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ACCELERATING BLOCKSPARSE DMRG WITH GPUS

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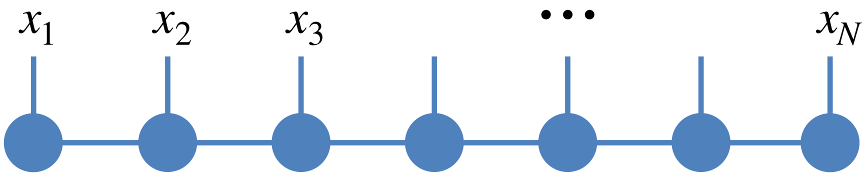
DMRG algorithm

A many variable function is represented as a tensor network

$$\psi(x_1, x_2, \ldots, x_N) \approx$$



The wave function is minimized variationally via the linear least squares algorithm

$$f(\psi) = \frac{1}{2} \| H \,|\psi\rangle - E \,|\psi\rangle \|^2$$

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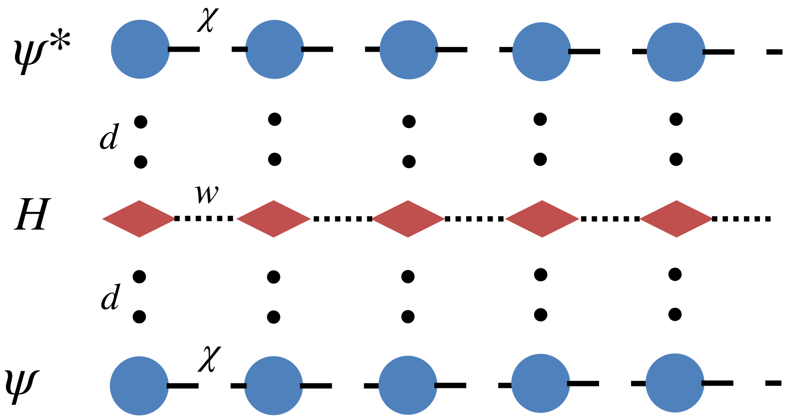
DMRG algorithm



$\chi \sim$ 100 to 10,000+
$w \sim$ 10 to 100
$d \sim$ 2 to 10

Pairs of blue nodes on this graph are optimized using a least squares algorithm.

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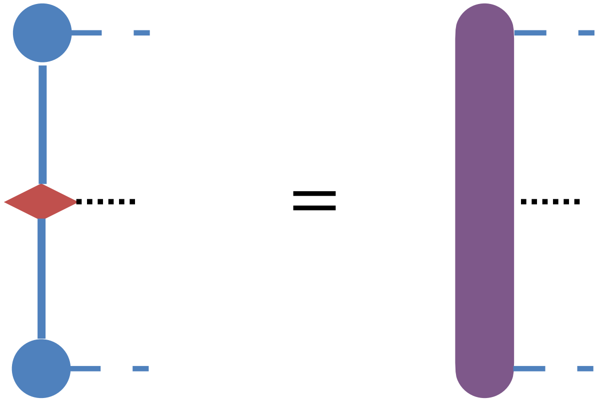
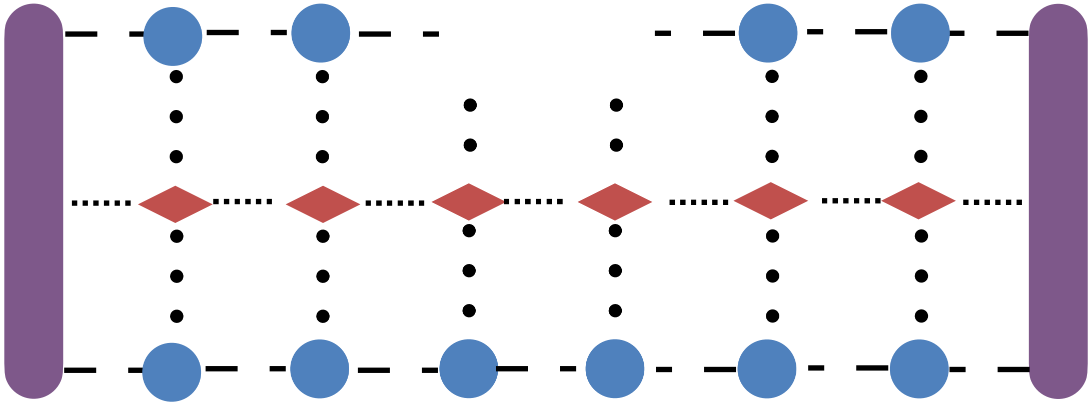
DMRG algorithm

Partial contractions are stored for convenience



DMRG algorithm

Take the derivative of the network with respect to wavefunction tensors



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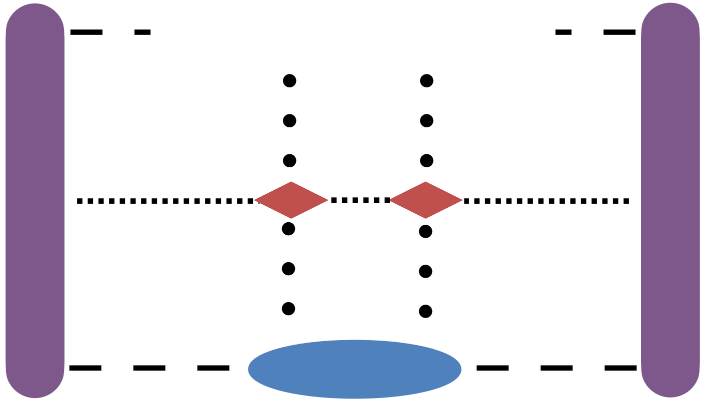
Consolidating the graph gives us the most expensive terms



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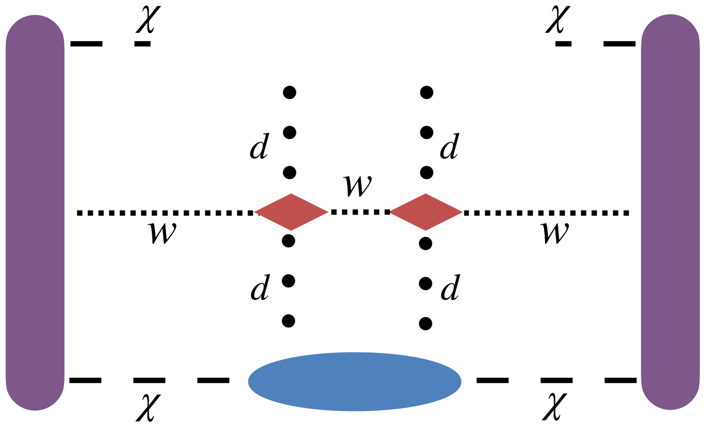

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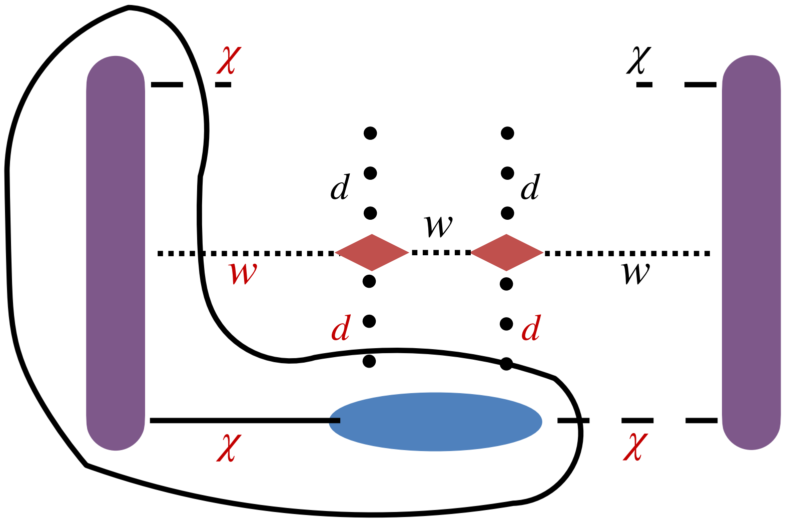

$\chi \sim$ 100 to 10,000+
$w \sim$ 10 to 100
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Contraction Cost: $\chi^3 w d^2$

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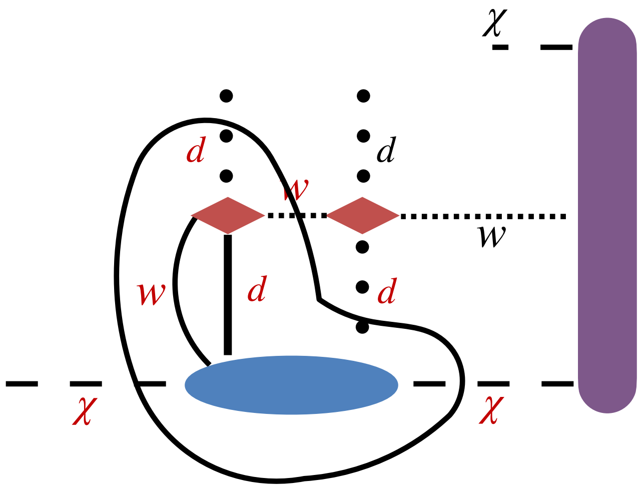

$\chi \sim$ 100 to 10,000+
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Contraction Cost: $d^3 w^2 \chi^2$

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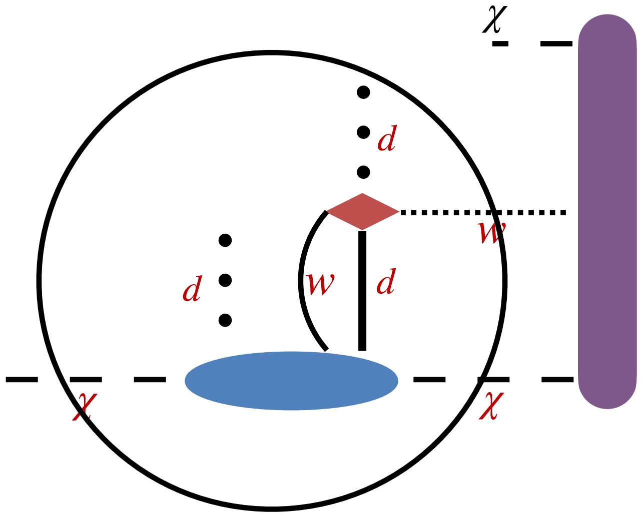

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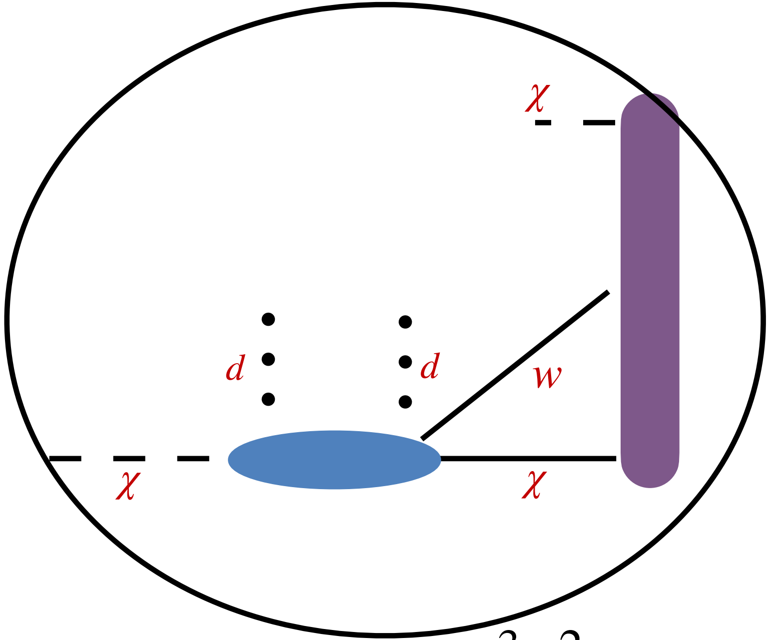

$\chi \sim 100$ to $10{,}000+$
$w \sim 10$ to 100
$d \sim 2$ to 10

Contraction Cost: $\chi^3 d^2 w$

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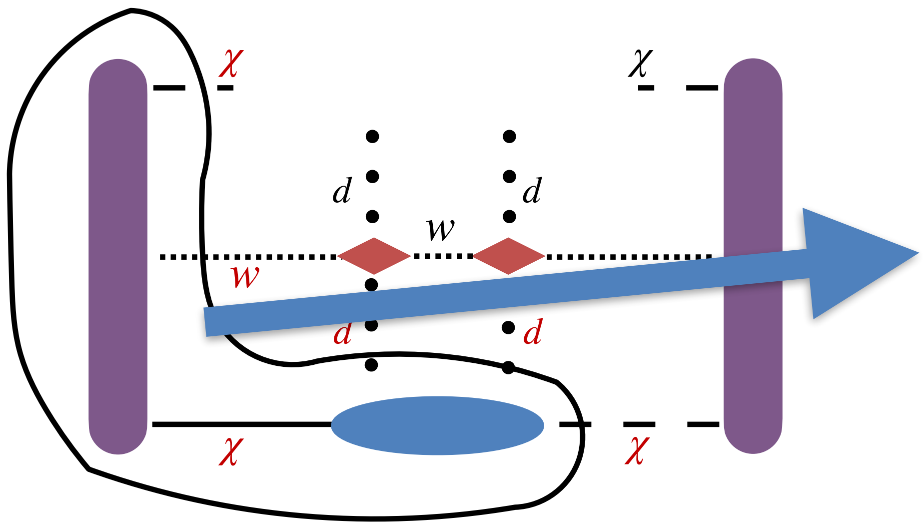
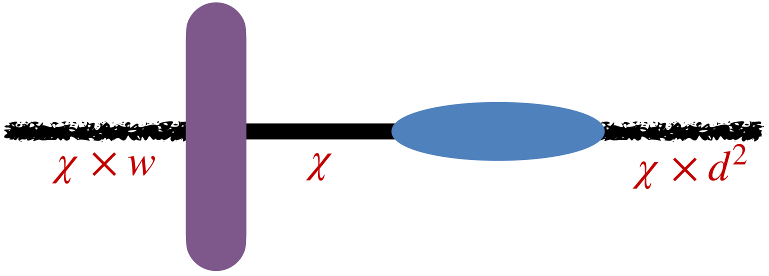
The term with the highest computational cost is relatively square





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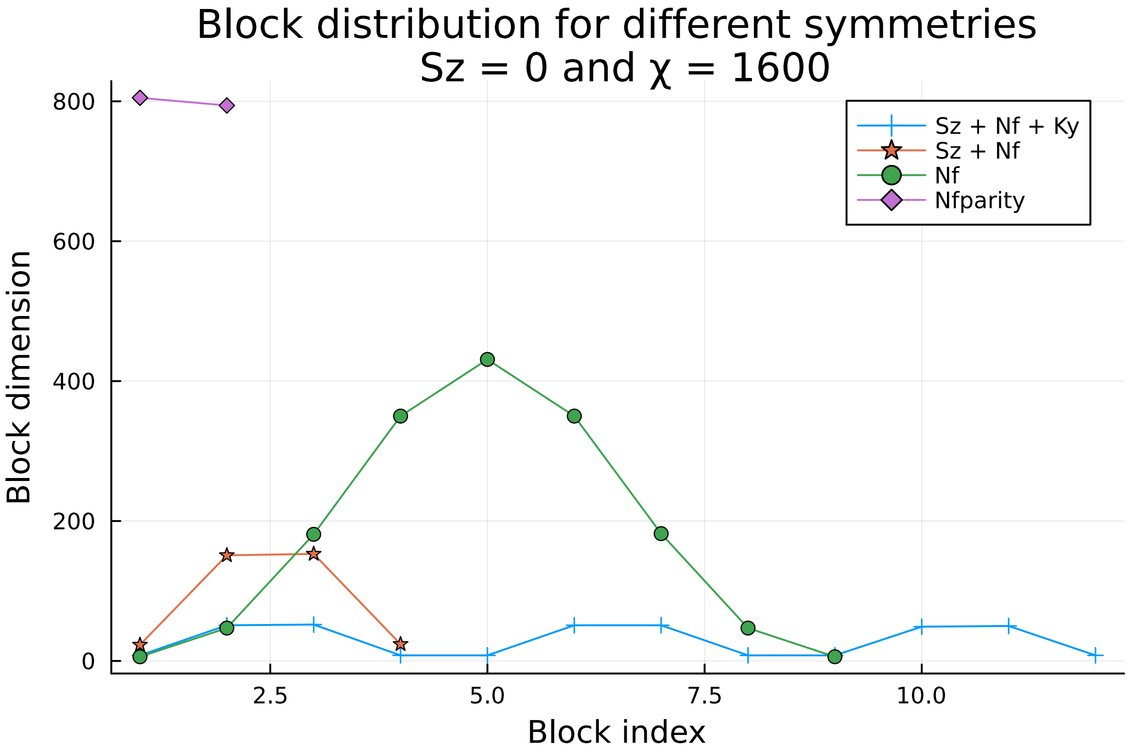
Typical block distribution of χ: 2D momentum Hubbard



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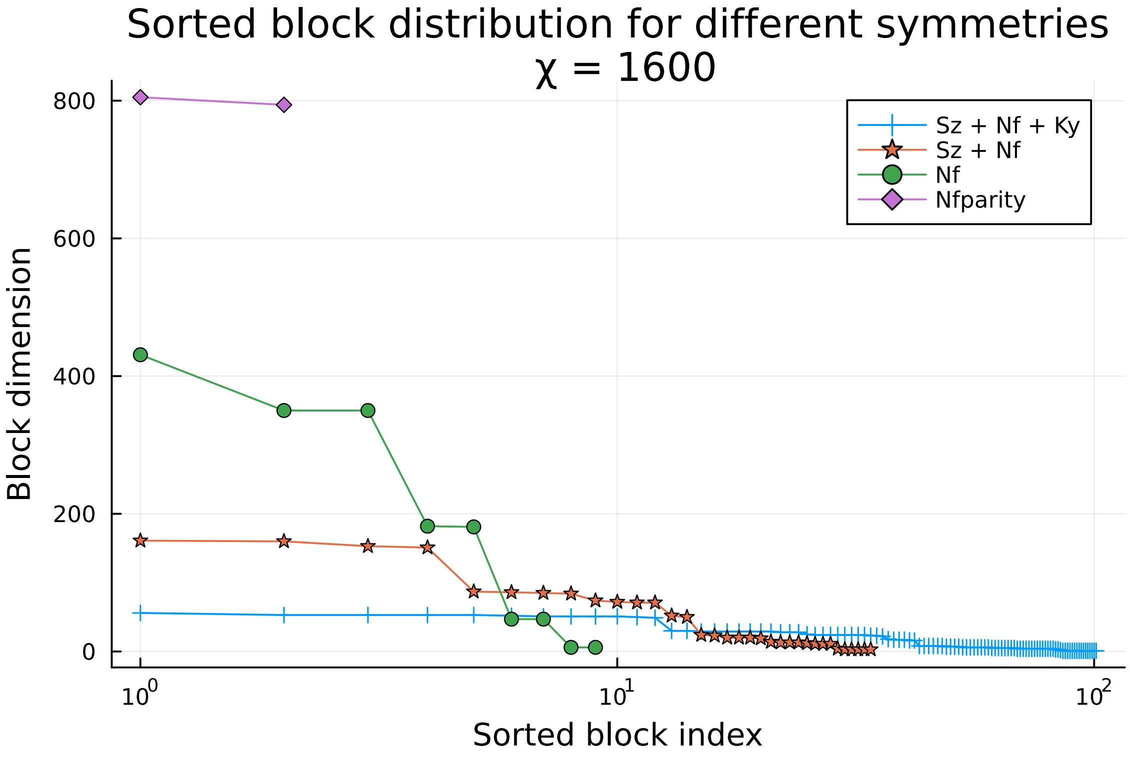
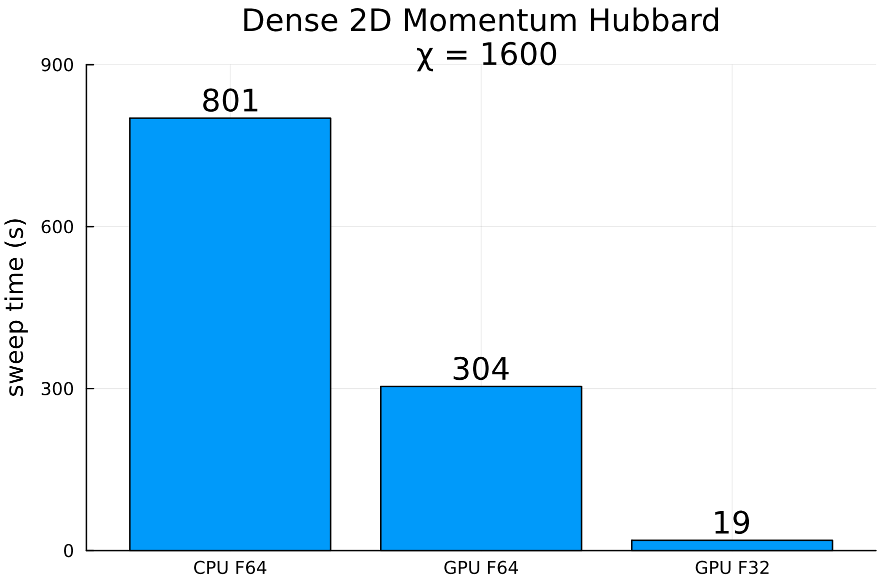
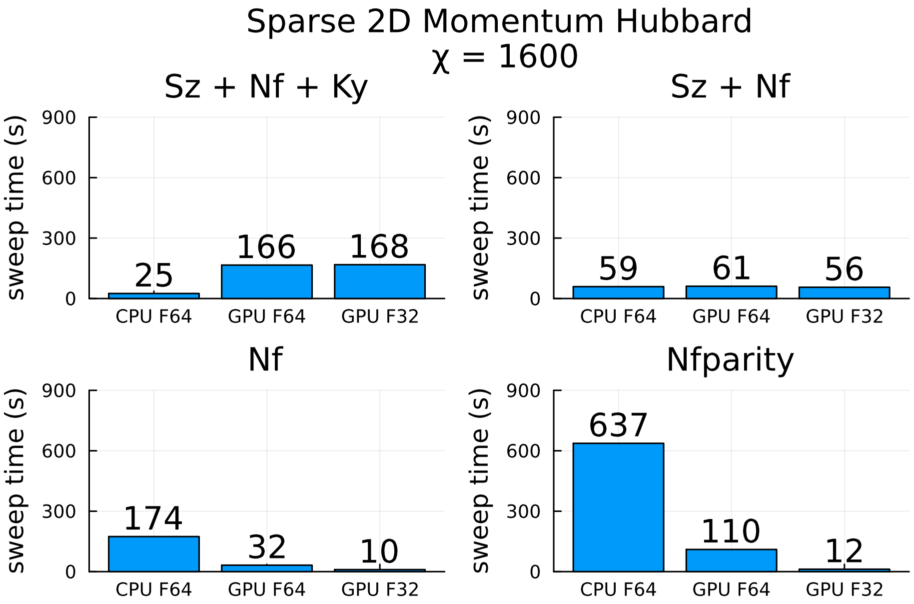
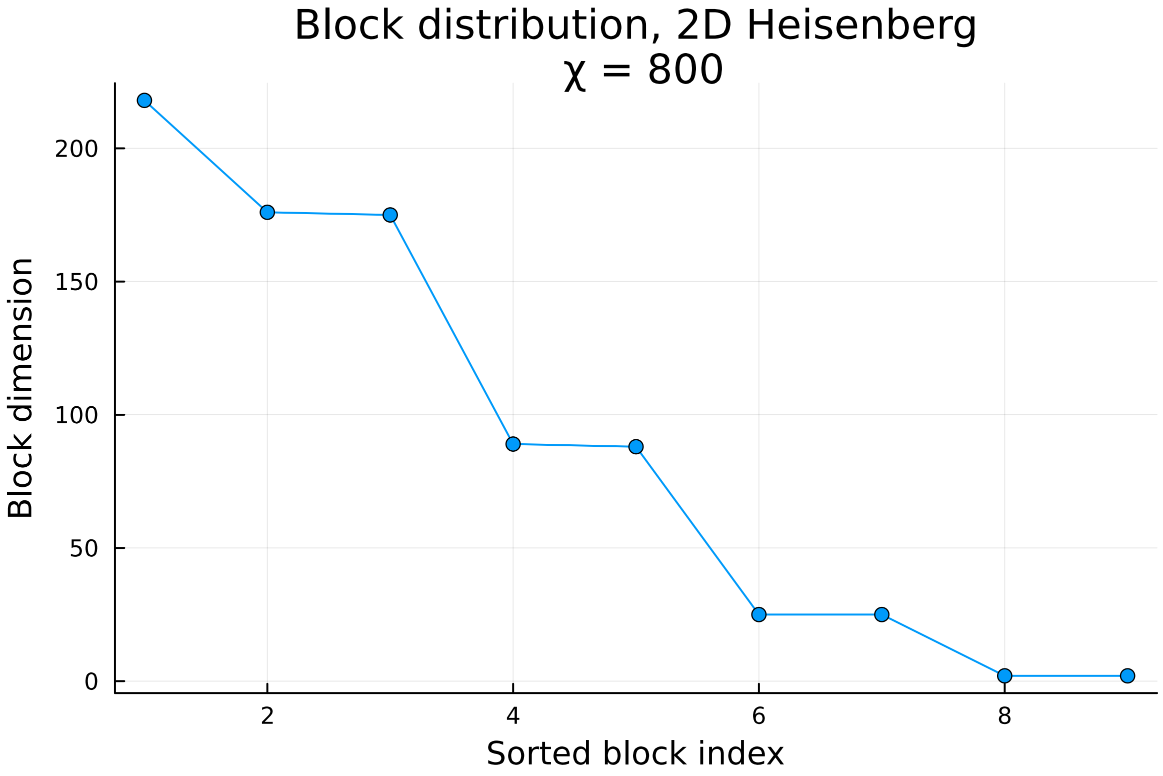


DMRG Timing: 2D Momentum Hubbard





Typical block distribution of χ: 2D Heisenberg



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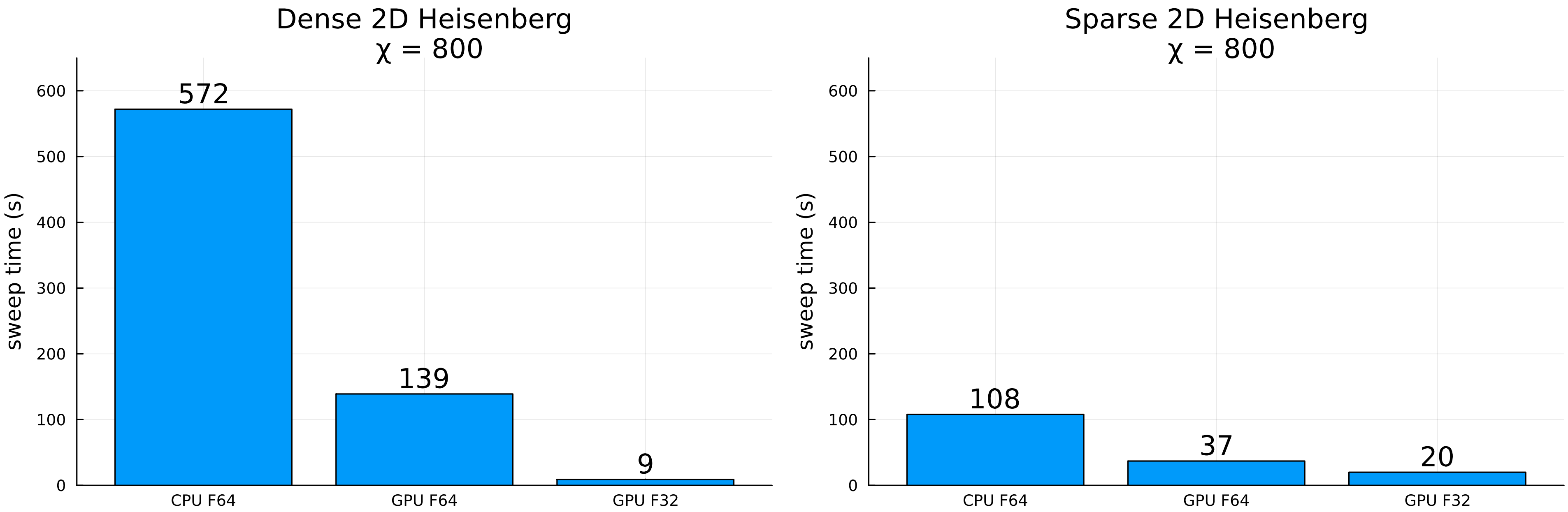
DMRG Timing: 2D Heisenberg



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