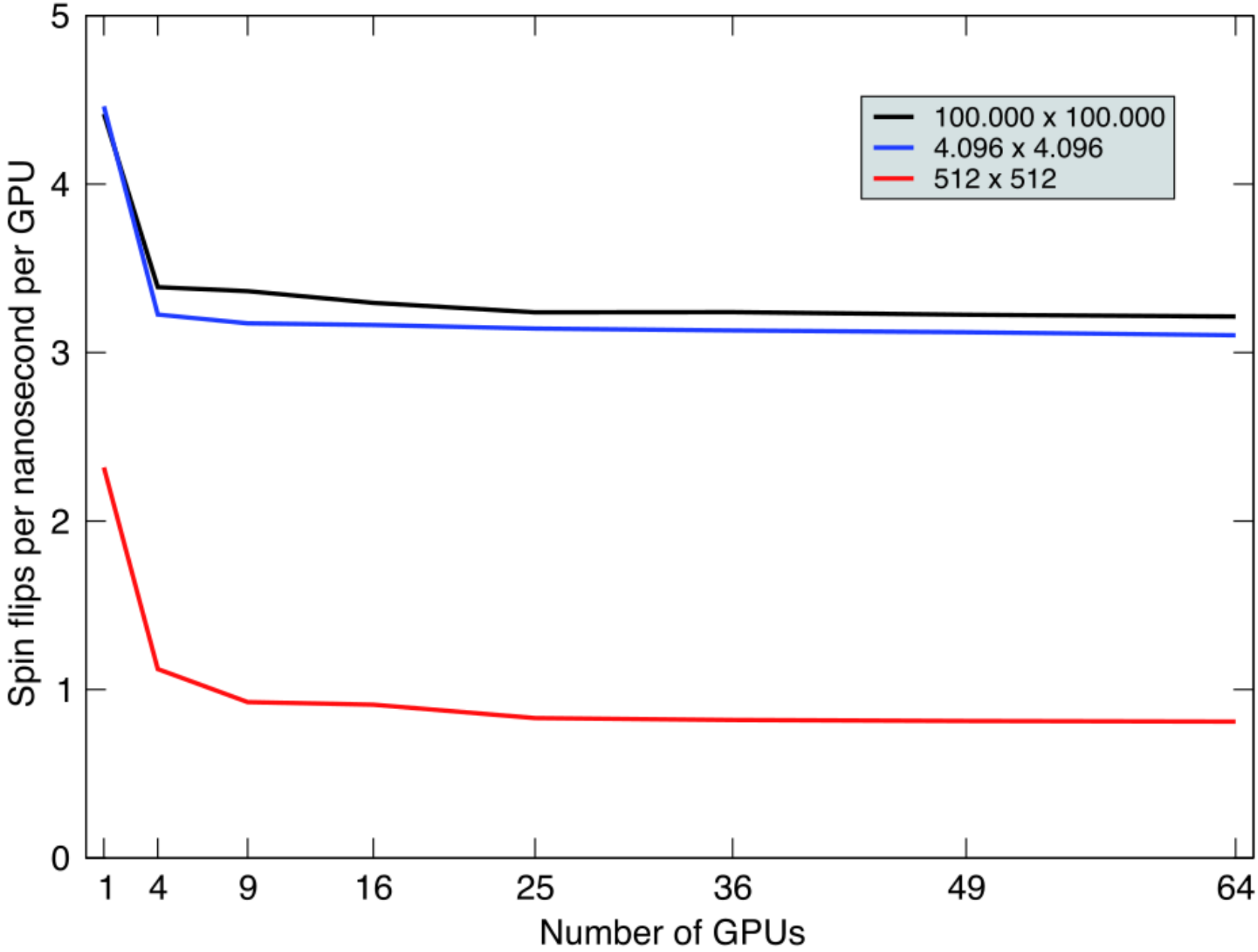
  5. Repeat or finish

Multi-GPU: Results



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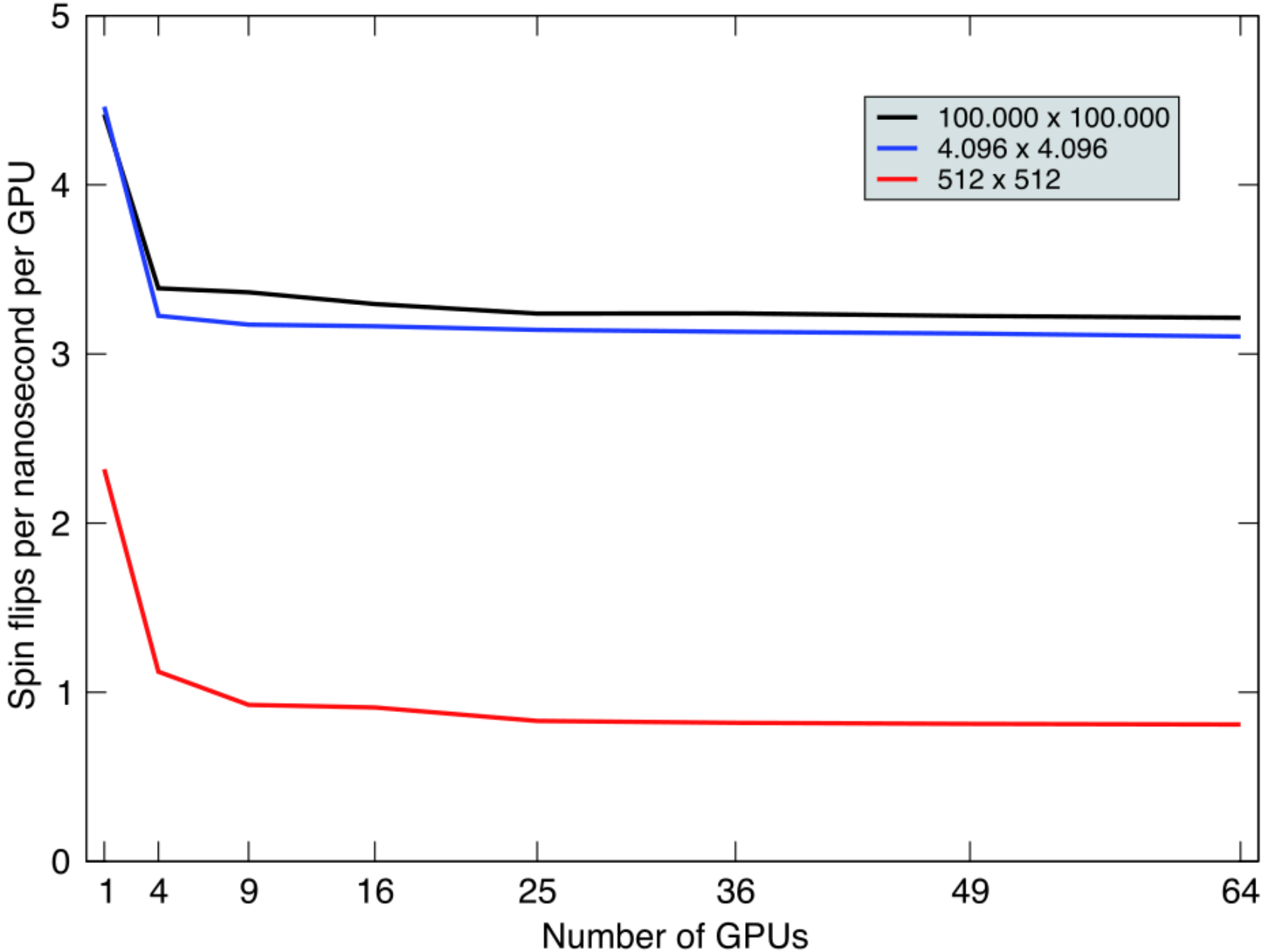

64 GPUs, $800'000 \times 800'000$: 3s

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Why this paper?!

Questions?