Benchmarking GPU Clusters with the Jülich Universal Quantum Computer Simulator

GTC21 | APRIL 14 I DR. DENNIS WILLSCH

JÜLICH Forschungszentrum
JÜLICH SUPERCOMPUTING CENTRE

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JÜLICH SUPERCOMPUTING CENTRE

Dr. Dennis Willsch

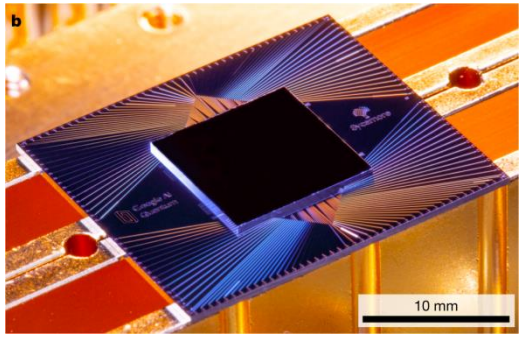
Prof. Dr. Hans De Raedt

Prof. Dr. Kristel Michielsen

QUANTUM COMPUTING

Ideal gate-based quantum computing

- What does a (gate-based) quantum computer do?



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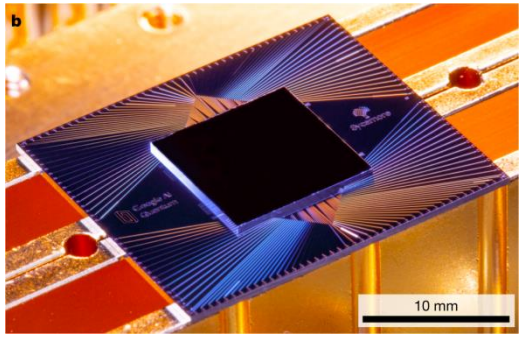

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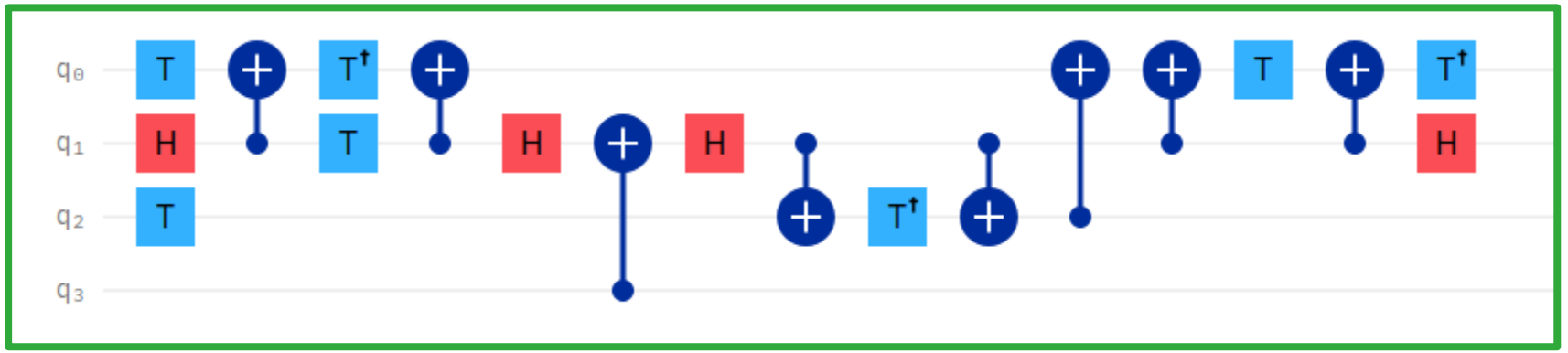

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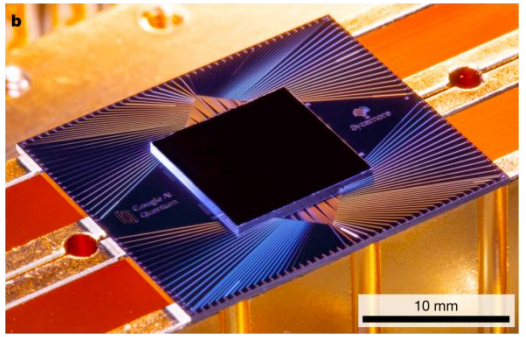

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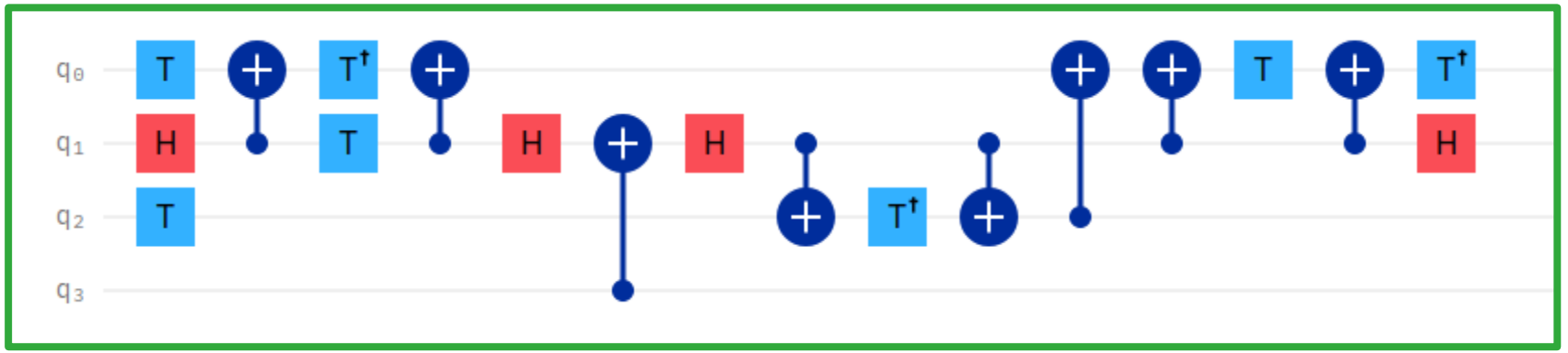

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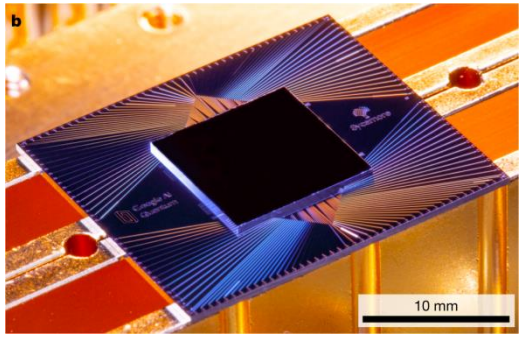

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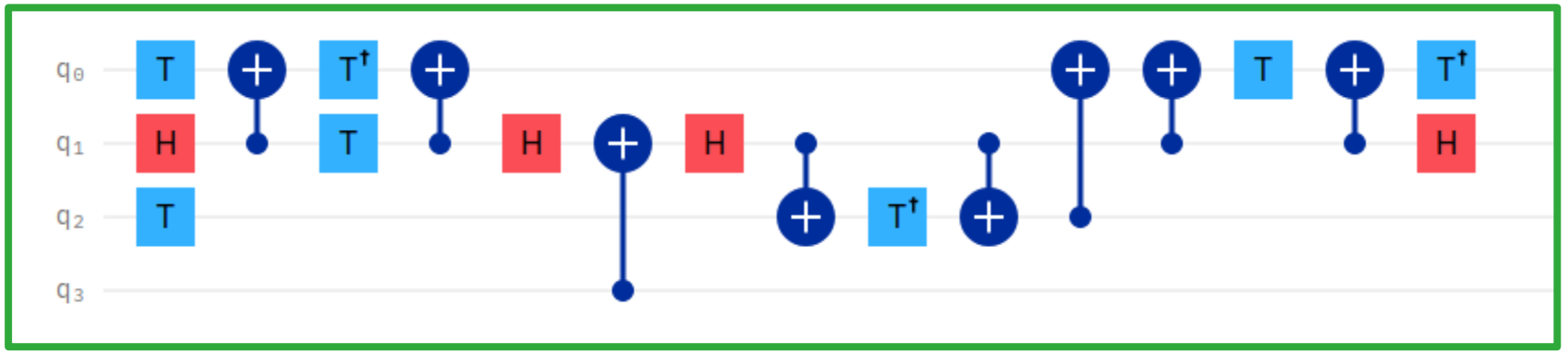

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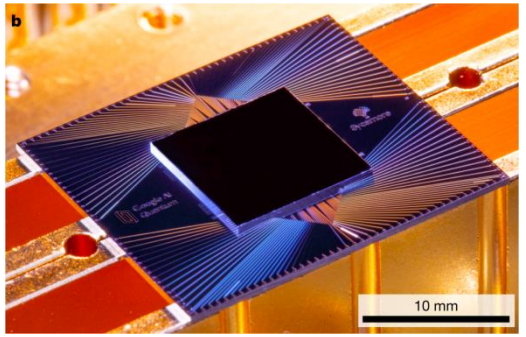

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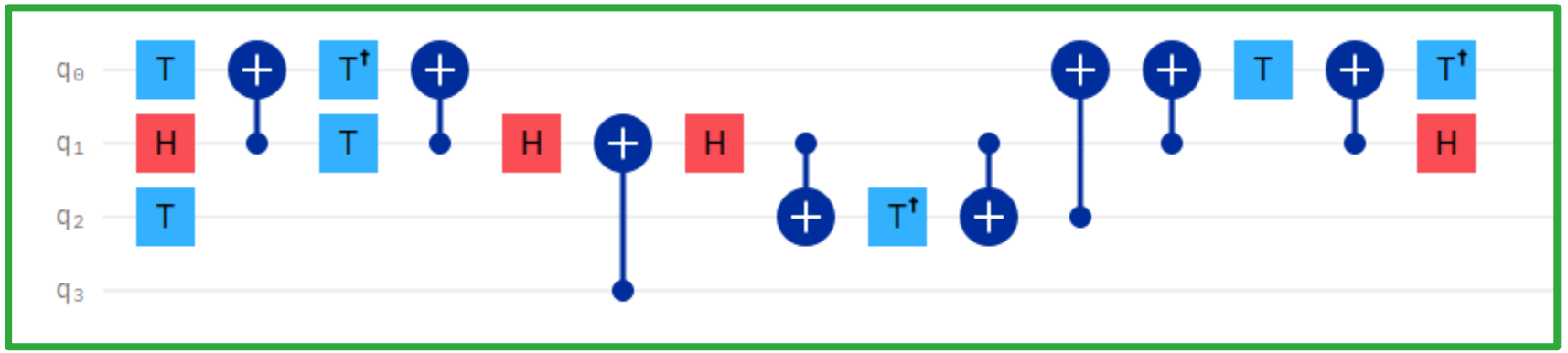

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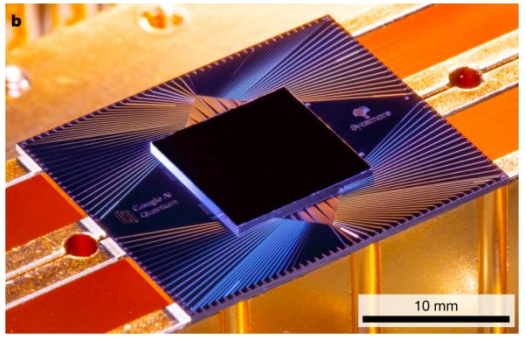

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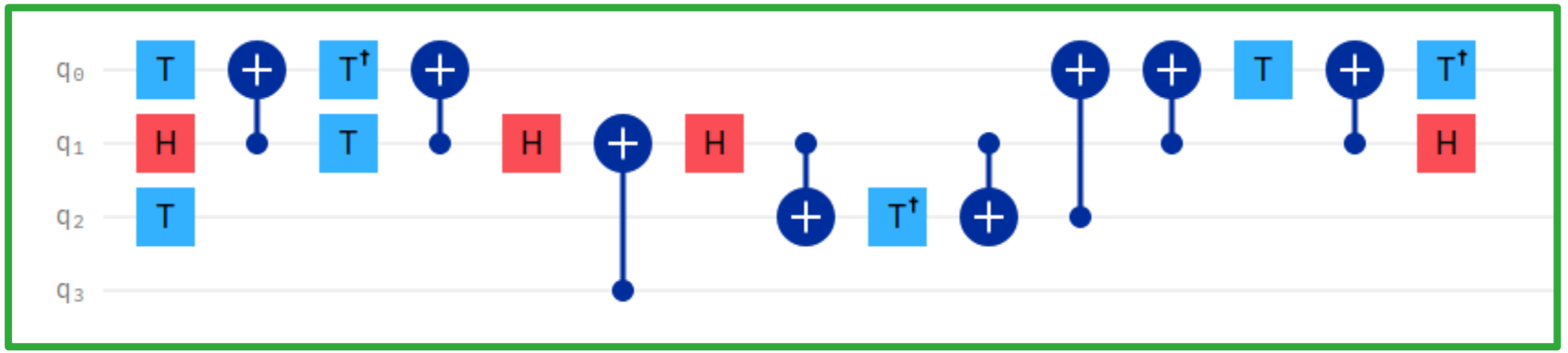

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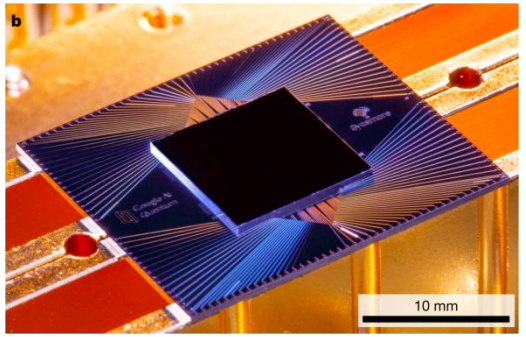

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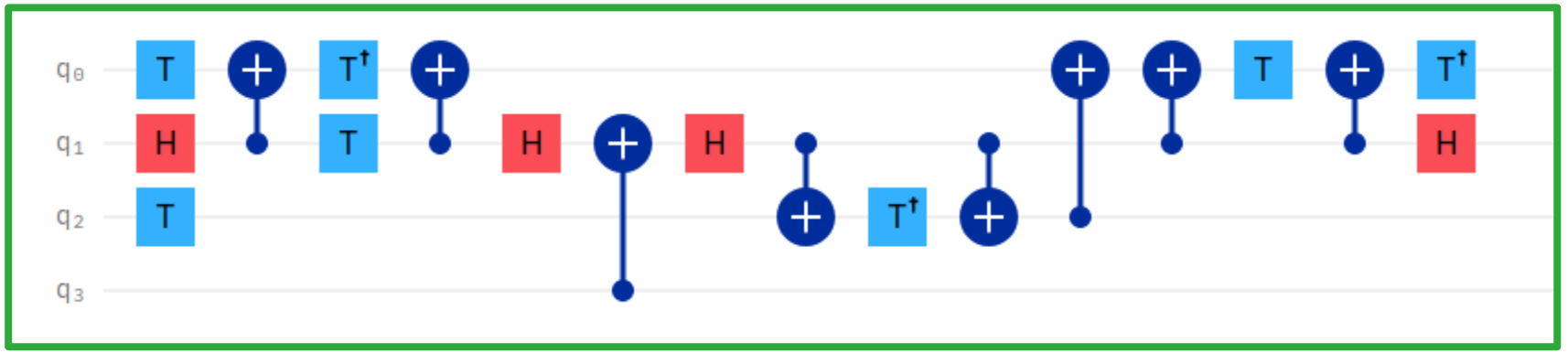

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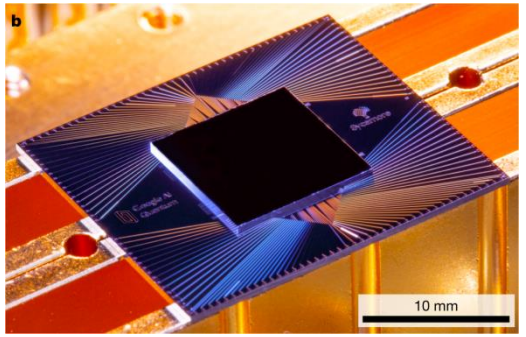

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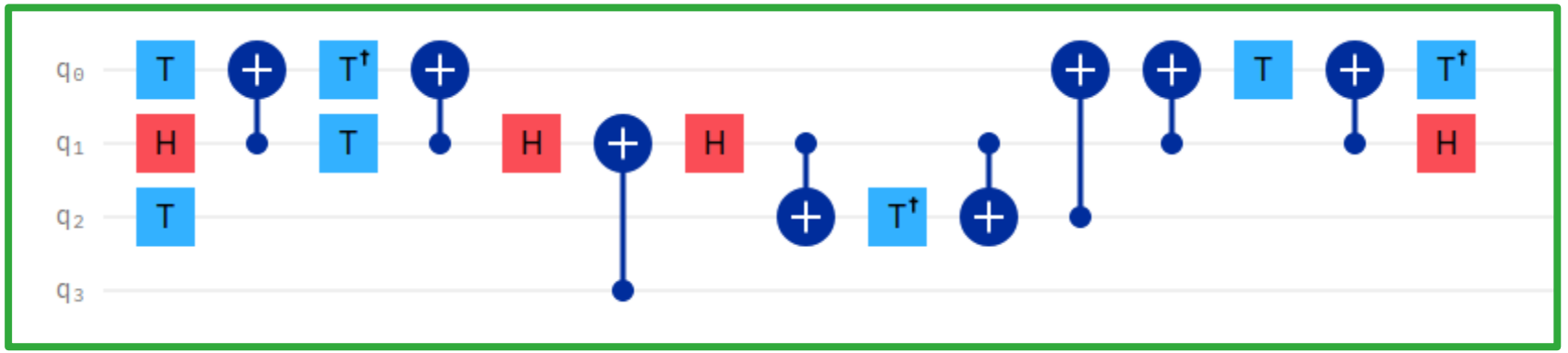

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  - It performs **matrix-vector multiplications** that are

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  - with **huge** vectors and **huge²** matrices

QUANTUM COMPUTING

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- What kind of sparse, unitary **matrix-vector multiplications**, precisely?

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vector = state of the QC = 2^n complex numbers

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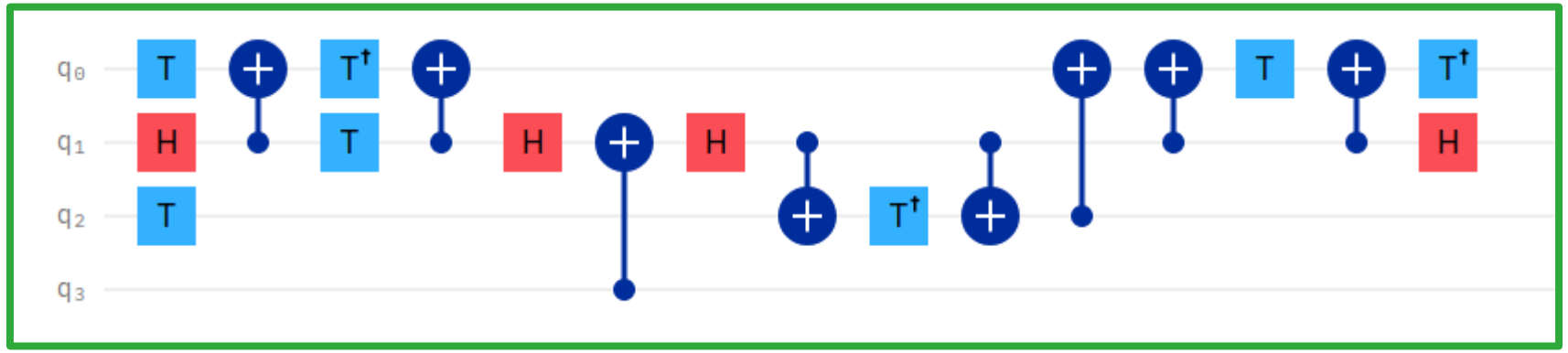

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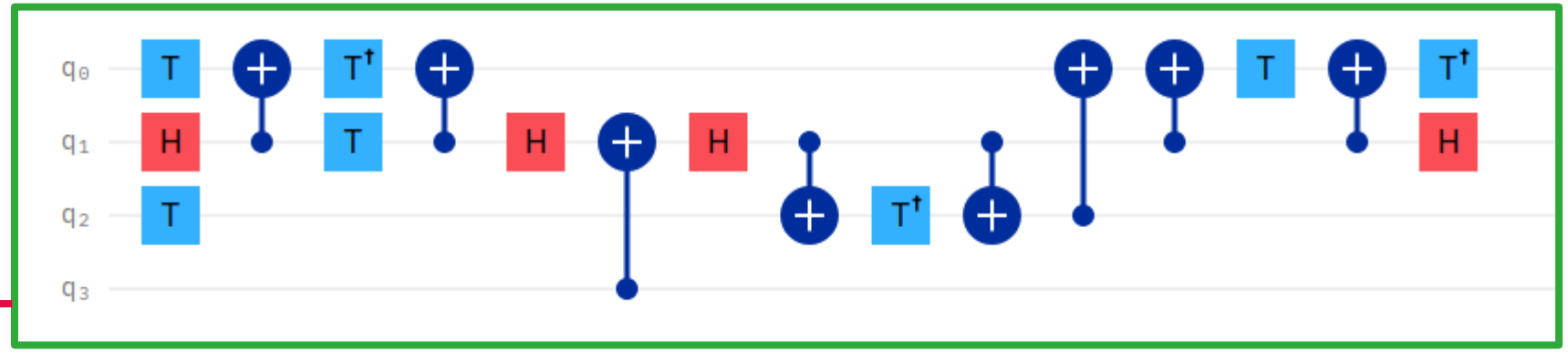

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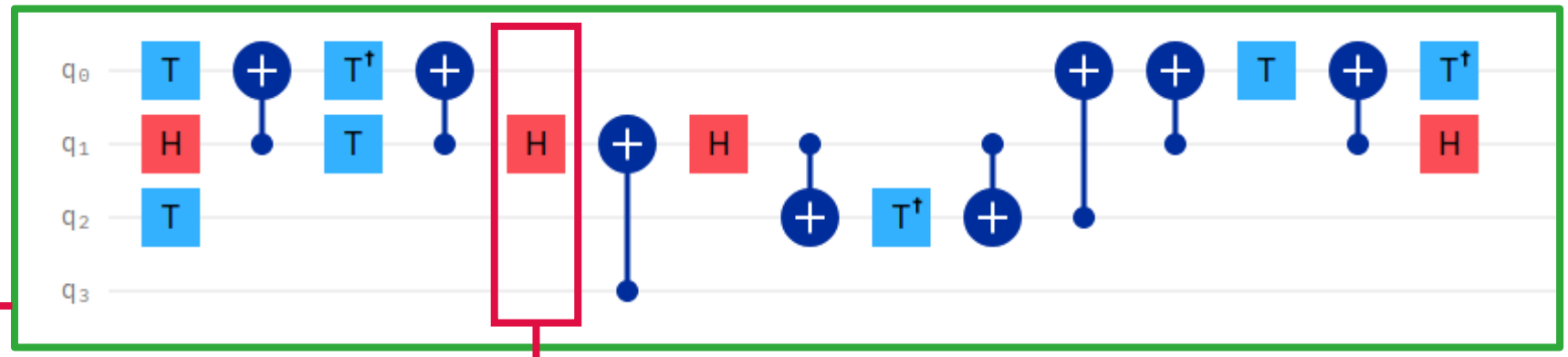

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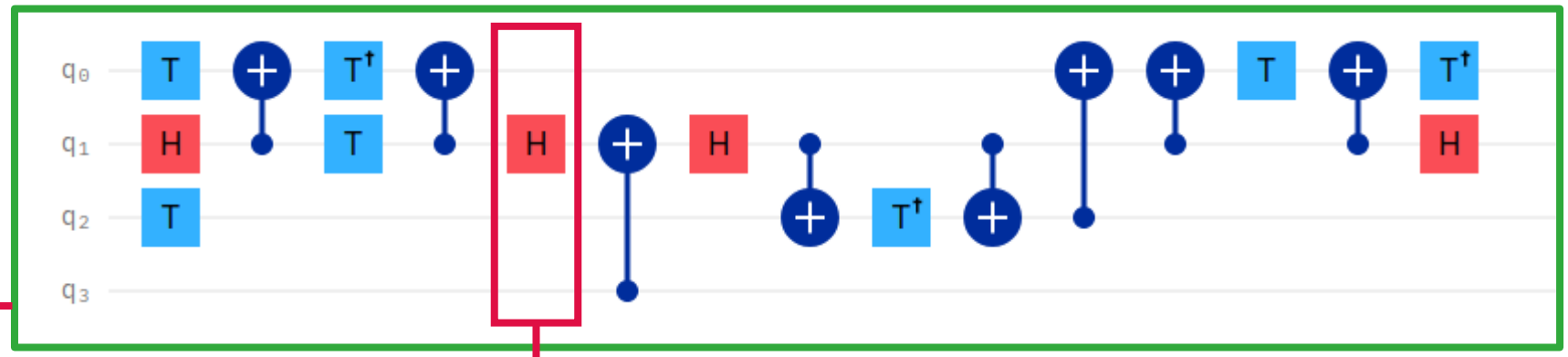

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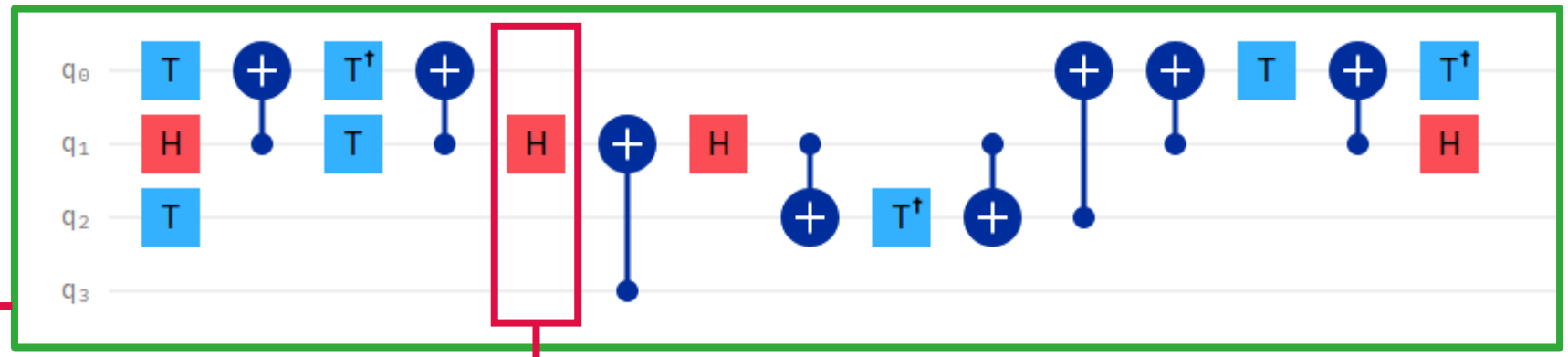

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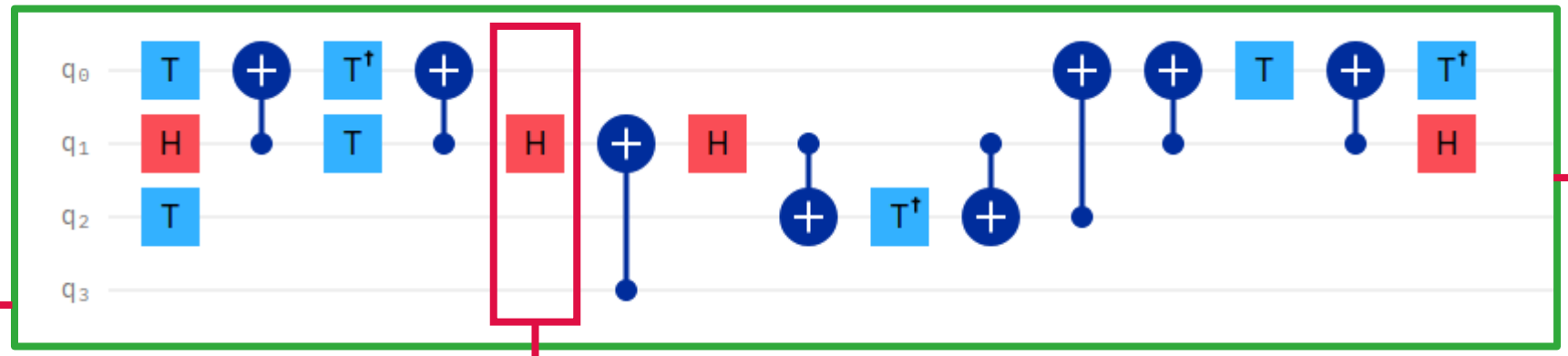

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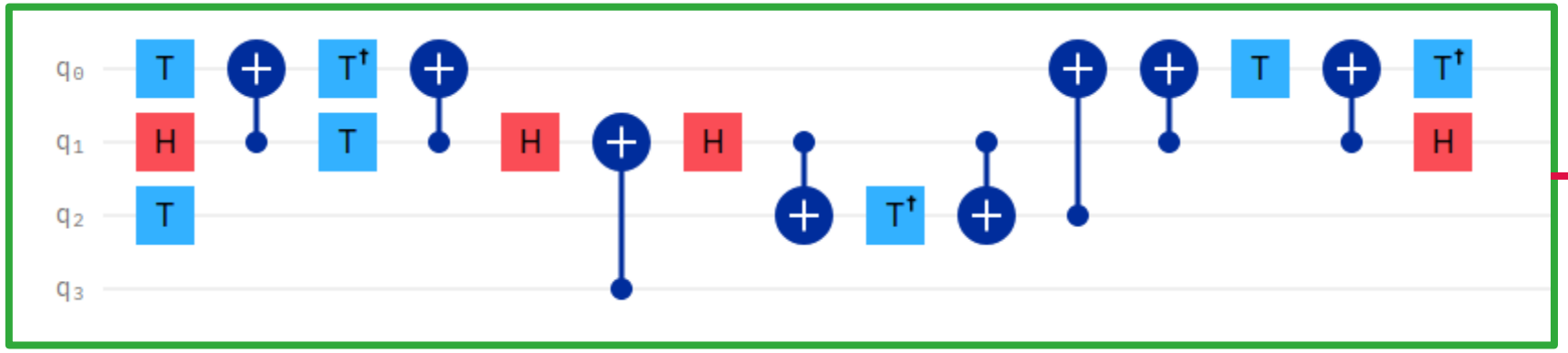

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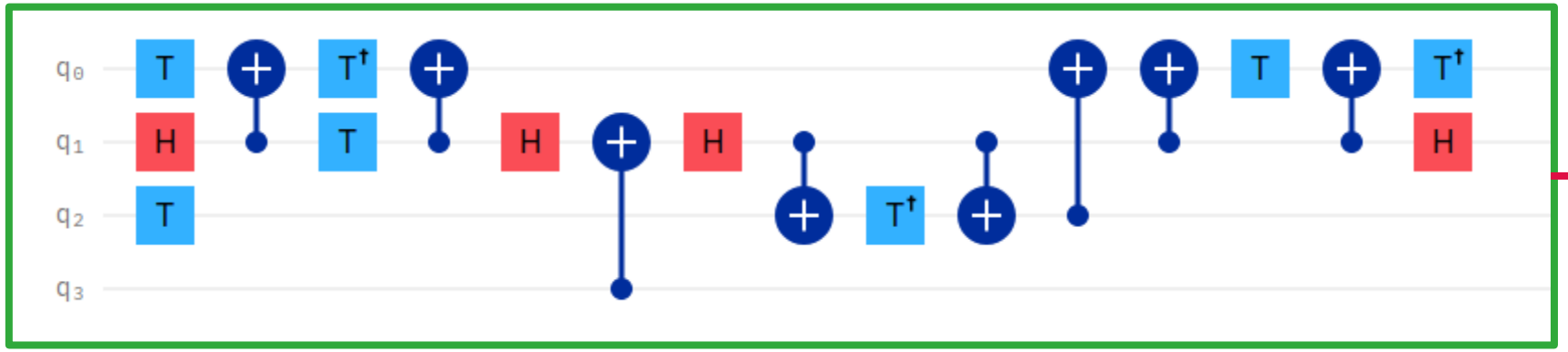

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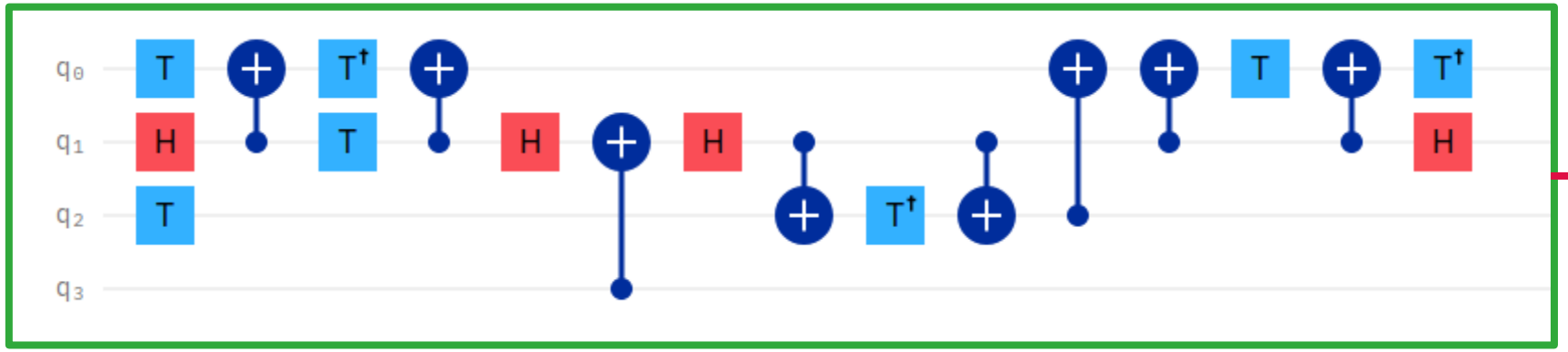

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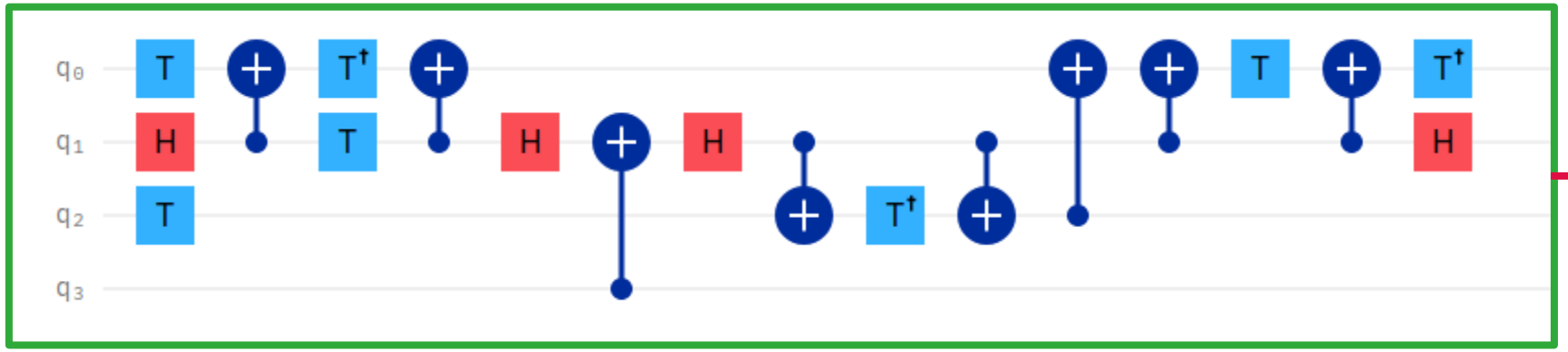

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For 40 qubits: 2^{40} ψ's = 16 TiB complex numbers

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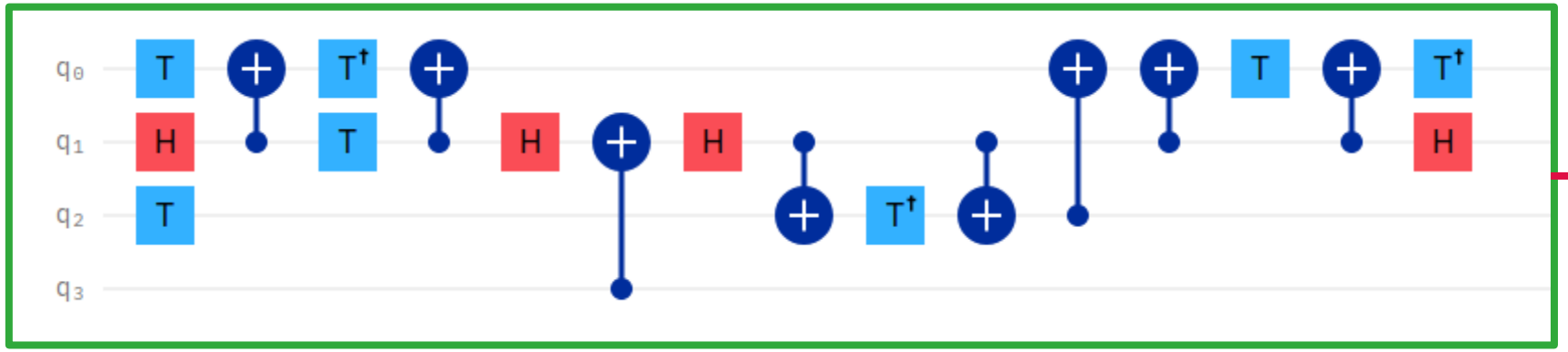

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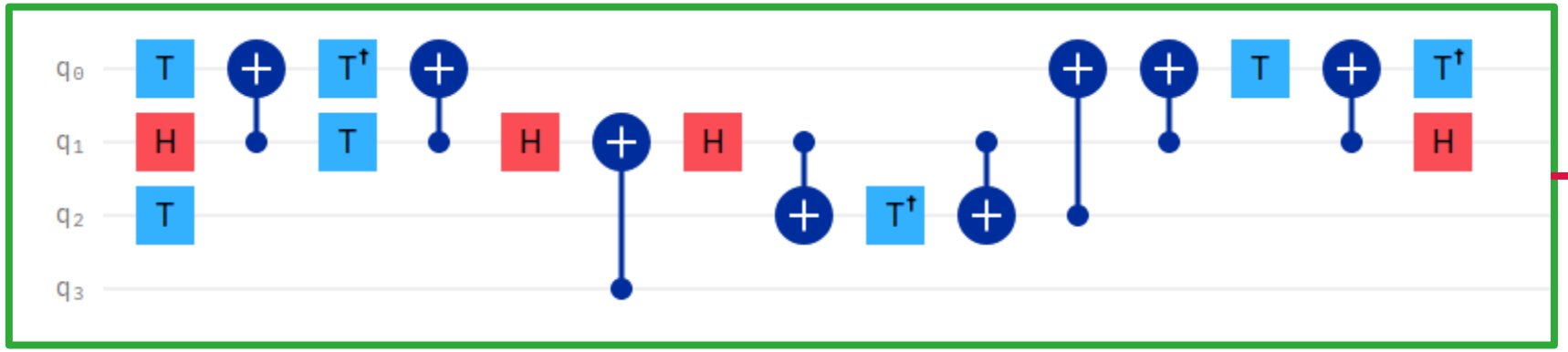

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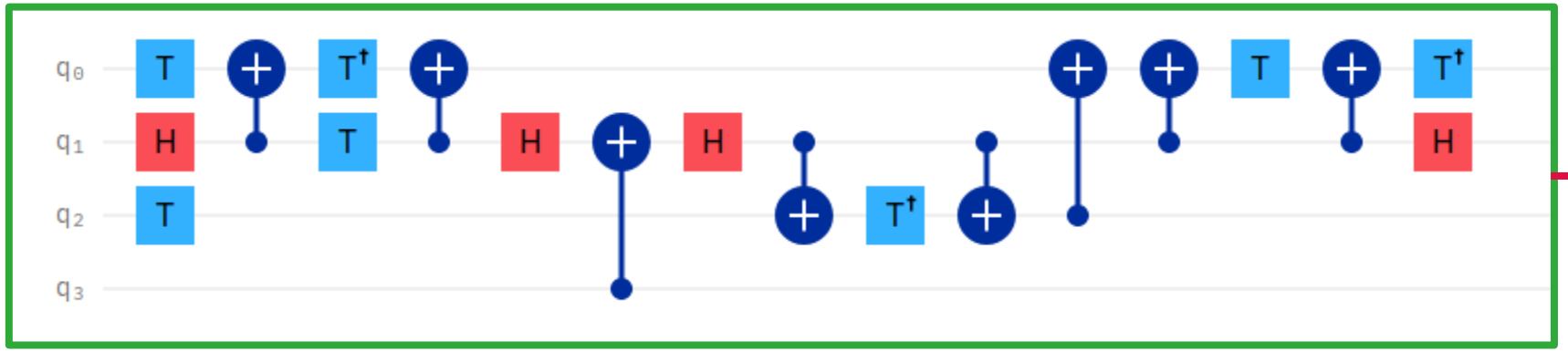

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  - Need to run circuit repeatedly to **sample** from the distribution

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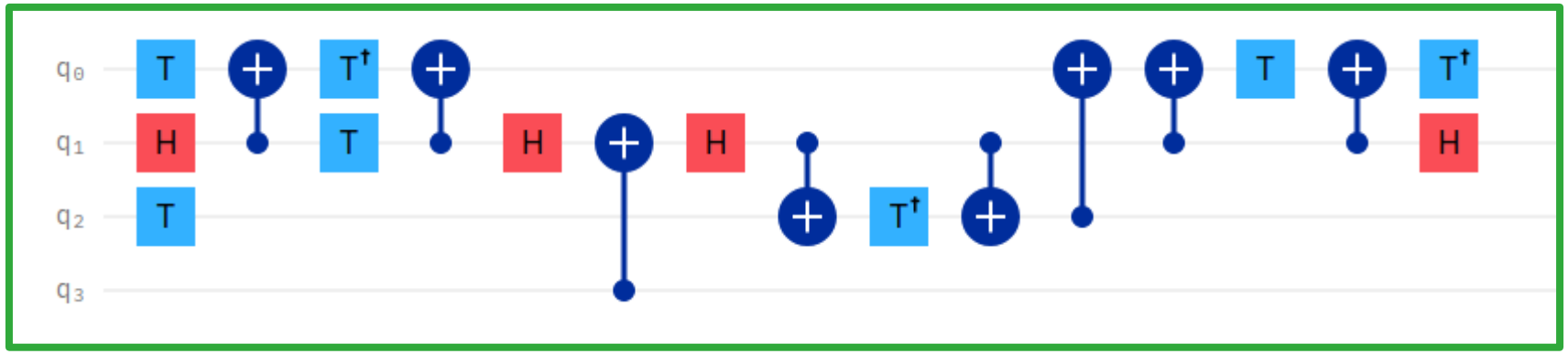

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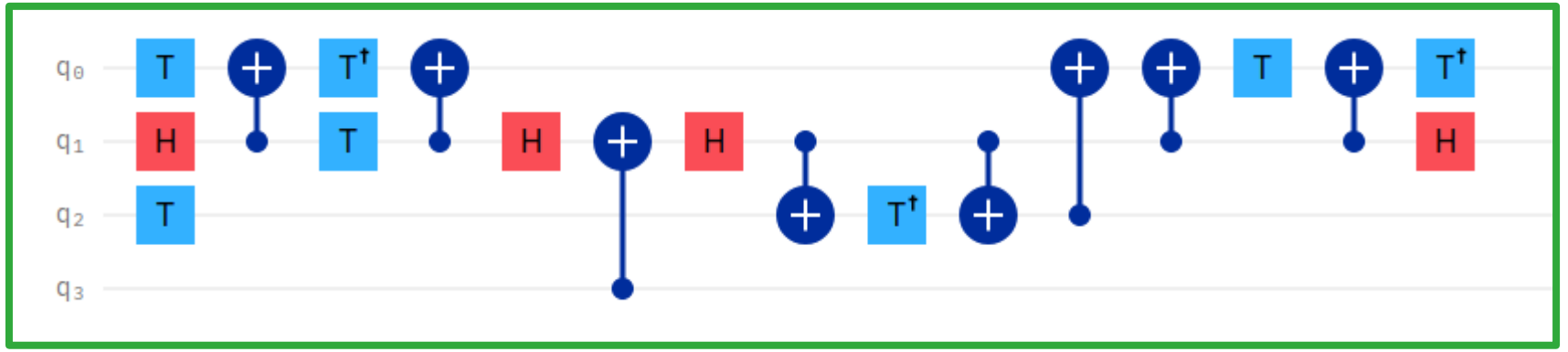

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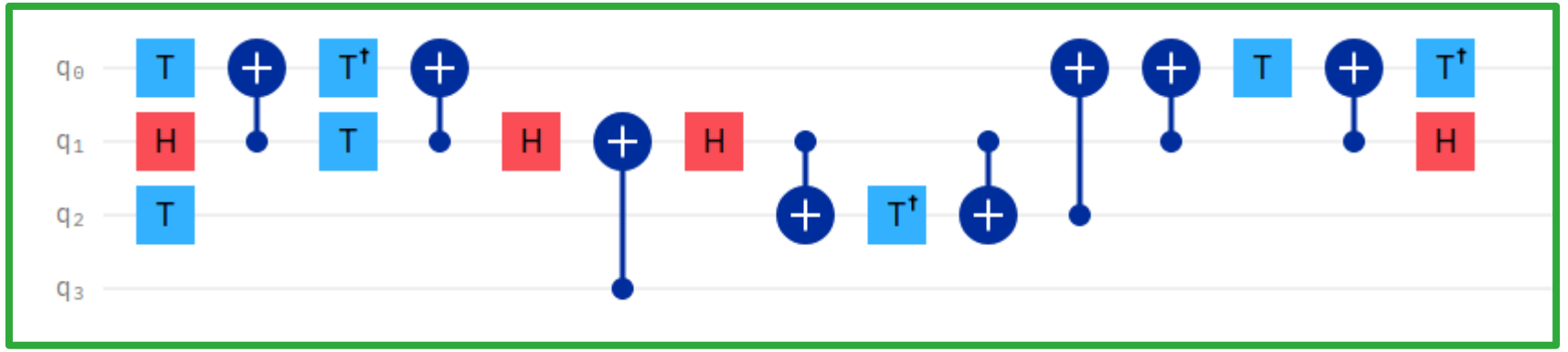

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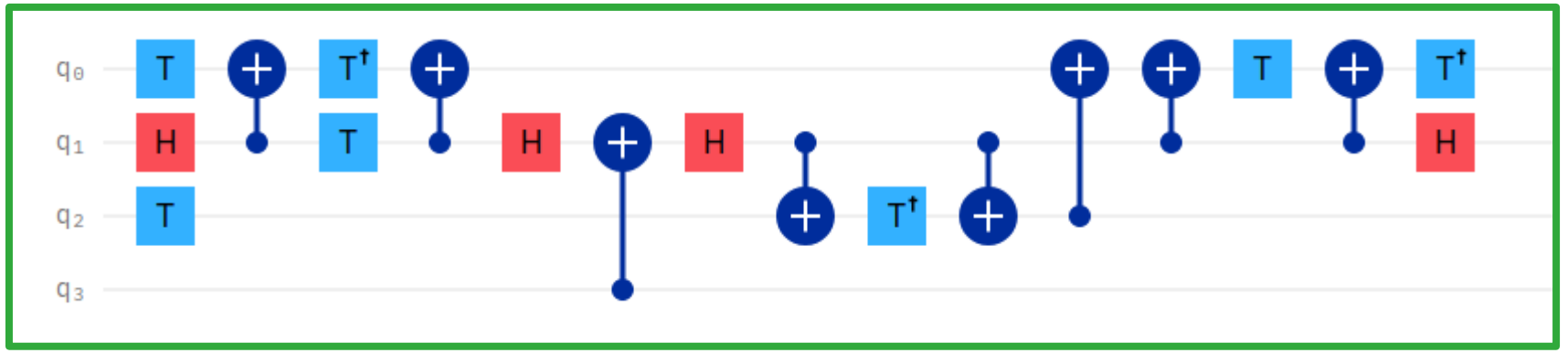

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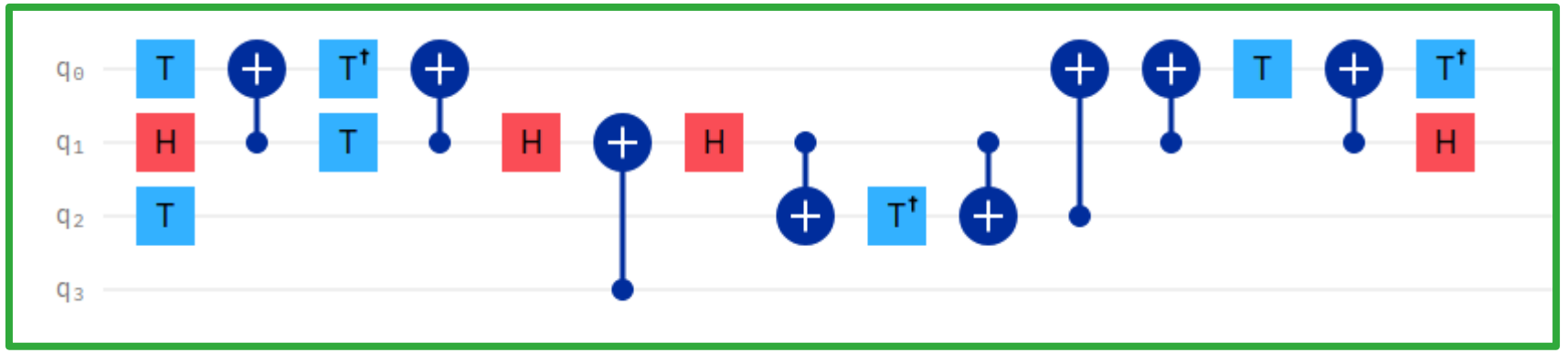
  - but also **superpositions**:

QUANTUM COMPUTING

Ideal gate-based quantum computing

- In particular, what does **this quantum circuit** do?



- 2-qubit adder

$$|q_3 q_2\rangle|q_1 q_0\rangle \mapsto |q_3 q_2\rangle|q_3 q_2 + q_1 q_0\rangle$$

  - e.g. $|2\rangle|1\rangle \mapsto |2\rangle|3\rangle$
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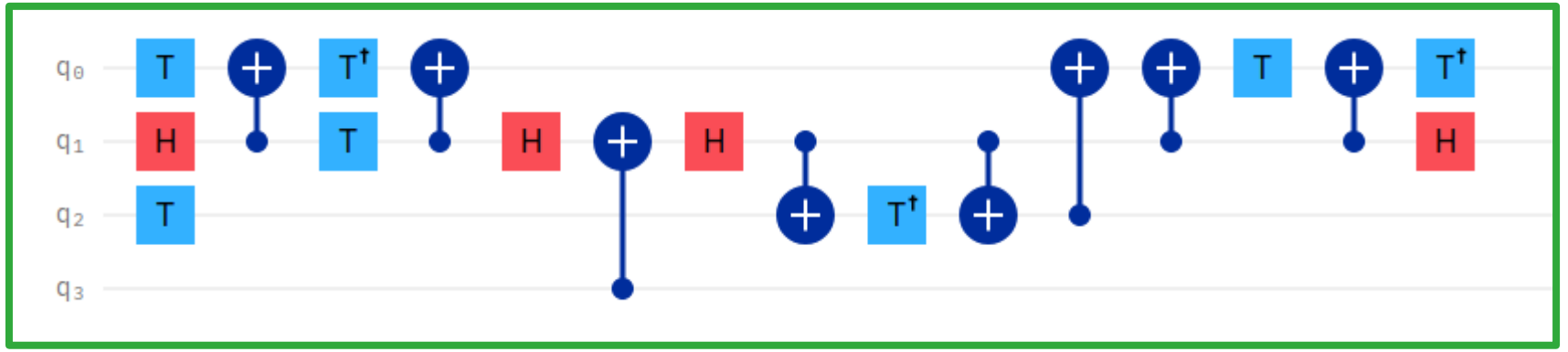

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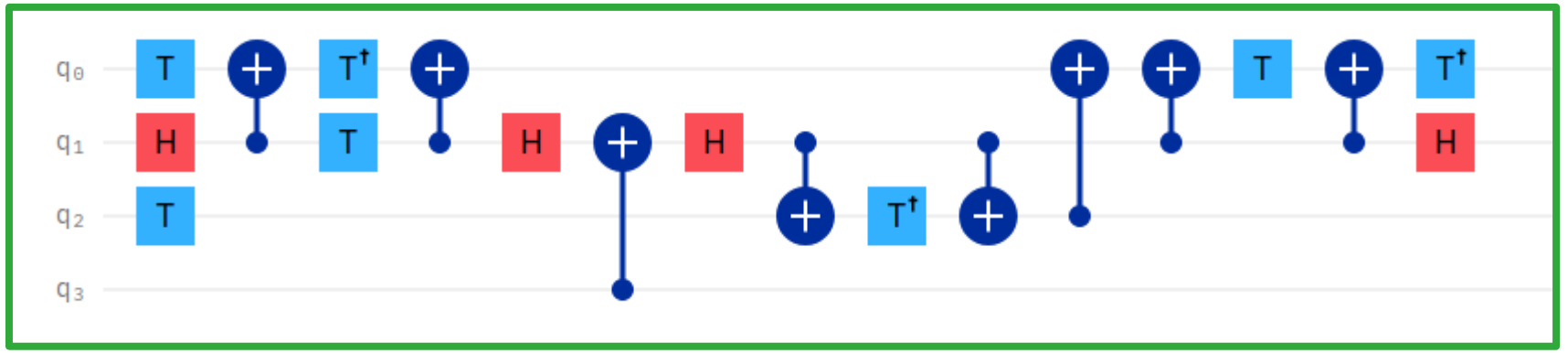

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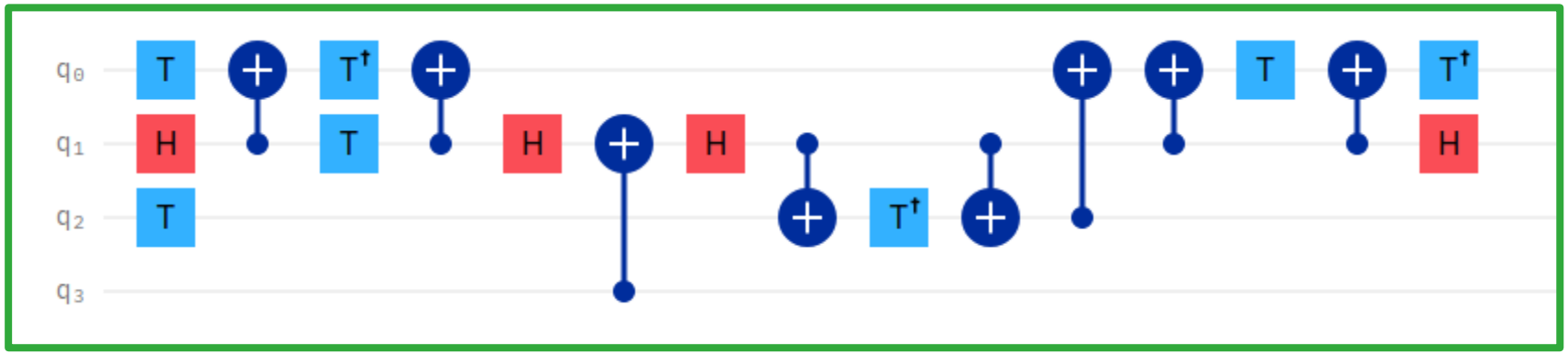
- Why? → Simulate with JUQCS

JUQCS

Jülich universal quantum computer simulator

- What does a quantum computer **simulator** do?
  - It runs a quantum circuit



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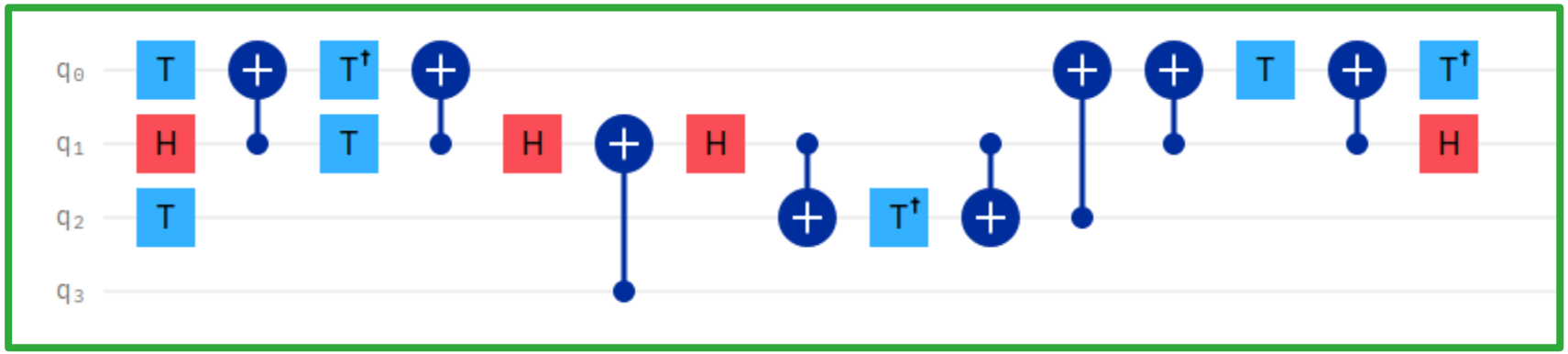

- What does this mean, actually?
  - It performs **matrix-vector multiplications** that are

sparse **complex** **unitary**

  - with **huge** vectors and **huge²** matrices

JUQCS

Distribution of the quantum state

How does the simulator manage all these complex numbers?

JUQCS

Distribution of the quantum state

How does the simulator manage all these complex numbers?

→ Distribute quantum state $|\psi\rangle = (\psi_{\ldots q_2 q_1 q_0})$ over multiple compute nodes

JUQCS

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For 40 qubits: 2^{40} $\psi'\mathrm{s}$ = 16 TiB complex numbers = 64 GiB per node with 256 nodes

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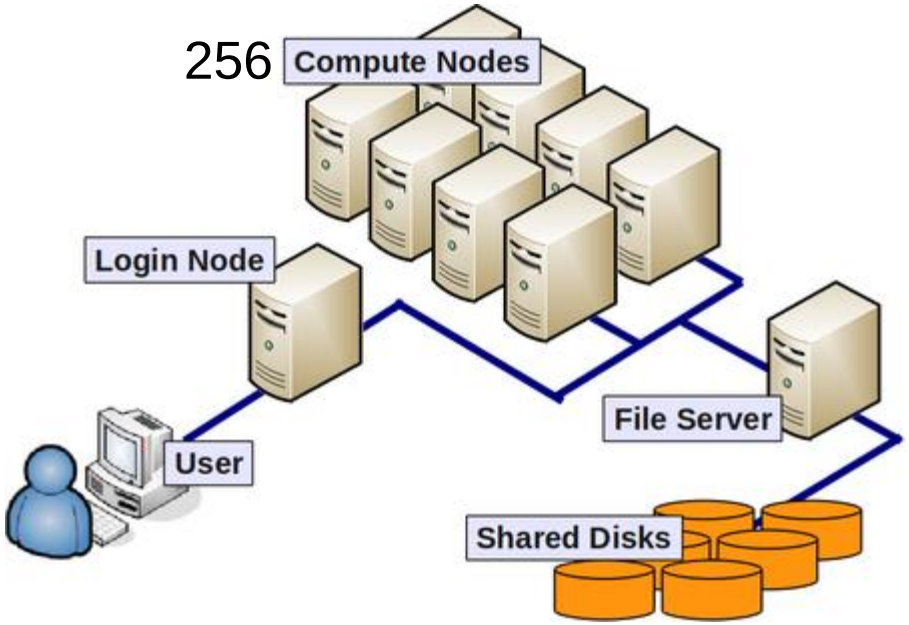

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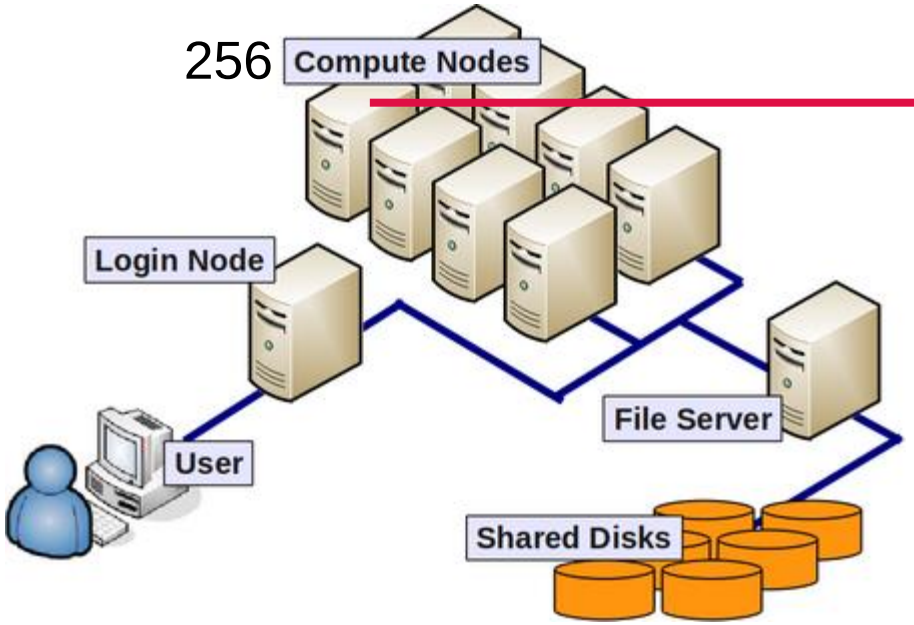

MPI rank 0 = 0b00000000:

$$\begin{pmatrix} \psi_{00000000\ 0\cdots0} \\ \vdots \\ \psi_{00000000\ 1\cdots1} \end{pmatrix}$$

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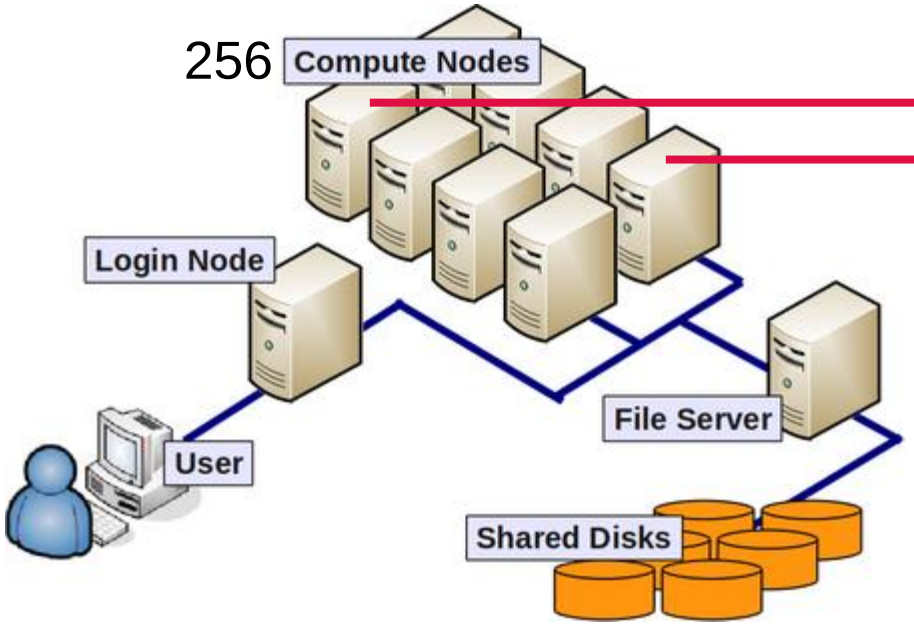

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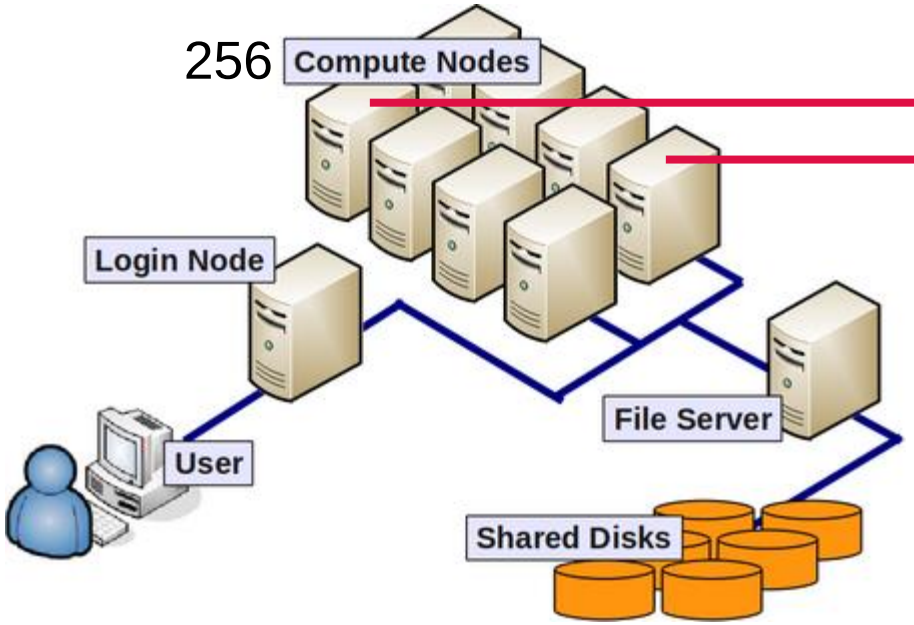

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8 **global** qubits

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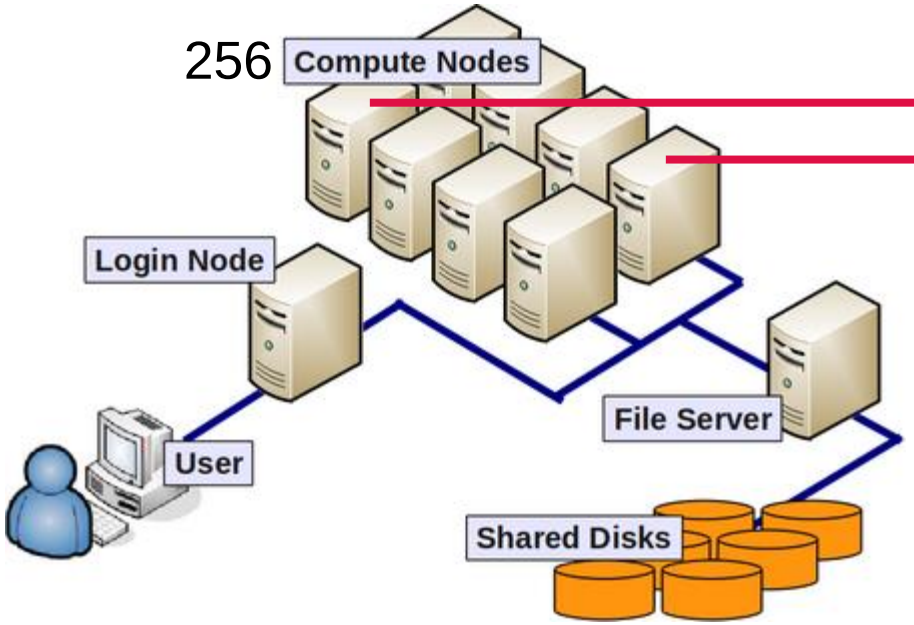

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8 **global** qubits
32 **local** qubits

JUQCS-G

Simulating quantum computers on GPUs CUDA MPI Fortran

- Distribute quantum state on GPUs (NVIDIA A100: 40GB per GPU)

  For 40 qubits: $2^{40}\ \psi's$ = 16 TiB complex numbers = 16 GiB per GPU with 4*256 GPUs

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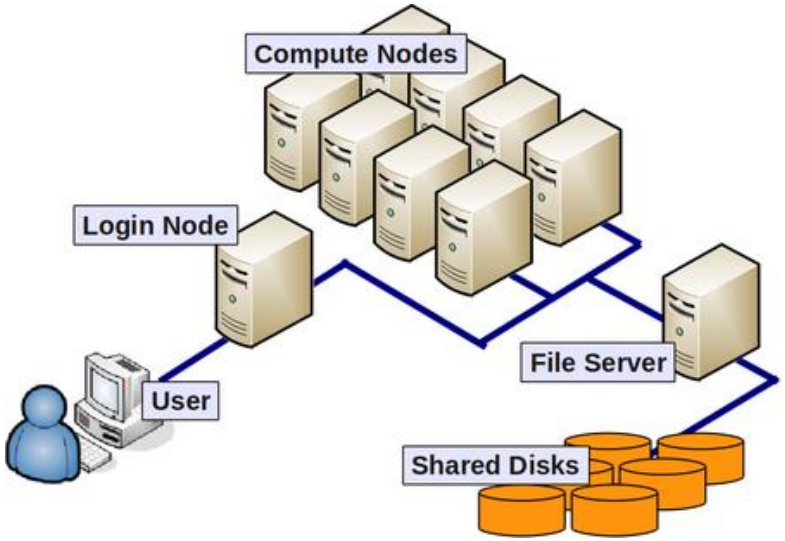

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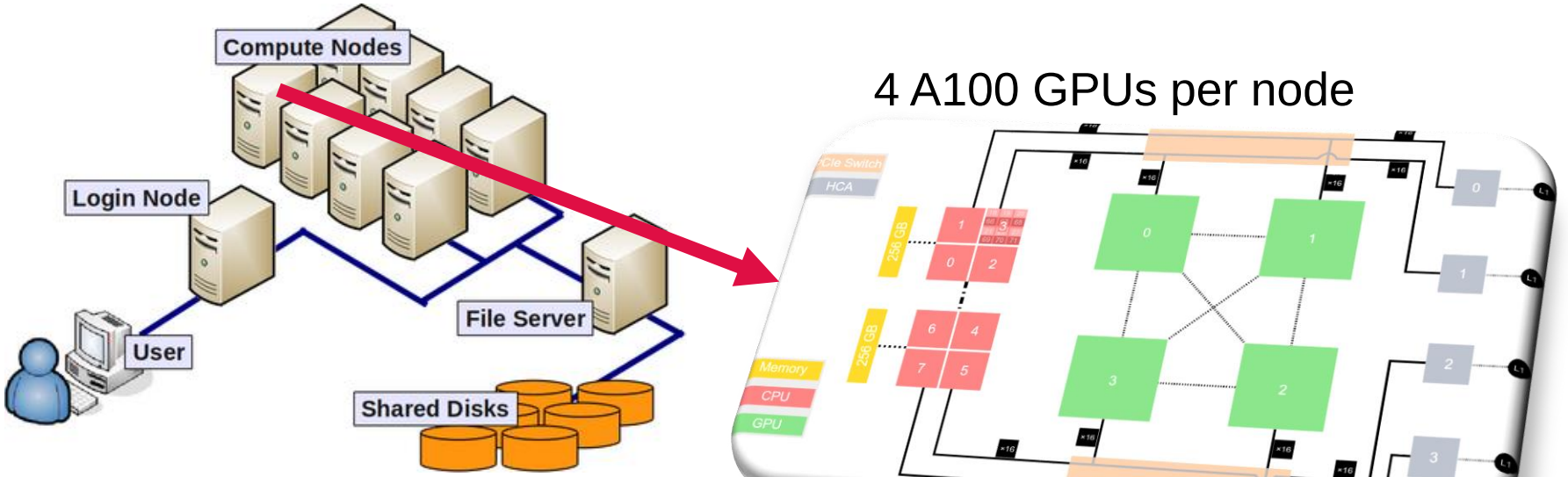

4 A100 GPUs per node

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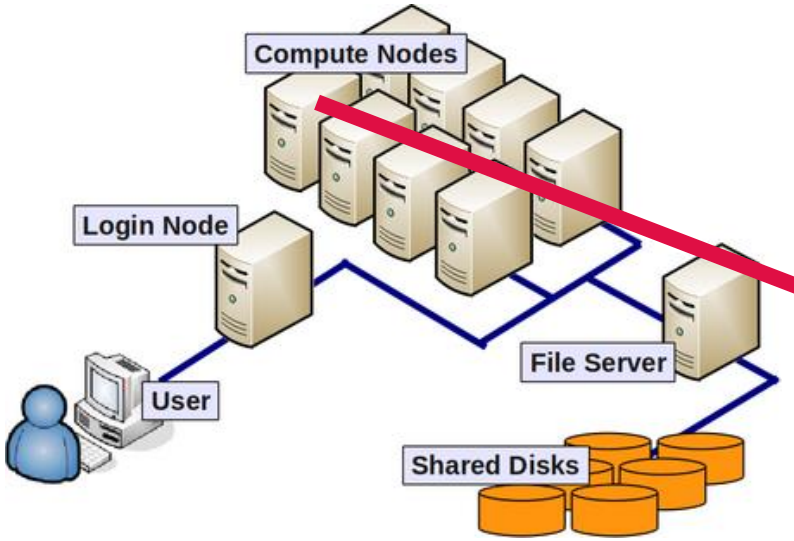

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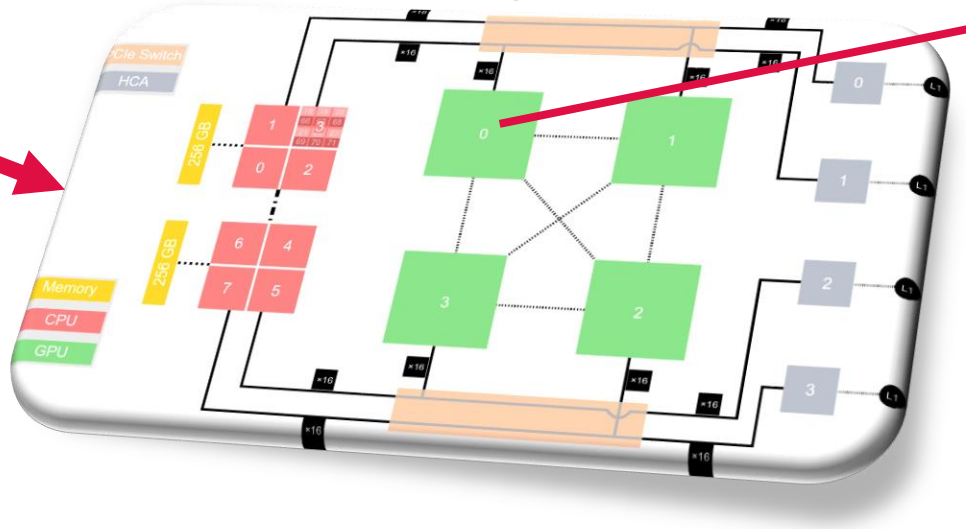

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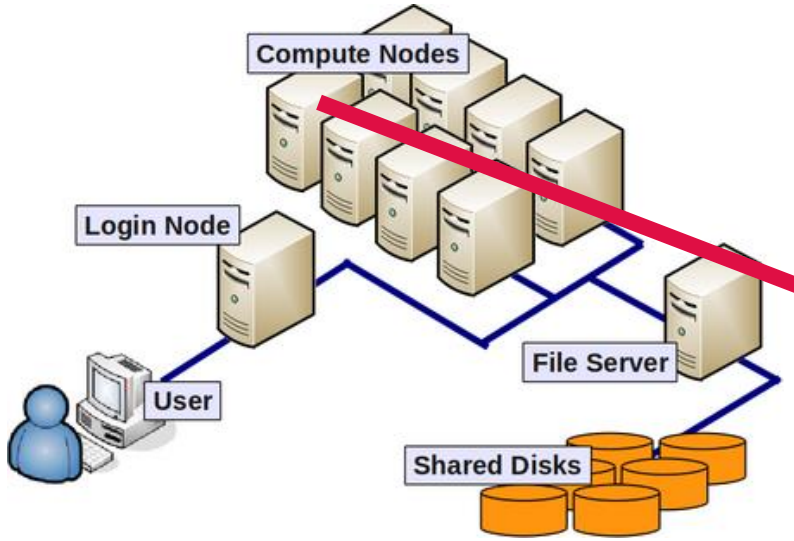

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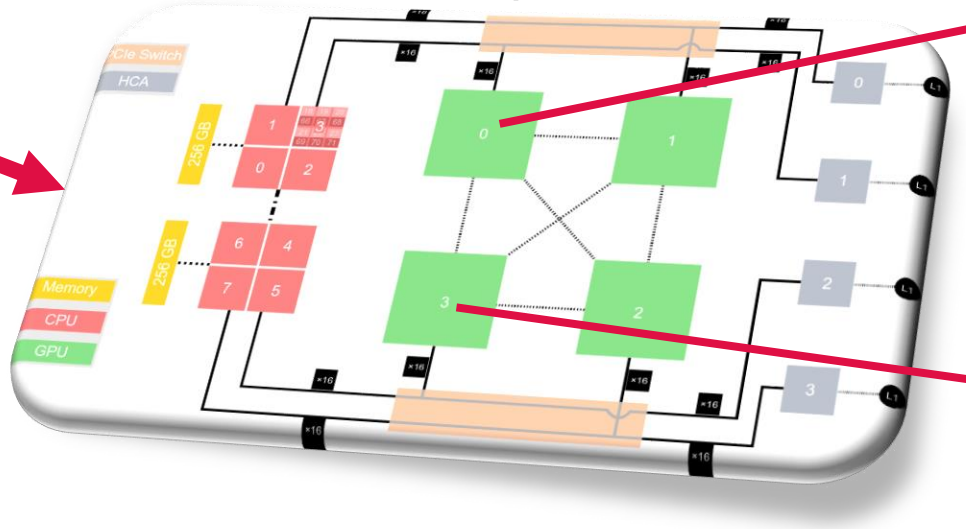

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GPU rank 3 = 0b0000000011:

$$\begin{pmatrix} \psi_{0000000011\,0\cdots0} \\ \vdots \\ \psi_{0000000011\,1\cdots1} \end{pmatrix}$$

JUQCS-G

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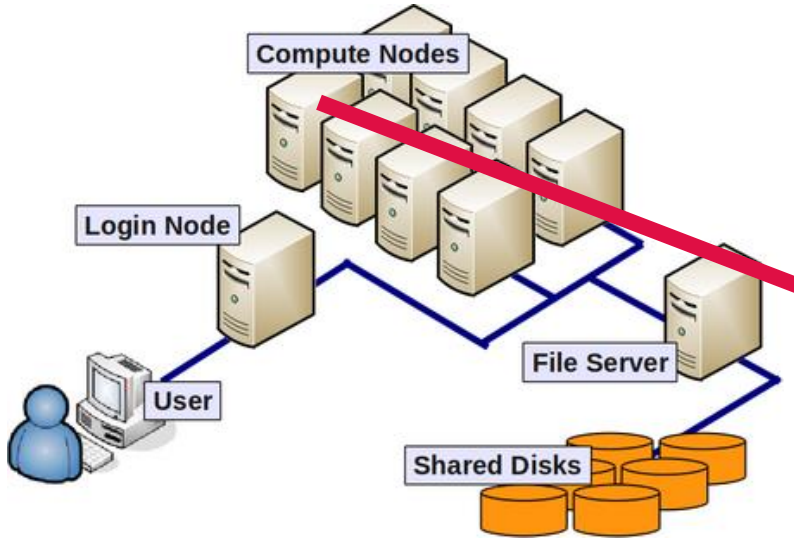

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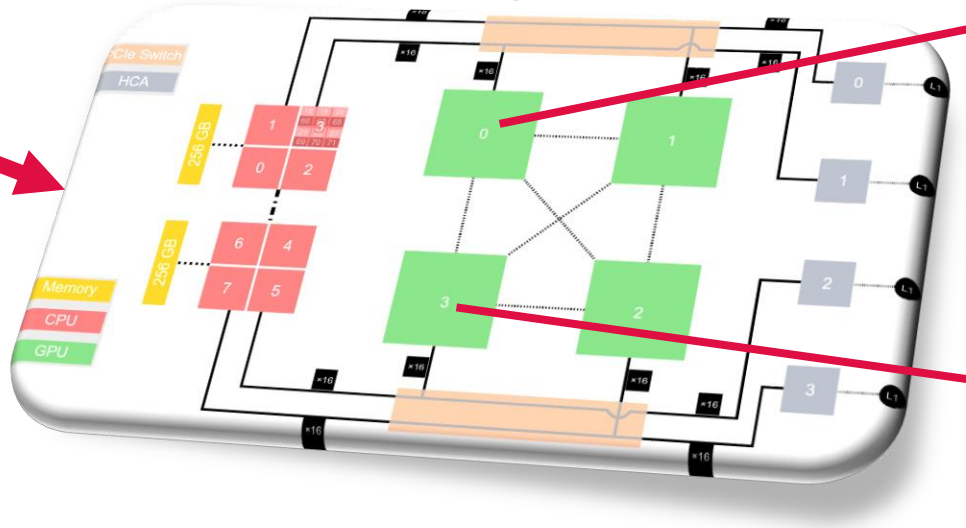

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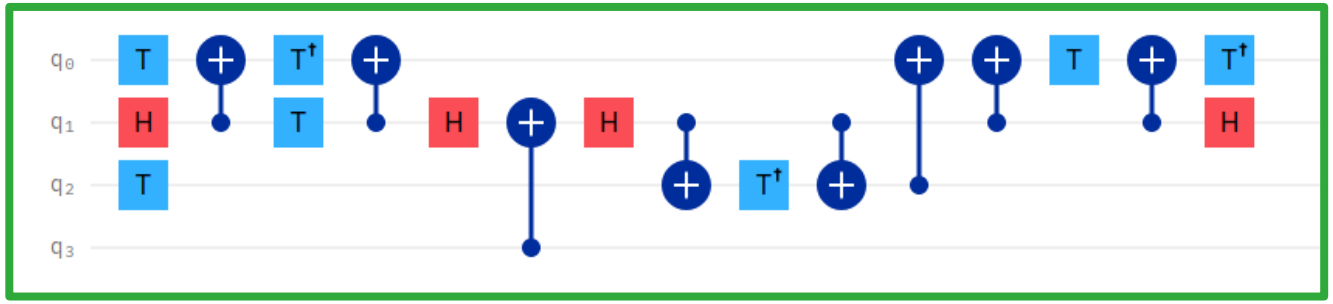
GPU rank 3 = 0b0000000011:

$$\begin{pmatrix} \psi_{0000000011\,0\cdots0} \\ \vdots \\ \psi_{0000000011\,1\cdots1} \end{pmatrix}$$

- The MPI communication scheme is the same

JUQCS-G

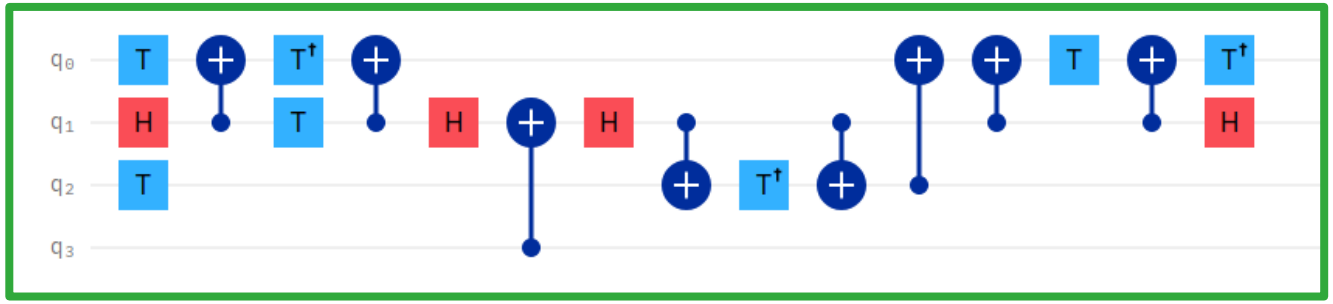
CUDA implementation



How to implement these **matrix-vector multiplications** in the most efficient way?

JUQCS-G

CUDA implementation



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JUQCS-G

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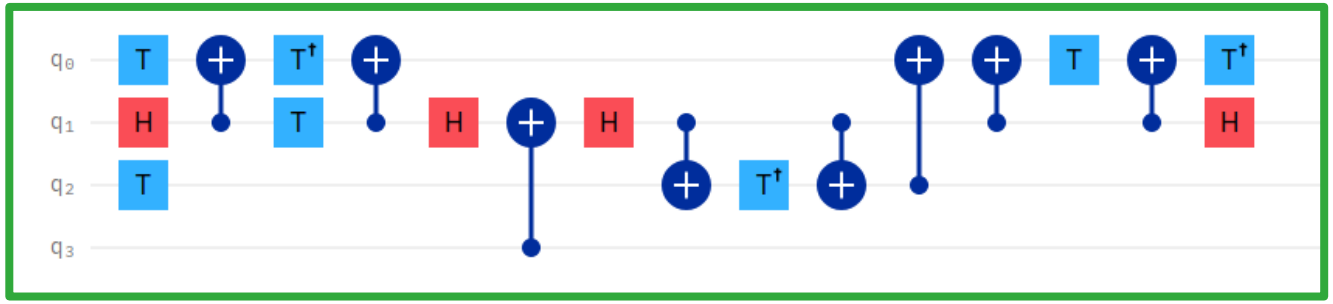

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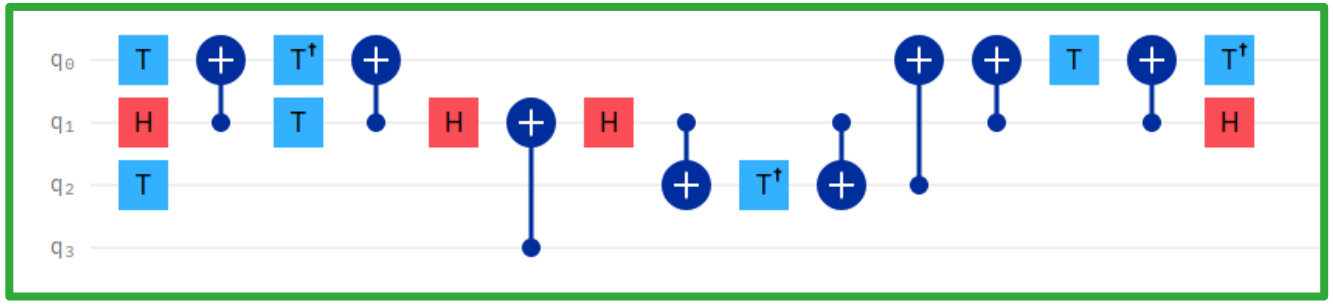
GPU rank 0

JUQCS-G

CUDA implementation



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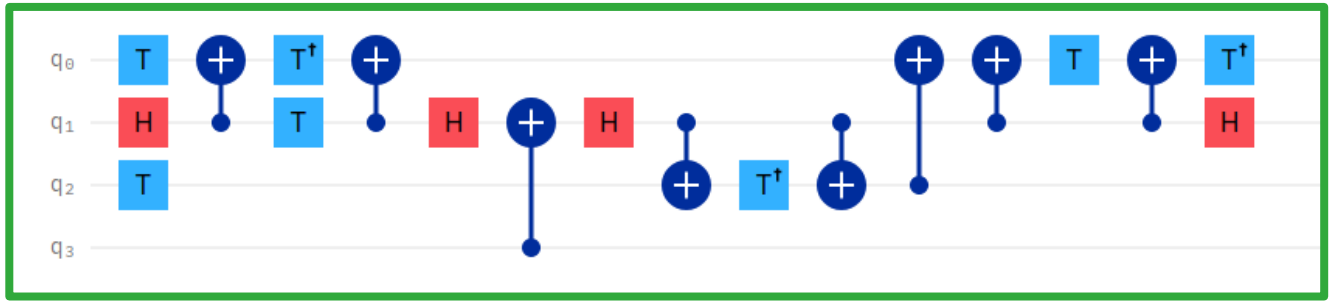

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Full quantum state:

$\psi_{00000000\,0\cdots0}$

GPU rank 0

$\psi_{00000000\,1\cdots1}$

$\psi_{00000001\,0\cdots0}$

GPU rank 1

$\psi_{00000001\,1\cdots1}$

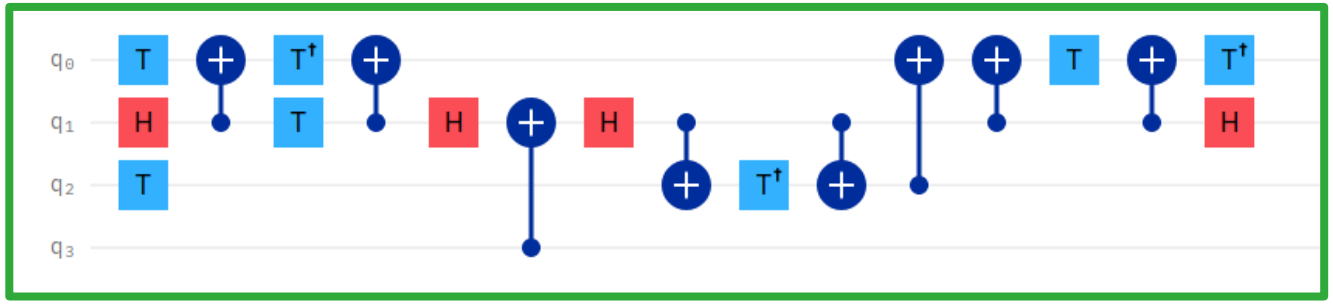
$\psi_{11111111\,0\cdots0}$

GPU rank 255

$\psi_{11111111\,1\cdots1}$

JUQCS-G

CUDA implementation



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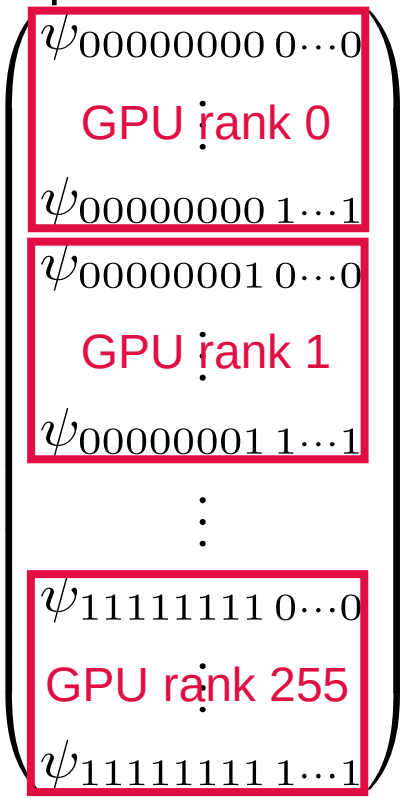
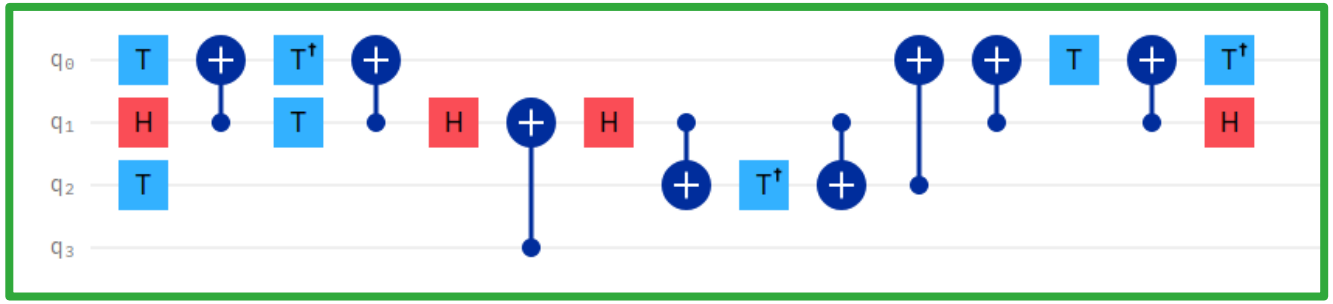


Quantum gate on **local** qubits:

JUQCS-G

CUDA implementation



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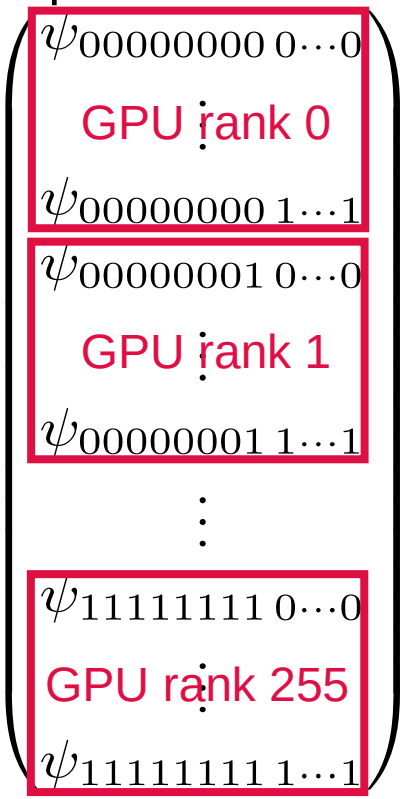

Quantum gate on **local** qubits:

e.g. H on qubit q_{30}

JUQCS-G

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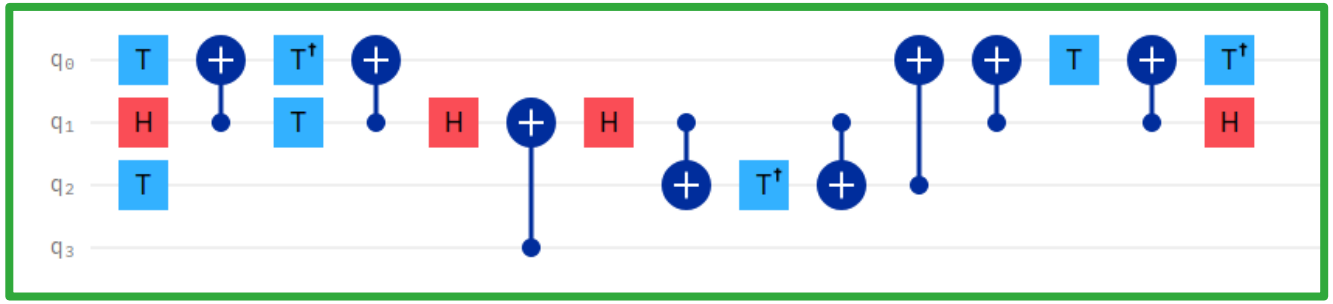

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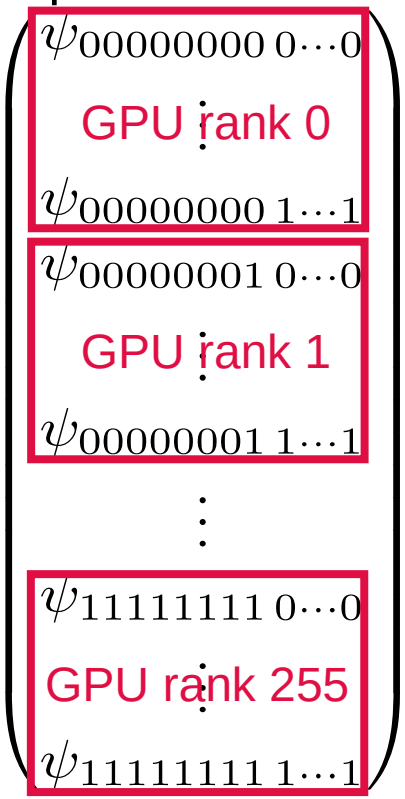

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→ Each MPI rank r performs local 2x2 updates of the form

JUQCS-G

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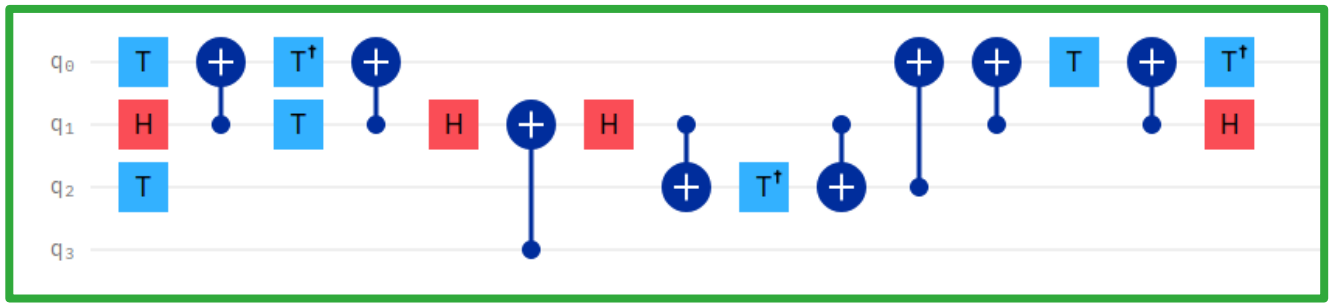

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$$\begin{pmatrix} \psi_{00000000\,0\cdots0} \\ \text{GPU rank 0} \\ \vdots \\ \psi_{00000000\,1\cdots1} \\ \psi_{00000001\,0\cdots0} \\ \text{GPU rank 1} \\ \vdots \\ \psi_{00000001\,1\cdots1} \\ \vdots \\ \psi_{11111111\,0\cdots0} \\ \text{GPU rank 255} \\ \vdots \\ \psi_{11111111\,1\cdots1} \end{pmatrix}$$

Quantum gate on **local** qubits:

e.g. H on qubit q_{30}

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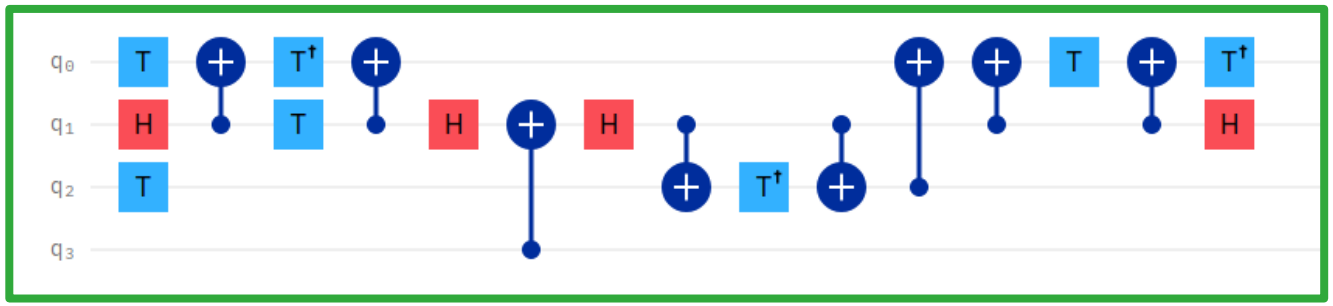
$$\begin{pmatrix} \psi_{rrrrrrrr\,*0*\cdots*} \\ \psi_{rrrrrrrr\,*1*\cdots*} \end{pmatrix} \leftarrow \mathrm{H} \begin{pmatrix} \psi_{rrrrrrrr\,*0*\cdots*} \\ \psi_{rrrrrrrr\,*1*\cdots*} \end{pmatrix}$$

JUQCS-G

CUDA implementation



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GPU rank 0

GPU rank 1

GPU rank 255

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$$\uparrow$$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

JUQCS-G

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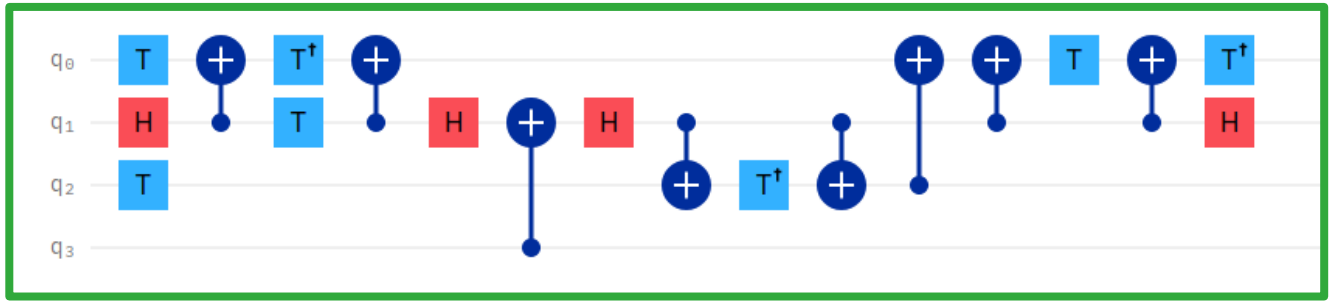

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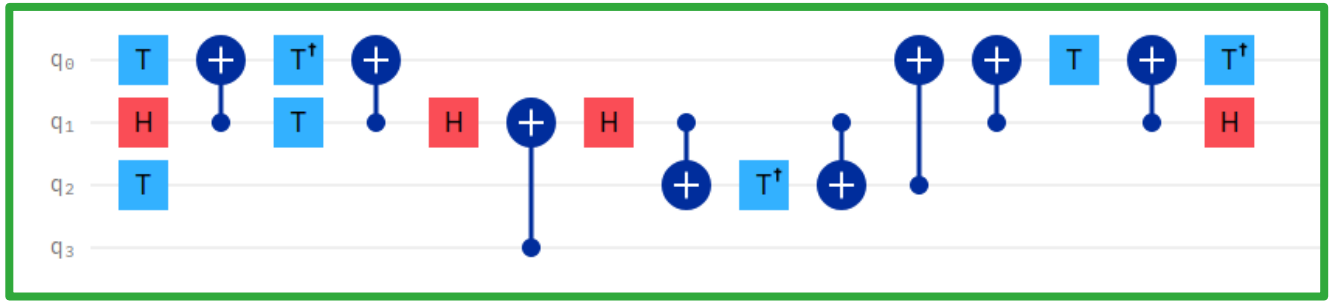
$$\begin{pmatrix} \psi_{rrrrrrrr\,*0*\cdots*} \\ \psi_{rrrrrrrr\,*1*\cdots*} \end{pmatrix} \leftarrow \boxed{\mathrm{H}} \begin{pmatrix} \psi_{rrrrrrrr\,*0*\cdots*} \\ \psi_{rrrrrrrr\,*1*\cdots*} \end{pmatrix}$$

$$\uparrow$$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

JUQCS-G

CUDA implementation



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JUQCS-G

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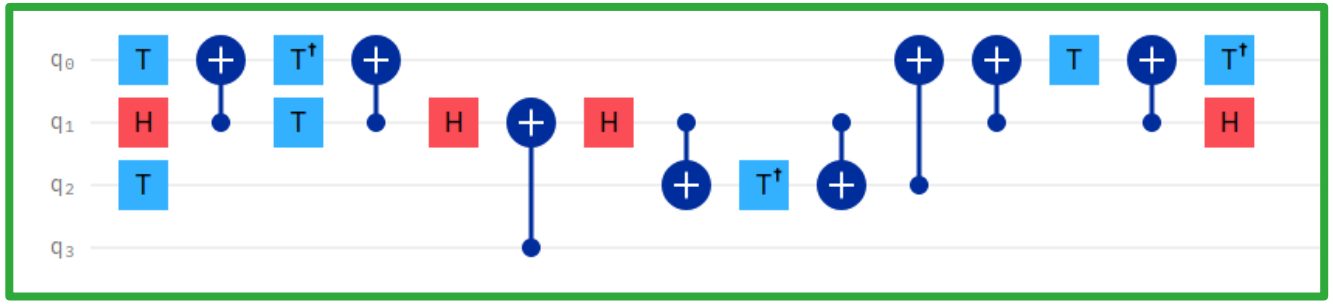

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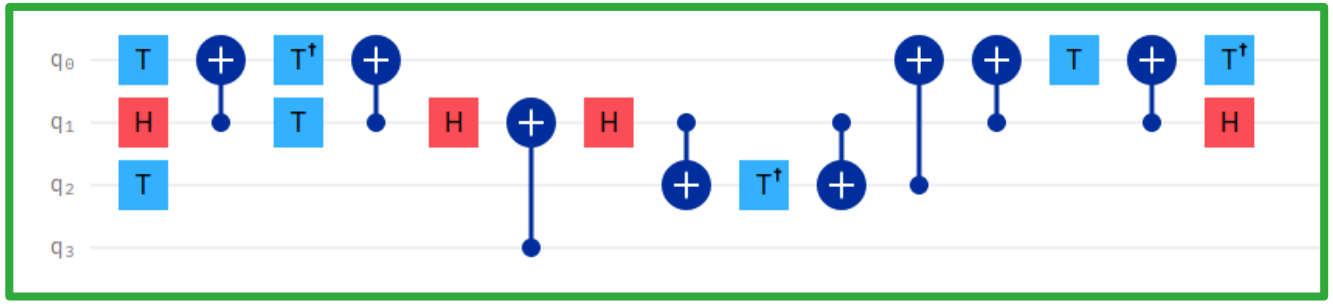

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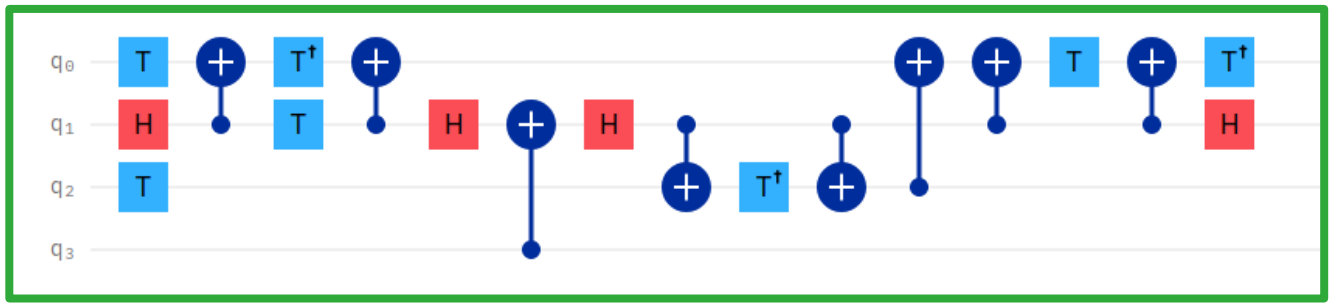

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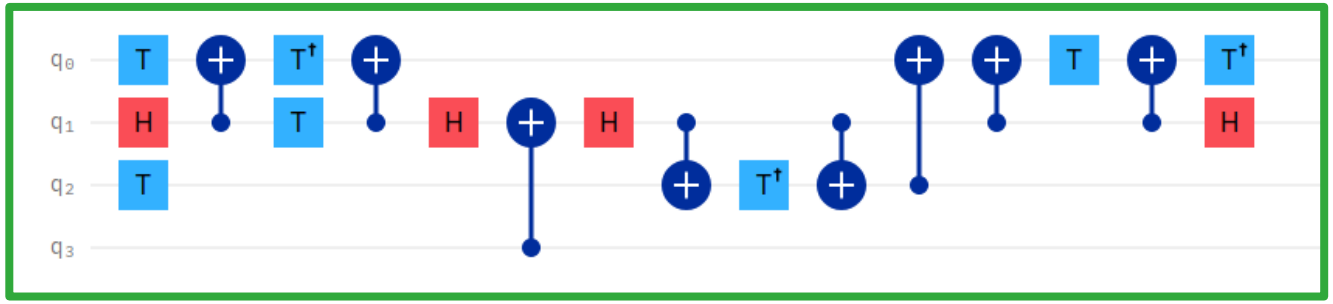

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JUQCS-G

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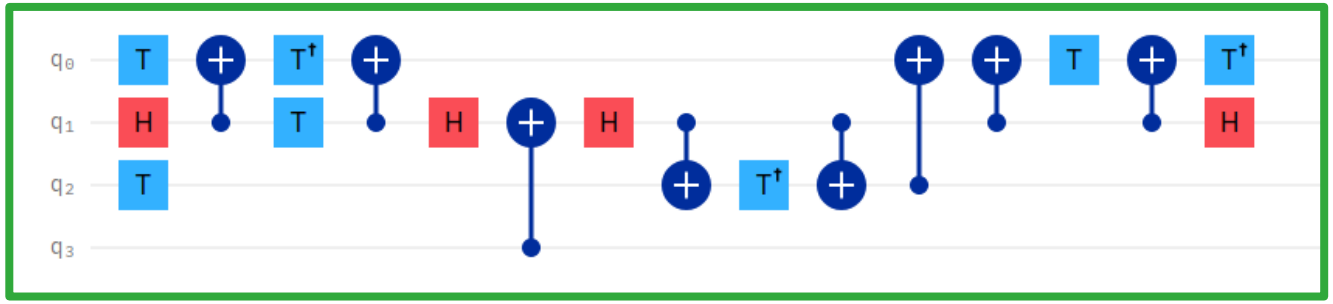

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Full quantum state:

$\psi_{00000000\,0\cdots0}$

GPU rank 0

$\psi_{00000000\,1\cdots1}$

$\psi_{00000001\,0\cdots0}$

GPU rank 1

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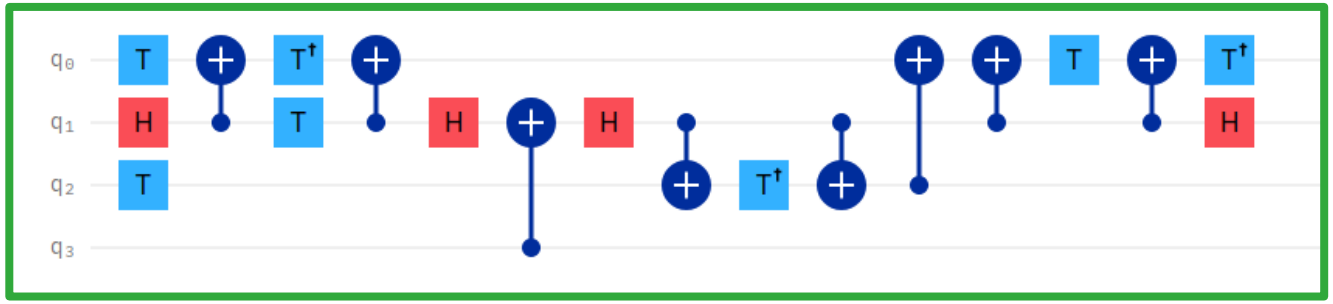
$\psi_{11111111\,0\cdots0}$

GPU rank 255

$\psi_{11111111\,1\cdots1}$

JUQCS-G

CUDA implementation



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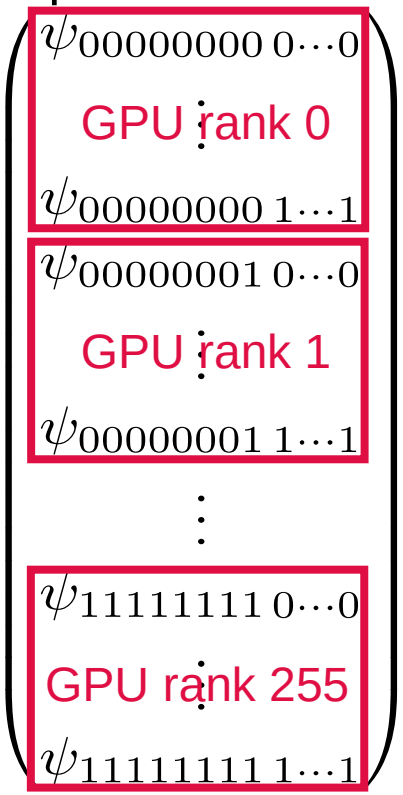

Quantum gate on **global** qubits:

JUQCS-G

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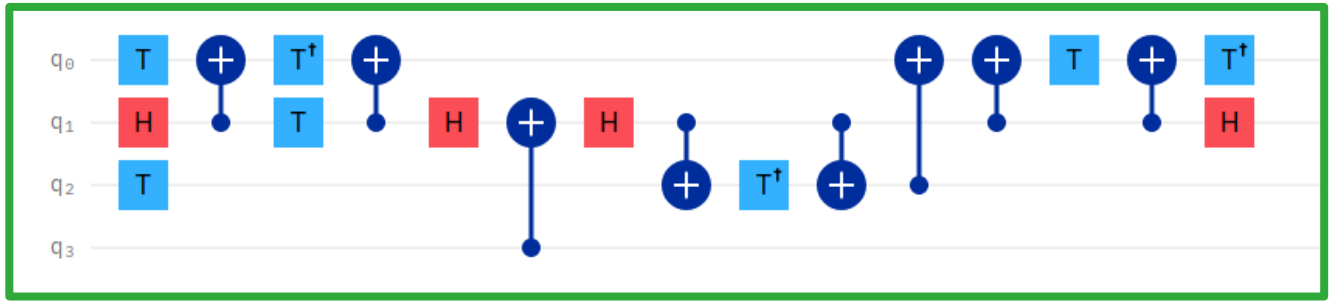

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Quantum gate on **global** qubits:

e.g. H on qubit q_{32}

JUQCS-G

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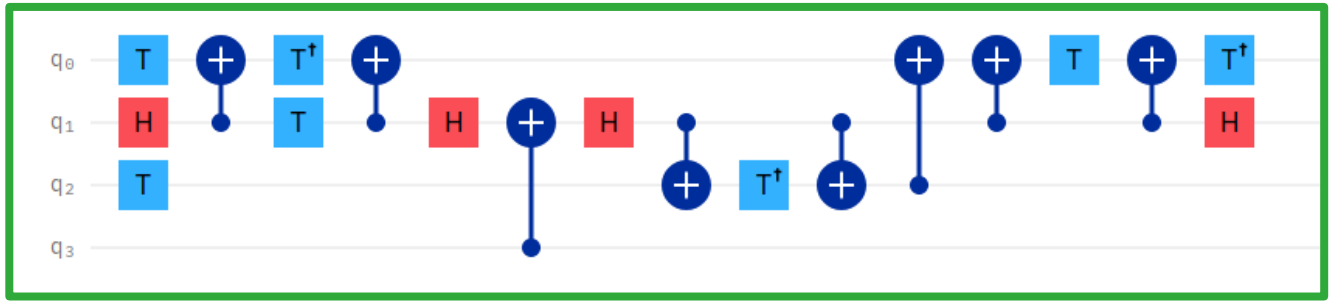

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JUQCS-G

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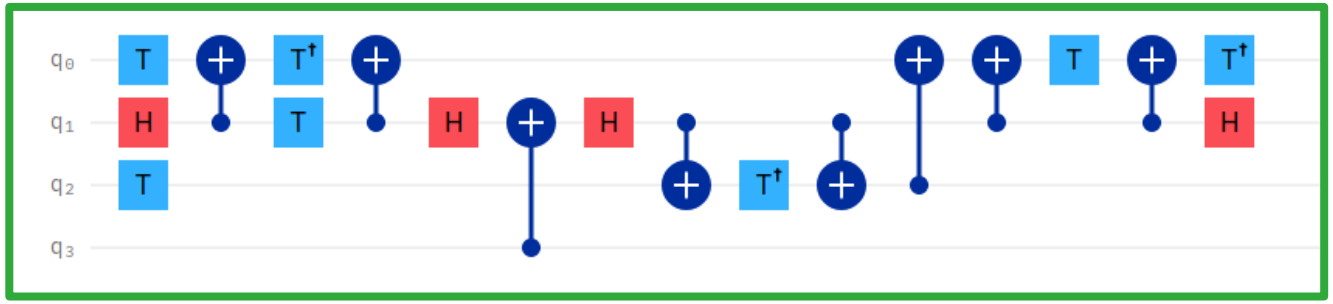

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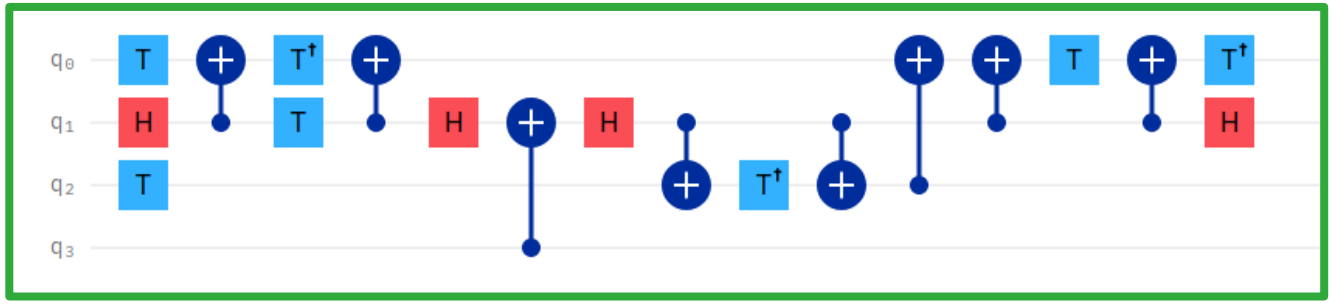

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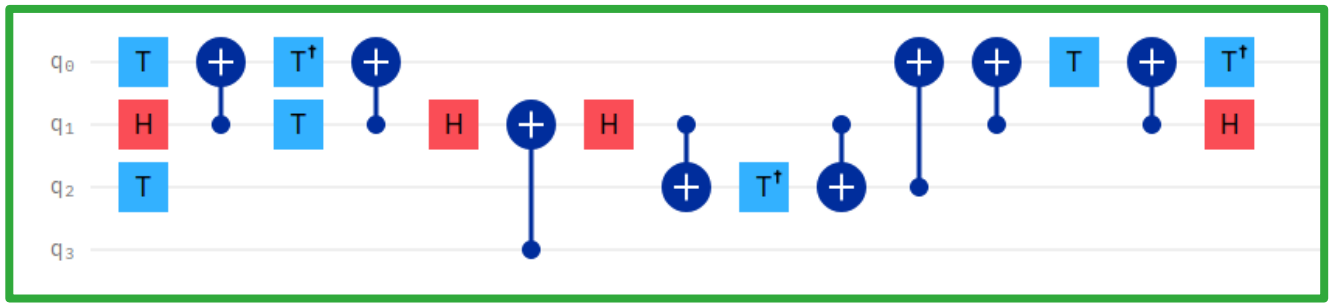

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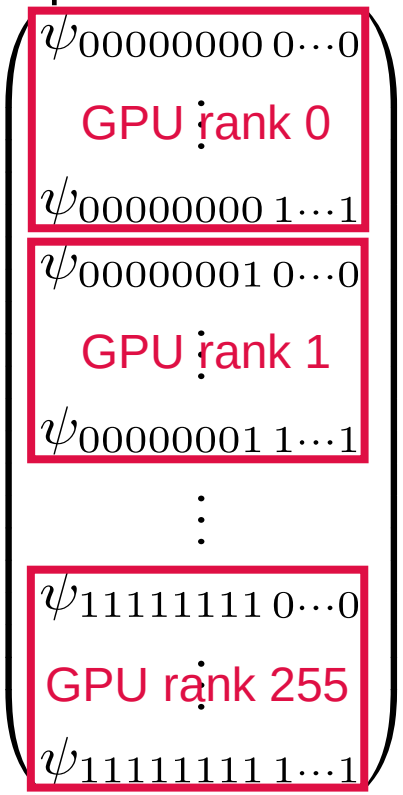

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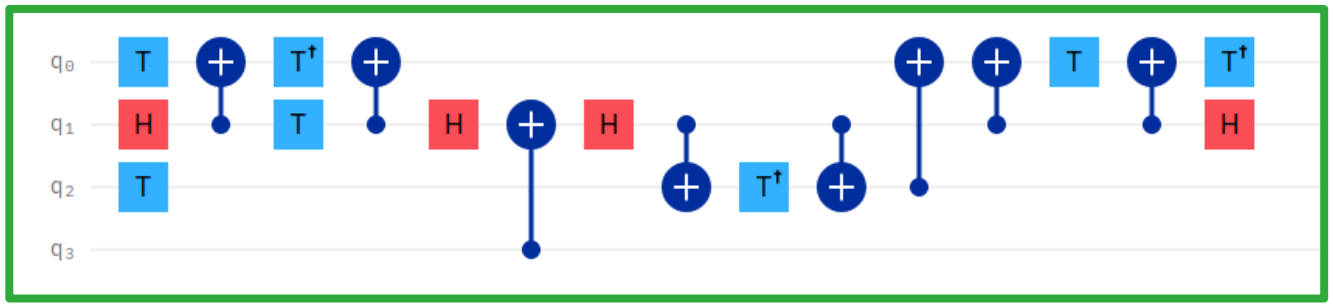

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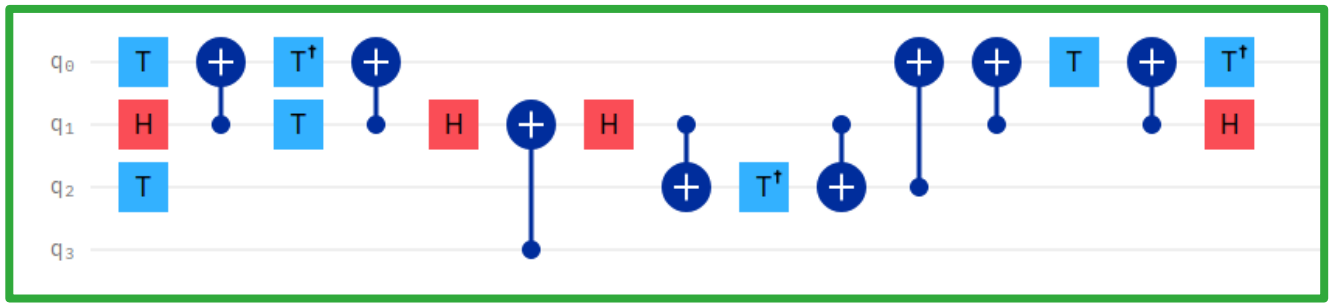

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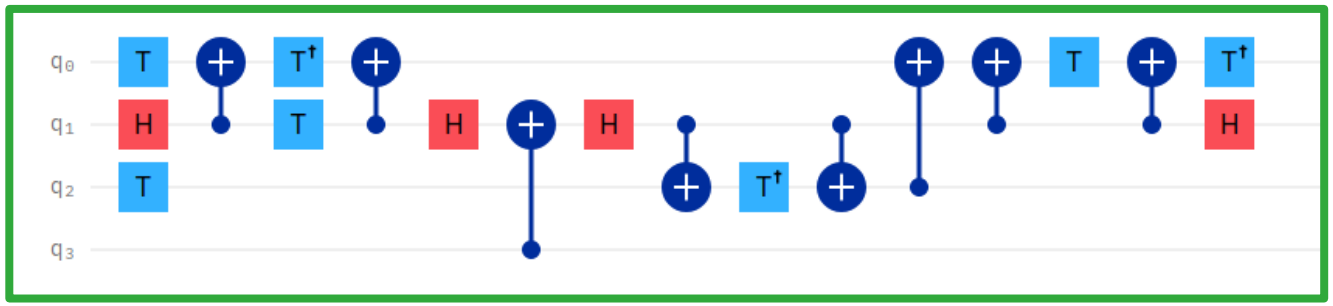

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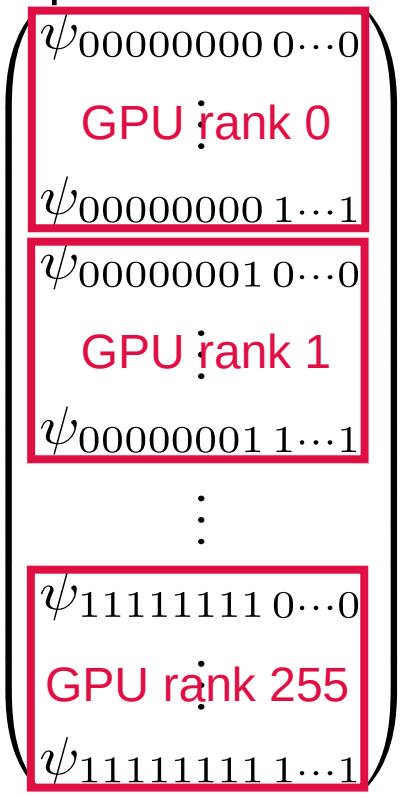

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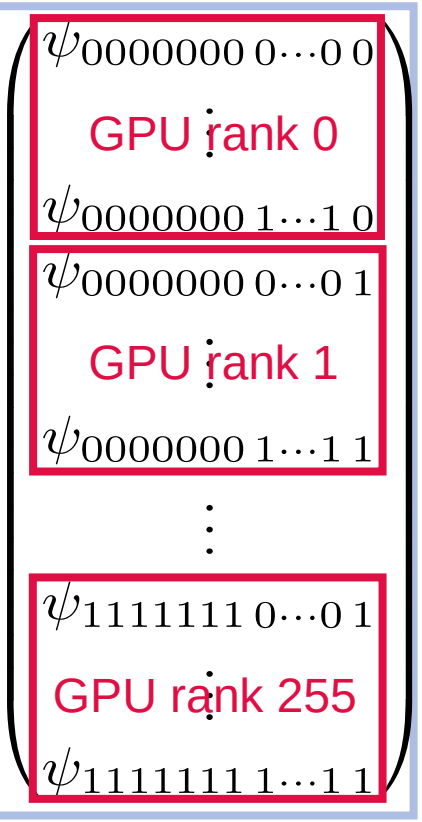
  - Keep track of qubit assignment in a permutation



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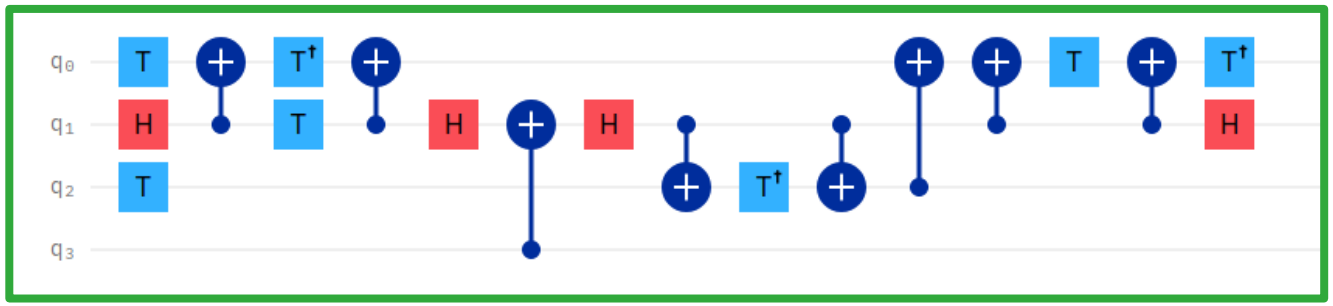

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- Problem: the numbers are on separate GPUs
- Naïve solution:
  - Transfer $2^n/2$ ψ's (8 TiB), perform H, transfer back
- Optimal solution:
  - Exchange global and local qubit, e.g. $q_{32} \leftrightarrow q_0$
  - Keep track of qubit assignment in a permutation
  - Transfer $2^n/2$ ψ's only **once**

$\psi_{0000000\,0\cdots0\,0}$

GPU rank 0

$\psi_{0000000\,1\cdots1\,0}$

$\psi_{0000000\,0\cdots0\,1}$

GPU rank 1

$\psi_{0000000\,1\cdots1\,1}$

$\psi_{1111111\,0\cdots0\,1}$

GPU rank 255

$\psi_{1111111\,1\cdots1\,1}$

JUQCS-G

MPI communication scheme

Before transfer:

$$\begin{pmatrix} \psi_{rrrrrrrr*\cdots*} \\ \psi_{rrrrrrrr*\cdots*} \end{pmatrix}$$

```
...
call psi2MPIbuf<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_I)
istat=cudaStreamSynchronize()
call MPI_SENDRECV(DD(0)%buf_I,m0,MPI_REAL8,idest,0,DD(0)%buf_R,m0,MPI_REAL8,idest,MPI_ANY_TAG,MPI_COMM_WORLD,MPI_STATUS_IGNORE,IERR)
call MPIbuf2psi<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_R)
istat=cudaStreamSynchronize()
...
```

JUQCS-G

MPI communication scheme

Before transfer:

$$\begin{pmatrix} \psi_{rrrrrrrr*\cdots*} \\ \psi_{rrrrrrrr*\cdots*} \end{pmatrix}$$

After transfer:

$$\begin{pmatrix} \psi_{rrrrrrr*\cdots*r} \\ \psi_{rrrrrrr*\cdots*r} \end{pmatrix}$$

```
...
call psi2MPIbuf<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_I)
istat=cudaStreamSynchronize()
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call MPIbuf2psi<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_R)
istat=cudaStreamSynchronize()
...
```

JUQCS-G

MPI communication scheme

Before transfer:

$$\begin{pmatrix} \psi_{rrrrrrrr*\cdots*} \\ \psi_{rrrrrrrr*\cdots*} \end{pmatrix}$$

After transfer:

$$\begin{pmatrix} \psi_{rrrrrrr*\cdots*r} \\ \psi_{rrrrrrr*\cdots*r} \end{pmatrix}$$

- Build buffer on each GPU

```
...
call psi2MPIbuf<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_I)
istat=cudaStreamSynchronize()
call MPI_SENDRECV(DD(0)%buf_I,m0,MPI_REAL8,idest,0,DD(0)%buf_R,m0,MPI_REAL8,idest,MPI_ANY_TAG,MPI_COMM_WORLD,MPI_STATUS_IGNORE,IERR)
call MPIbuf2psi<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_R)
istat=cudaStreamSynchronize()
...
```

JUQCS-G

MPI communication scheme

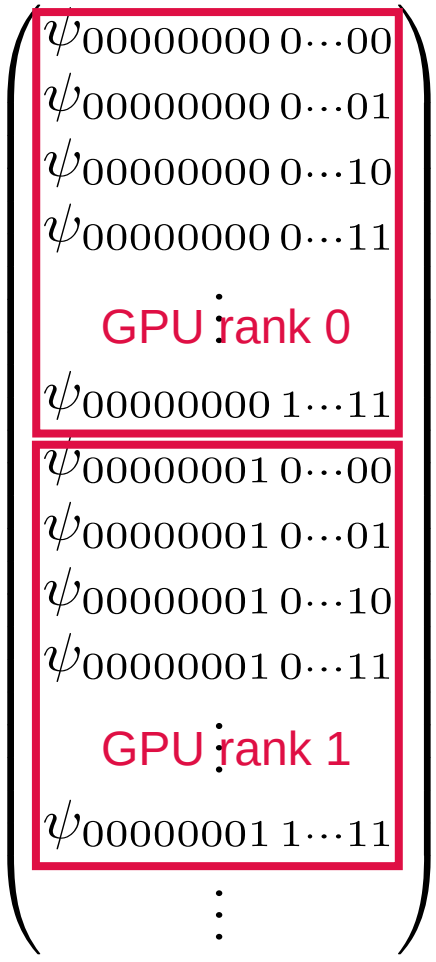
Before transfer:

$$\begin{pmatrix} \psi_{rrrrrrrr*\cdots*} \\ \psi_{rrrrrrrr*\cdots*} \end{pmatrix}$$

After transfer:

$$\begin{pmatrix} \psi_{rrrrrrr*\cdots*r} \\ \psi_{rrrrrrr*\cdots*r} \end{pmatrix}$$

- Build buffer on each GPU




```
...
call psi2MPIbuf<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_I)
istat=cudaStreamSynchronize()
call MPI_SENDRECV(DD(0)%buf_I,m0,MPI_REAL8,idest,0,DD(0)%buf_R,m0,MPI_REAL8,idest,MPI_ANY_TAG,MPI_COMM_WORLD,MPI_STATUS_IGNORE,IERR)
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istat=cudaStreamSynchronize()
...
```

JUQCS-G

MPI communication scheme

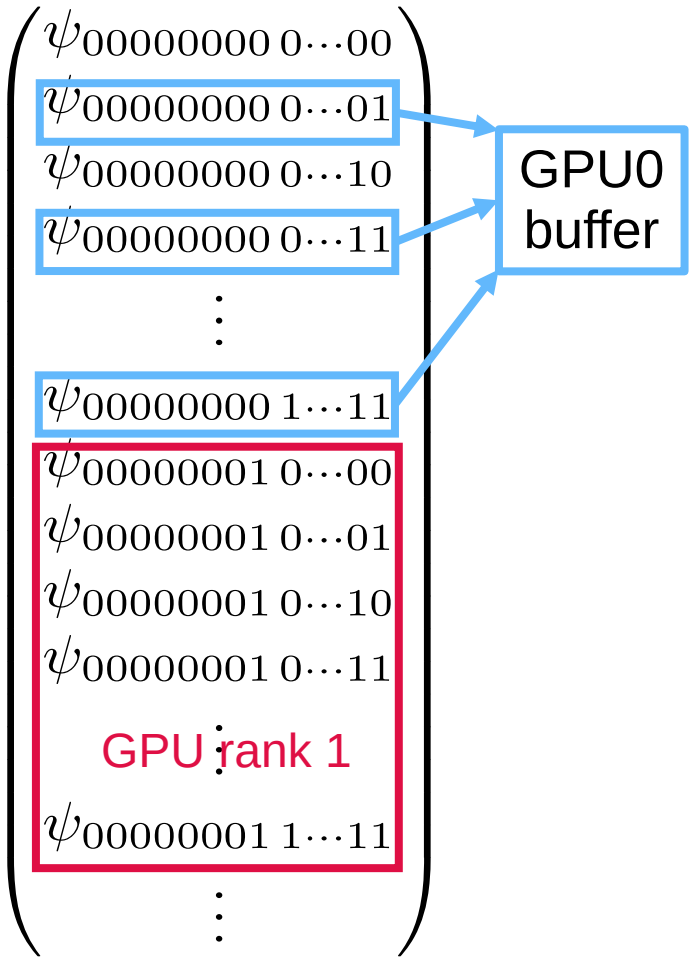
Before transfer:

$$\begin{pmatrix} \psi_{rrrrrrrr*\cdots*} \\ \psi_{rrrrrrrr*\cdots*} \end{pmatrix}$$

After transfer:

$$\begin{pmatrix} \psi_{rrrrrrr*\cdots*r} \\ \psi_{rrrrrrr*\cdots*r} \end{pmatrix}$$

- Build buffer on each GPU




```
...
call psi2MPIbuf<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_I)
istat=cudaStreamSynchronize()
call MPI_SENDRECV(DD(0)%buf_I,m0,MPI_REAL8,idest,0,DD(0)%buf_R,m0,MPI_REAL8,idest,MPI_ANY_TAG,MPI_COMM_WORLD,MPI_STATUS_IGNORE,IERR)
call MPIbuf2psi<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_R)
istat=cudaStreamSynchronize()
...
```

JUQCS-G

MPI communication scheme

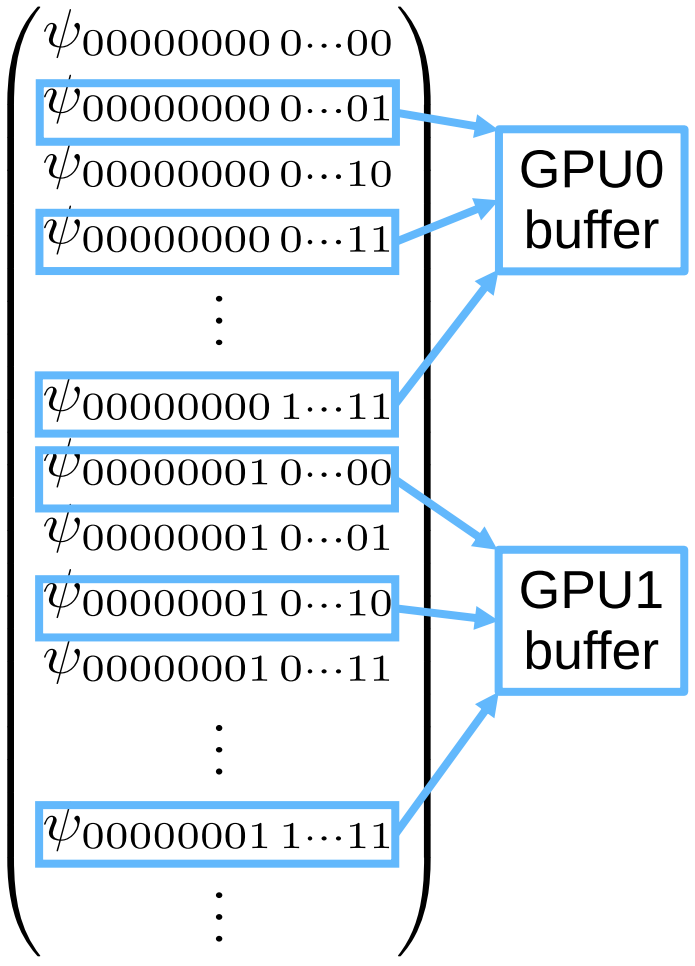
Before transfer:

$$\begin{pmatrix} \psi_{rrrrrrrr*\cdots*} \\ \psi_{rrrrrrrr*\cdots*} \end{pmatrix}$$

After transfer:

$$\begin{pmatrix} \psi_{rrrrrrr*\cdots*r} \\ \psi_{rrrrrrr*\cdots*r} \end{pmatrix}$$

- Build buffer on each GPU




```
...
call psi2MPIbuf<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_I)
istat=cudaStreamSynchronize()
call MPI_SENDRECV(DD(0)%buf_I,m0,MPI_REAL8,idest,0,DD(0)%buf_R,m0,MPI_REAL8,idest,MPI_ANY_TAG,MPI_COMM_WORLD,MPI_STATUS_IGNORE,IERR)
call MPIbuf2psi<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_R)
istat=cudaStreamSynchronize()
...
```

JUQCS-G

MPI communication scheme

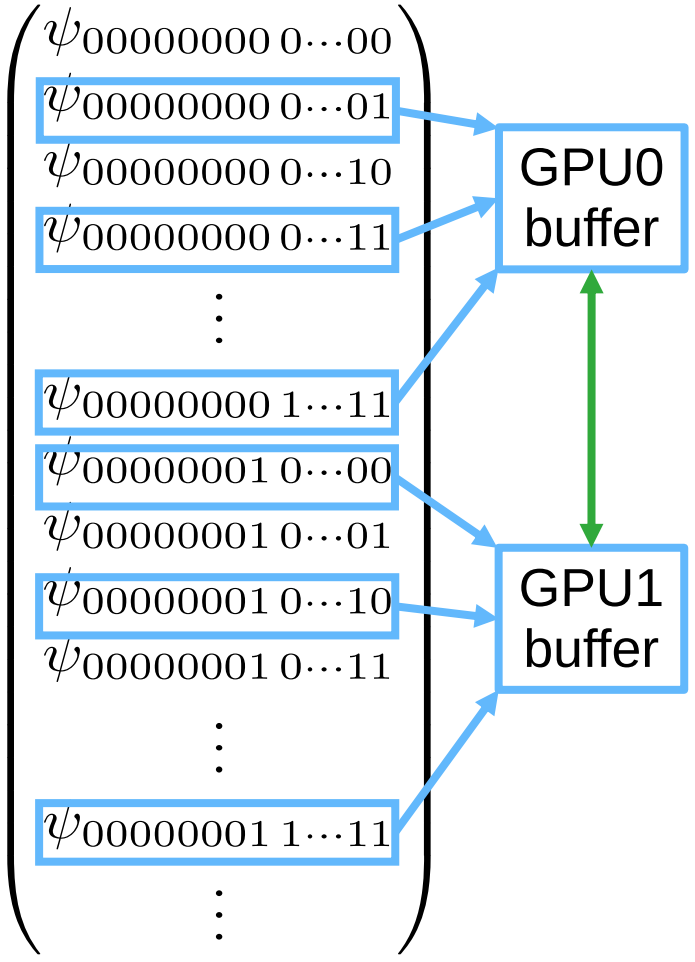
Before transfer:

$$\begin{pmatrix} \psi_{rrrrrrrr*\cdots*} \\ \psi_{rrrrrrrr*\cdots*} \end{pmatrix}$$

After transfer:

$$\begin{pmatrix} \psi_{rrrrrrr*\cdots*r} \\ \psi_{rrrrrrr*\cdots*r} \end{pmatrix}$$

- Build buffer on each GPU
- Transfer with MPI




```
...
call psi2MPIbuf<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_I)
istat=cudaStreamSynchronize()
call MPI_SENDRECV(DD(0)%buf_I,m0,MPI_REAL8,idest,0,DD(0)%buf_R,m0,MPI_REAL8,idest,MPI_ANY_TAG,MPI_COMM_WORLD,MPI_STATUS_IGNORE,IERR)
call MPIbuf2psi<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_R)
istat=cudaStreamSynchronize()
...
```

JUQCS-G

MPI communication scheme

Before transfer:

$$\begin{pmatrix} \psi_{rrrrrrrr*\cdots*} \\ \psi_{rrrrrrrr*\cdots*} \end{pmatrix}$$

After transfer:

$$\begin{pmatrix} \psi_{rrrrrrr*\cdots*r} \\ \psi_{rrrrrrr*\cdots*r} \end{pmatrix}$$

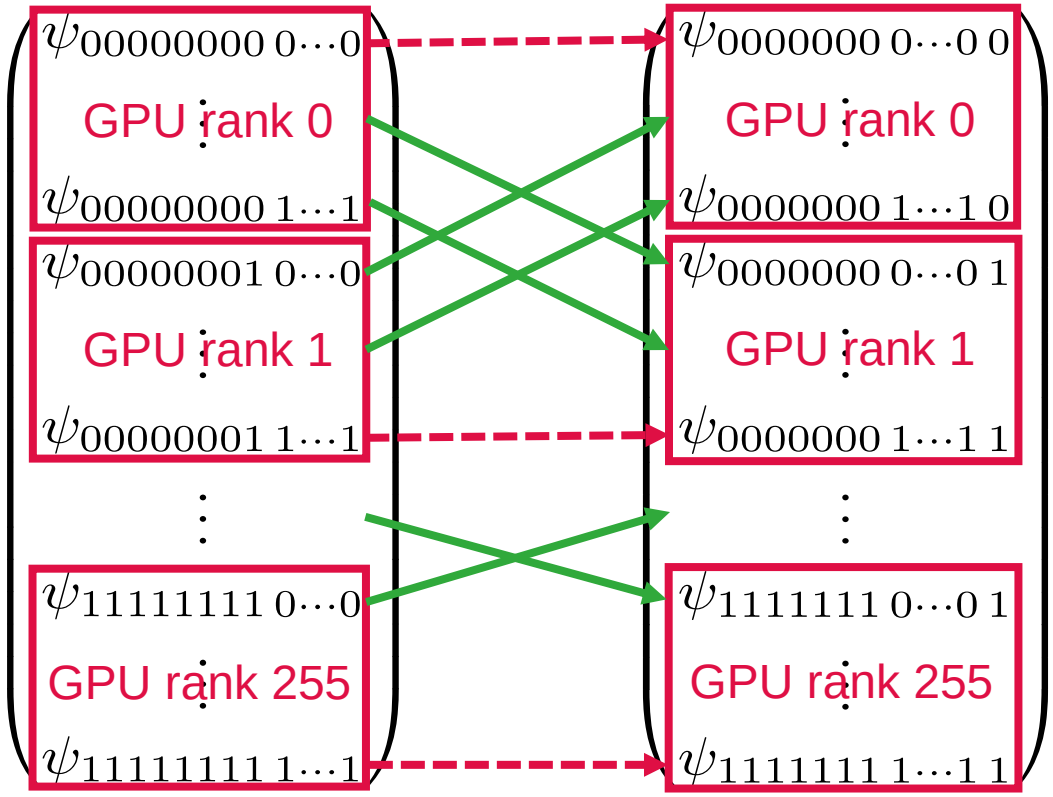
- Build buffer on each GPU
- Transfer with MPI

$$\begin{pmatrix} \psi_{00000000\,0\cdots00} \\ \psi_{00000000\,0\cdots01} \\ \psi_{00000000\,0\cdots10} \\ \psi_{00000000\,0\cdots11} \\ \vdots \\ \psi_{00000000\,1\cdots11} \\ \psi_{00000001\,0\cdots00} \\ \psi_{00000001\,0\cdots01} \\ \psi_{00000001\,0\cdots10} \\ \psi_{00000001\,0\cdots11} \\ \vdots \\ \psi_{00000001\,1\cdots11} \\ \vdots \end{pmatrix}$$

GPU0 buffer

GPU1 buffer

```
n=blockidx%x-1
n=n*blockdim%x+threadidx%x-1
idx=n+noff
do i=0,nswap-1
j=bitmasklist(i)
idx=ishft(iand(idx,not(j)),one)+iand(idx,j)
enddo
buf(n)=phi(ior(idx,jsourmask))
```




```
...
call psi2MPIbuf<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_I)
istat=cudaStreamSynchronize()
call MPI_SENDRECV(DD(0)%buf_I,m0,MPI_REAL8,idest,0,DD(0)%buf_R,m0,MPI_REAL8,idest,MPI_ANY_TAG,MPI_COMM_WORLD,MPI_STATUS_IGNORE,IERR)
call MPIbuf2psi<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_R)
istat=cudaStreamSynchronize()
...
```

JUQCS-G

MPI communication scheme

Before transfer:

$$\begin{pmatrix} \psi_{rrrrrrrr*\cdots*} \\ \psi_{rrrrrrrr*\cdots*} \end{pmatrix}$$

After transfer:

$$\begin{pmatrix} \psi_{rrrrrrr*\cdots*r} \\ \psi_{rrrrrrr*\cdots*r} \end{pmatrix}$$

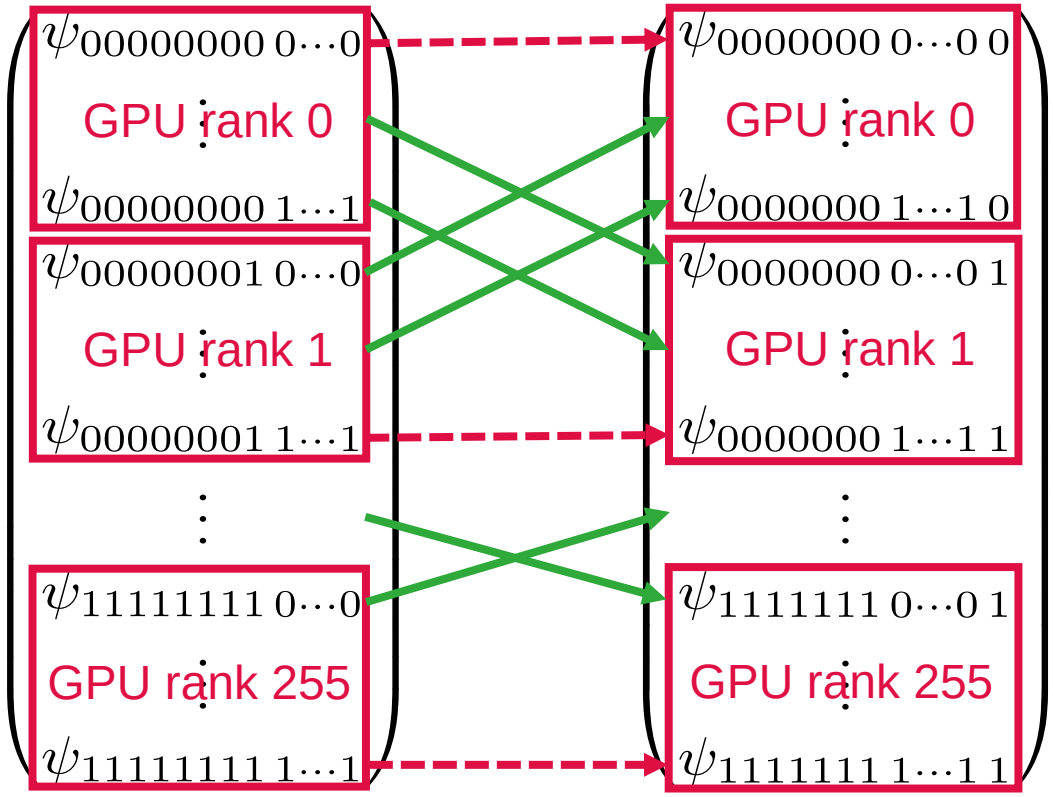
- Build buffer on each GPU
- Transfer with MPI
- Retrieve from buffer

$$\begin{pmatrix} \psi_{00000000\,0\cdots00} \\ \psi_{00000000\,0\cdots01} \\ \psi_{00000000\,0\cdots10} \\ \psi_{00000000\,0\cdots11} \\ \vdots \\ \psi_{00000000\,1\cdots11} \\ \psi_{00000001\,0\cdots00} \\ \psi_{00000001\,0\cdots01} \\ \psi_{00000001\,0\cdots10} \\ \psi_{00000001\,0\cdots11} \\ \vdots \\ \psi_{00000001\,1\cdots11} \\ \vdots \end{pmatrix}$$

GPU0 buffer

GPU1 buffer

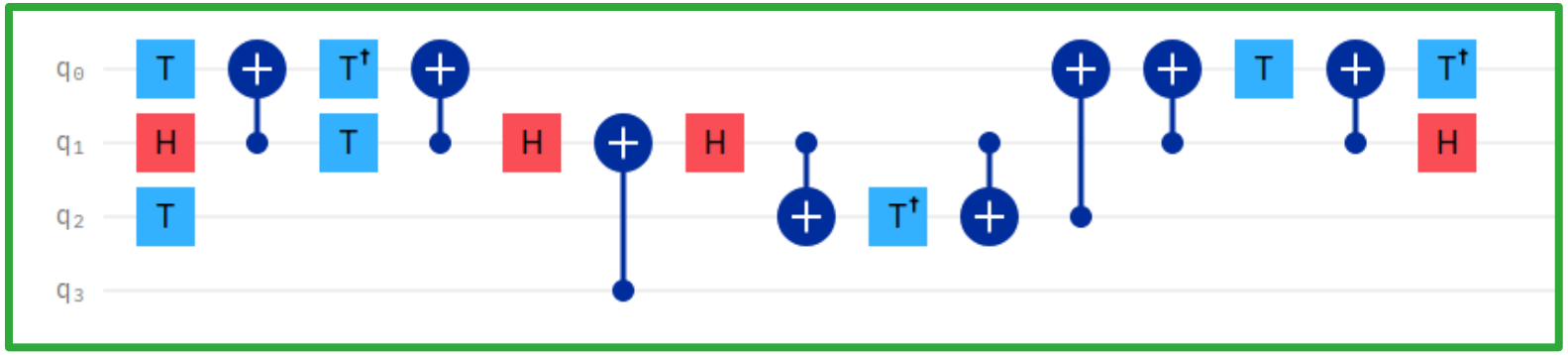
```
n=blockidx%x-1
n=n*blockdim%x+threadidx%x-1
idx=n+noff
do i=0,nswap-1
j=bitmasklist(i)
idx=ishft(iand(idx,not(j)),one)+iand(idx,j)
enddo
buf(n)=phi(ior(idx,jsourmask))
```




```
...
call psi2MPIbuf<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_I)
istat=cudaStreamSynchronize()
call MPI_SENDRECV(DD(0)%buf_I,m0,MPI_REAL8,idest,0,DD(0)%buf_R,m0,MPI_REAL8,idest,MPI_ANY_TAG,MPI_COMM_WORLD,MPI_STATUS_IGNORE,IERR)
call MPIbuf2psi<<<m,n>>> (nbits,nstatesGPU,m0,n0,nswap,isourmask,DD(0)%bitmasklist,DD(0)%phi_R,DD(0)%buf_R)
istat=cudaStreamSynchronize()
...
```

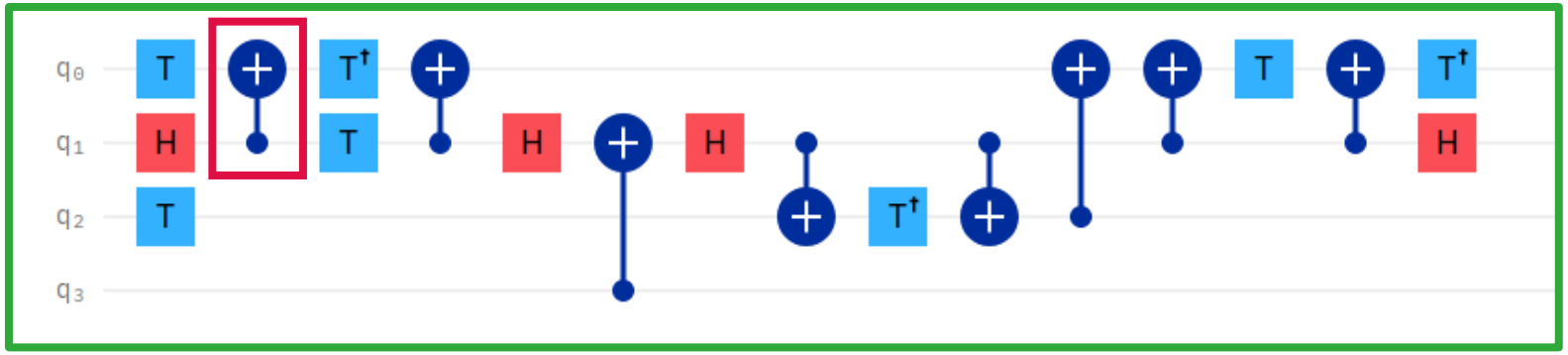
JUQCS-G

MPI communication: Two-qubit gates



JUQCS-G

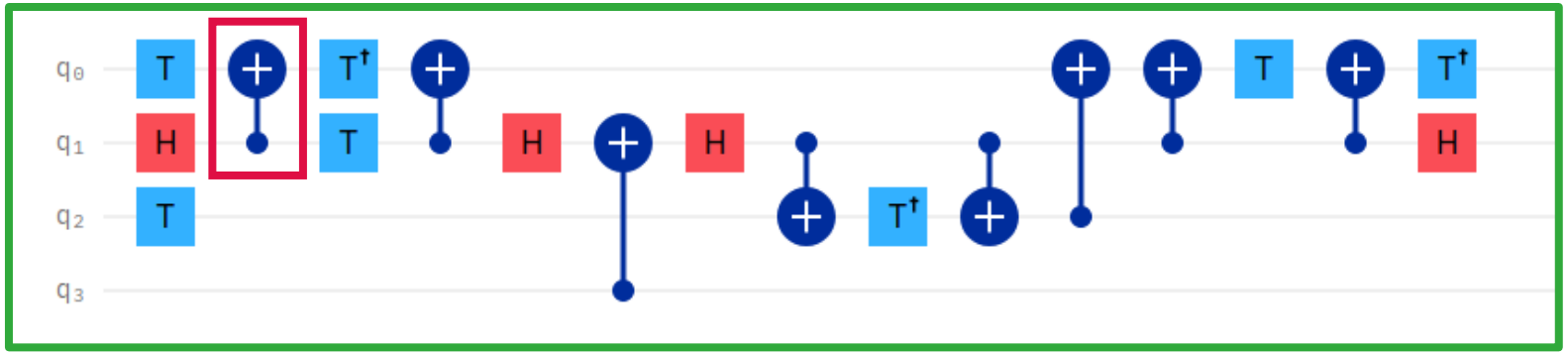
MPI communication: Two-qubit gates



➢ CNOT gate (controlled-NOT):

JUQCS-G

MPI communication: Two-qubit gates



- CNOT gate (controlled-NOT):
  - Swap all coefficients where control qubit C is 1

$$\begin{array}{cccc} \text{CT} & \text{CT} & \text{CT} & \text{CT} \\ 00 & 01 & 10 & 11 \end{array}$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

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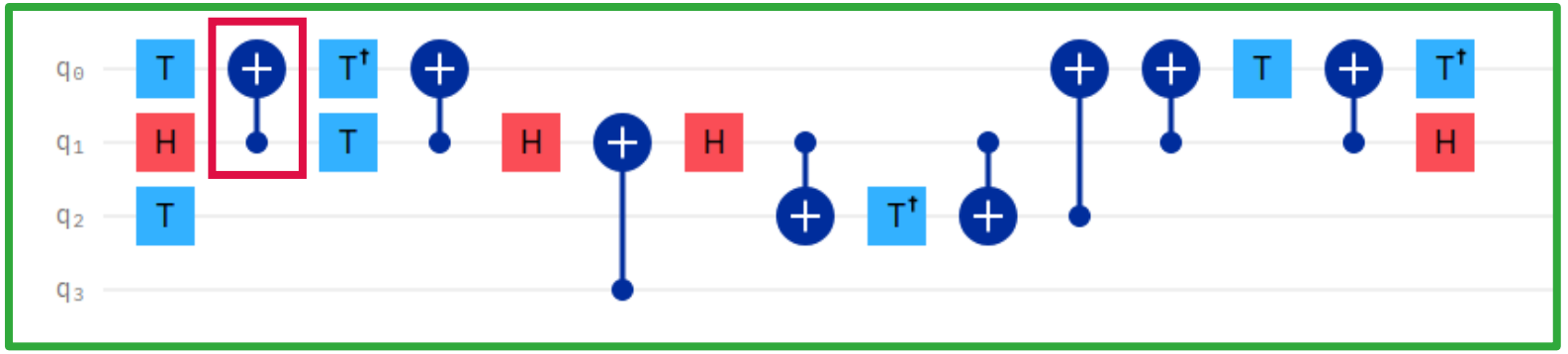
MPI communication: Two-qubit gates



- CNOT gate (controlled-NOT):
  - Swap all coefficients where control qubit C is 1

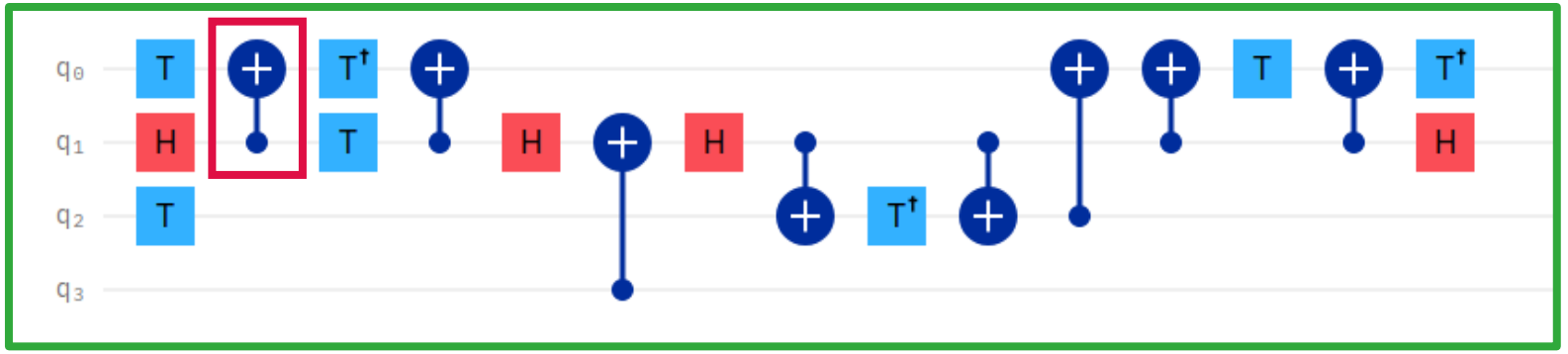
$$\begin{array}{cccc} \mathrm{CT} & \mathrm{CT} & \mathrm{CT} & \mathrm{CT} \\ 00 & 01 & 10 & 11 \end{array}$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\psi_{q_3 q_2 q_1 q_0}$$

GPU0	GPU1	GPU2	GPU3
$\psi_{00\,00}$	$\psi_{01\,00}$	$\psi_{10\,00}$	$\psi_{11\,00}$
$\psi_{00\,01}$	$\psi_{01\,01}$	$\psi_{10\,01}$	$\psi_{11\,01}$
$\psi_{00\,10}$	$\psi_{01\,10}$	$\psi_{10\,10}$	$\psi_{11\,10}$
$\psi_{00\,11}$	$\psi_{01\,11}$	$\psi_{10\,11}$	$\psi_{11\,11}$

JUQCS-G

MPI communication: Two-qubit gates



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$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

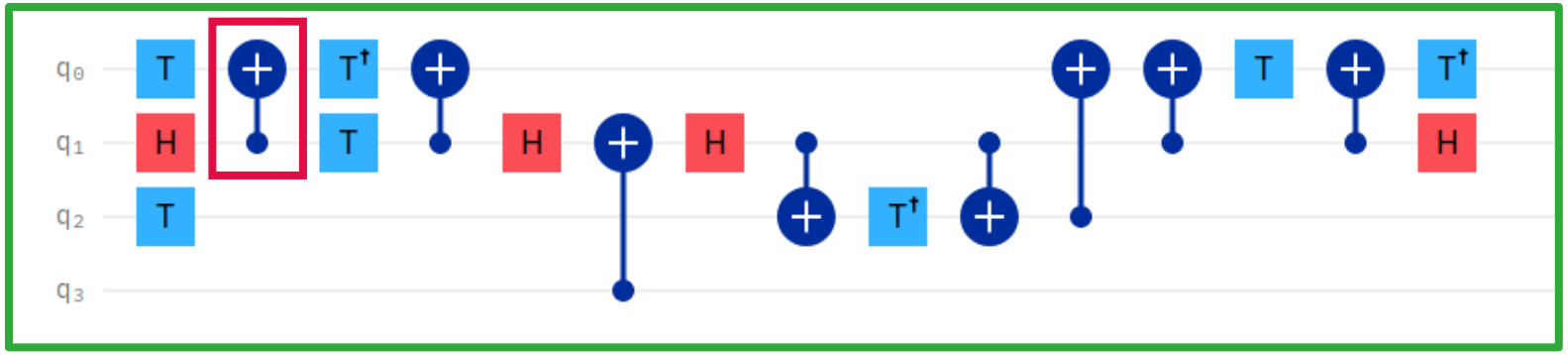
$$\psi_{q_3 q_2 q_1 q_0}$$
C T

GPU0	GPU1	GPU2	GPU3
$\psi_{00\,00}$	$\psi_{01\,00}$	$\psi_{10\,00}$	$\psi_{11\,00}$
$\psi_{00\,01}$	$\psi_{01\,01}$	$\psi_{10\,01}$	$\psi_{11\,01}$
$\psi_{00\,10}$	$\psi_{01\,10}$	$\psi_{10\,10}$	$\psi_{11\,10}$
$\psi_{00\,11}$	$\psi_{01\,11}$	$\psi_{10\,11}$	$\psi_{11\,11}$

  - “2 local”: GPUs swap locally

JUQCS-G

MPI communication: Two-qubit gates



- CNOT gate (controlled-NOT):
  - Swap all coefficients where control qubit C is 1

$$\begin{array}{cccc} \text{CT} & \text{CT} & \text{CT} & \text{CT} \\ 00 & 01 & 10 & 11 \end{array}$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\psi_{q_3 q_2 q_1 q_0}$$
C T

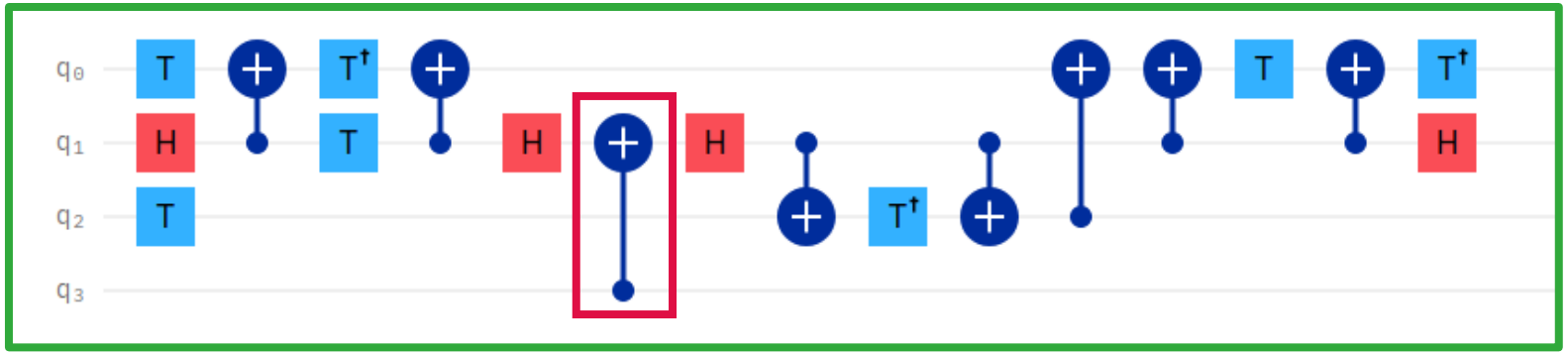
GPU0 GPU1 GPU2 GPU3

$$\begin{pmatrix} \psi_{00\,00} \\ \psi_{00\,01} \\ \psi_{00\,10} \\ \psi_{00\,11} \end{pmatrix} \quad \begin{pmatrix} \psi_{01\,00} \\ \psi_{01\,01} \\ \psi_{01\,10} \\ \psi_{01\,11} \end{pmatrix} \quad \begin{pmatrix} \psi_{10\,00} \\ \psi_{10\,01} \\ \psi_{10\,10} \\ \psi_{10\,11} \end{pmatrix} \quad \begin{pmatrix} \psi_{11\,00} \\ \psi_{11\,01} \\ \psi_{11\,10} \\ \psi_{11\,11} \end{pmatrix}$$

  - “2 local”: GPUs swap locally

JUQCS-G

MPI communication: Two-qubit gates



- CNOT gate (controlled-NOT):
  - Swap all coefficients where control qubit C is 1

$$\begin{array}{cccc} \mathrm{CT} & \mathrm{CT} & \mathrm{CT} & \mathrm{CT} \\ 00 & 01 & 10 & 11 \end{array}$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

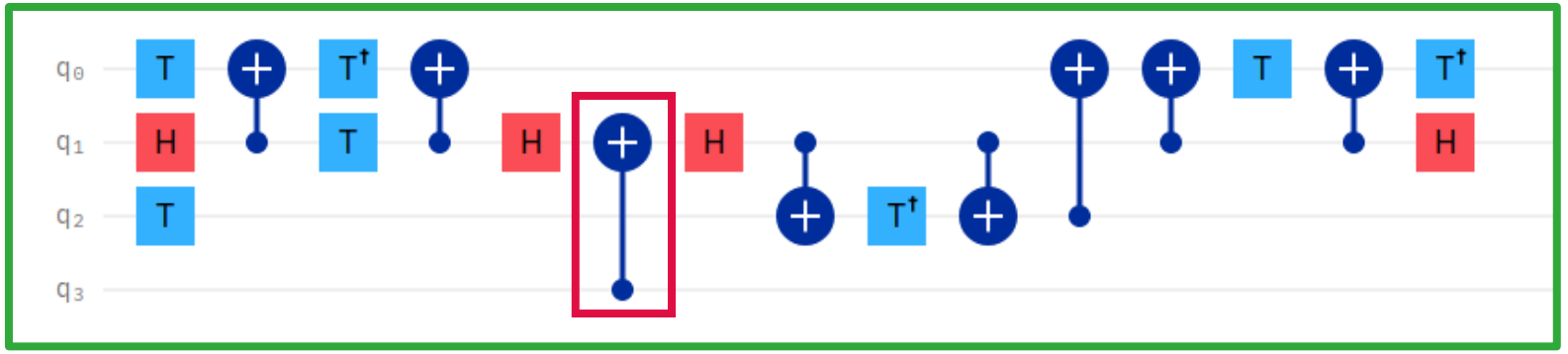
$$\psi_{q_3 q_2 q_1 q_0}$$
C T

GPU0	GPU1	GPU2	GPU3
$\psi_{00\,00}$	$\psi_{01\,00}$	$\psi_{10\,00}$	$\psi_{11\,00}$
$\psi_{00\,01}$	$\psi_{01\,01}$	$\psi_{10\,01}$	$\psi_{11\,01}$
$\psi_{00\,10}$	$\psi_{01\,10}$	$\psi_{10\,10}$	$\psi_{11\,10}$
$\psi_{00\,11}$	$\psi_{01\,11}$	$\psi_{10\,11}$	$\psi_{11\,11}$

  - “2 local”: GPUs swap locally
  - “C global, T local”: GPUs swap locally

JUQCS-G

MPI communication: Two-qubit gates



- CNOT gate (controlled-NOT):
  - Swap all coefficients where control qubit C is 1

$$\begin{array}{cccc} \mathrm{CT} & \mathrm{CT} & \mathrm{CT} & \mathrm{CT} \\ 00 & 01 & 10 & 11 \end{array}$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\psi_{q_3 q_2 q_1 q_0}$$
C T

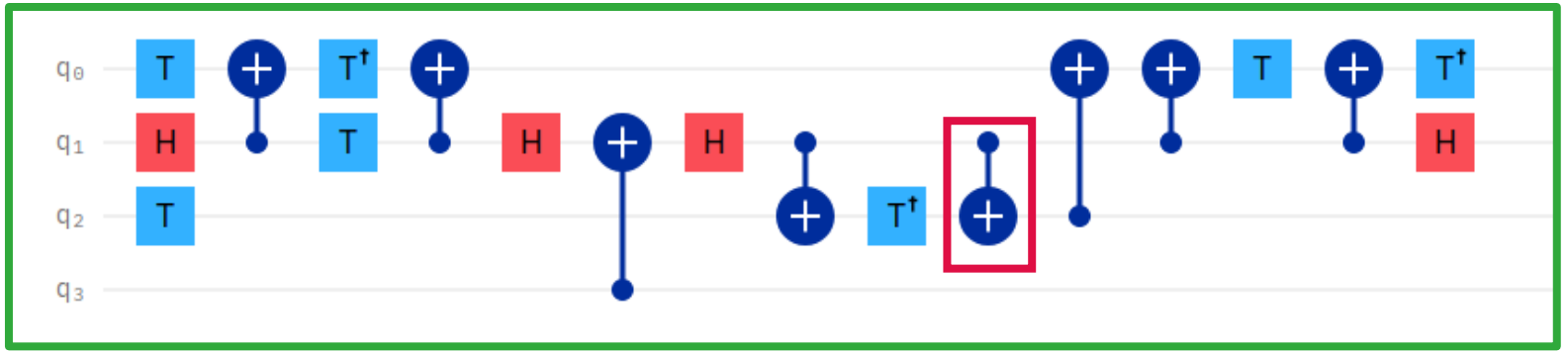
GPU0 GPU1 GPU2 GPU3

$$\begin{pmatrix} \psi_{00\,00} \\ \psi_{00\,01} \\ \psi_{00\,10} \\ \psi_{00\,11} \end{pmatrix} \quad \begin{pmatrix} \psi_{01\,00} \\ \psi_{01\,01} \\ \psi_{01\,10} \\ \psi_{01\,11} \end{pmatrix} \quad \begin{pmatrix} \psi_{10\,00} \\ \psi_{10\,01} \\ \psi_{10\,10} \\ \psi_{10\,11} \end{pmatrix} \quad \begin{pmatrix} \psi_{11\,00} \\ \psi_{11\,01} \\ \psi_{11\,10} \\ \psi_{11\,11} \end{pmatrix}$$

  - “2 local”: GPUs swap locally
  - “C global, T local”: GPUs swap locally

JUQCS-G

MPI communication: Two-qubit gates



- CNOT gate (controlled-NOT):
  - Swap all coefficients where control qubit C is 1

$$\begin{array}{cccc} \text{CT} & \text{CT} & \text{CT} & \text{CT} \\ 00 & 01 & 10 & 11 \end{array}$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

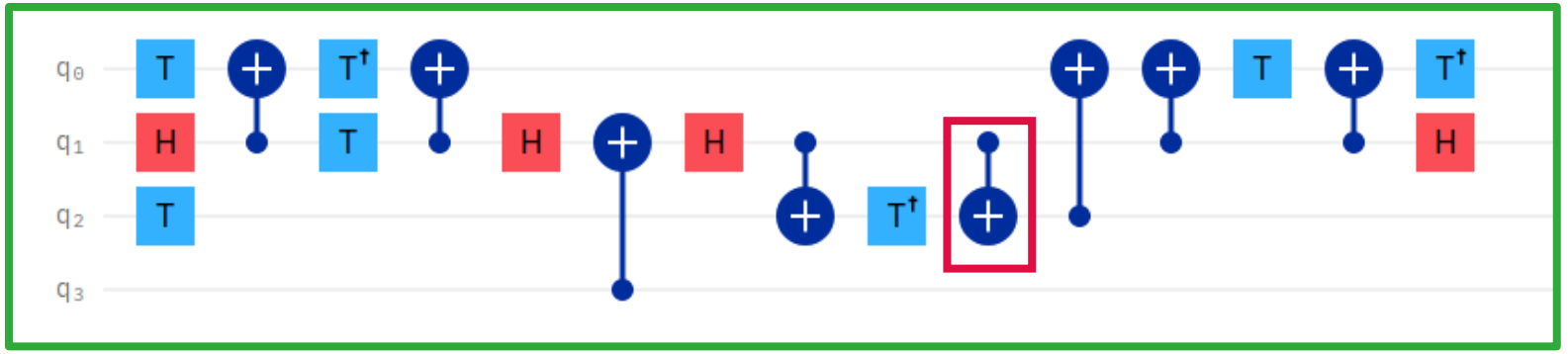
$$\psi_{q_3 q_2 q_1 q_0}$$
T C

GPU0	GPU1	GPU2	GPU3
$\psi_{00\,00}$	$\psi_{01\,00}$	$\psi_{10\,00}$	$\psi_{11\,00}$
$\psi_{00\,01}$	$\psi_{01\,01}$	$\psi_{10\,01}$	$\psi_{11\,01}$
$\psi_{00\,10}$	$\psi_{01\,10}$	$\psi_{10\,10}$	$\psi_{11\,10}$
$\psi_{00\,11}$	$\psi_{01\,11}$	$\psi_{10\,11}$	$\psi_{11\,11}$

  - “2 local”: GPUs swap locally
  - “C global, T local”: GPUs swap locally
  - “C local, T global”: MPI transfer ½ of all coefficients

JUQCS-G

MPI communication: Two-qubit gates



- CNOT gate (controlled-NOT):
  - Swap all coefficients where control qubit C is 1

$$\begin{array}{cccc} \text{CT} & \text{CT} & \text{CT} & \text{CT} \\ 00 & 01 & 10 & 11 \end{array}$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\psi_{q_3 q_2 q_1 q_0}$$
T C

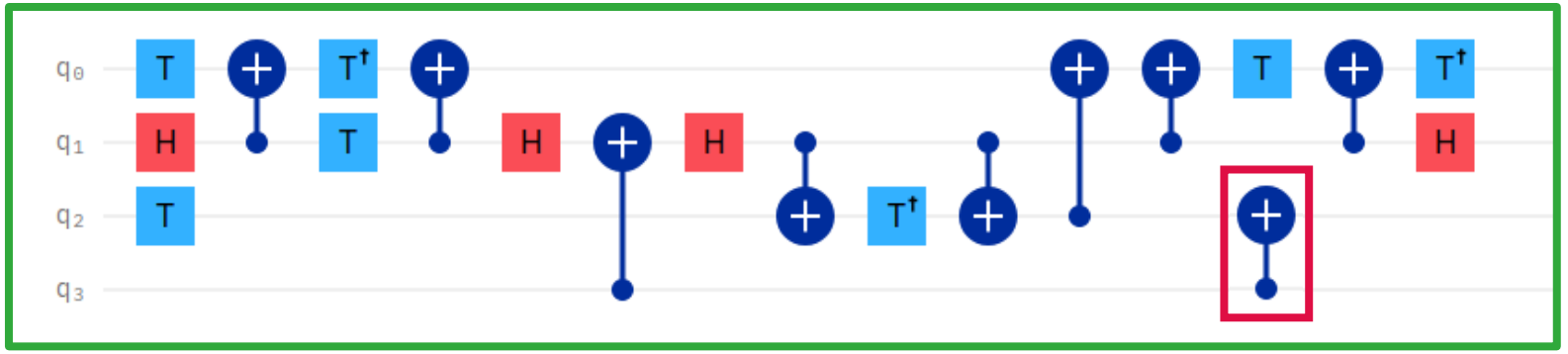
GPU0 GPU1 GPU2 GPU3

$$\begin{pmatrix} \psi_{00\,00} \\ \psi_{00\,01} \\ \psi_{00\,10} \\ \psi_{00\,11} \end{pmatrix} \begin{pmatrix} \psi_{01\,00} \\ \psi_{01\,01} \\ \psi_{01\,10} \\ \psi_{01\,11} \end{pmatrix} \begin{pmatrix} \psi_{10\,00} \\ \psi_{10\,01} \\ \psi_{10\,10} \\ \psi_{10\,11} \end{pmatrix} \begin{pmatrix} \psi_{11\,00} \\ \psi_{11\,01} \\ \psi_{11\,10} \\ \psi_{11\,11} \end{pmatrix}$$

  - “2 local”: GPUs swap locally
  - “C global, T local”: GPUs swap locally
  - “C local, T global”: MPI transfer ½ of all coefficients

JUQCS-G

MPI communication: Two-qubit gates



- CNOT gate (controlled-NOT):
  - Swap all coefficients where control qubit C is 1

$$\begin{array}{cccc} \text{CT} & \text{CT} & \text{CT} & \text{CT} \\ 00 & 01 & 10 & 11 \end{array}$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\psi_{q_3 q_2 q_1 q_0}$$
C T

GPU0	GPU1	GPU2	GPU3
$\psi_{00\,00}$	$\psi_{01\,00}$	$\psi_{10\,00}$	$\psi_{11\,00}$
$\psi_{00\,01}$	$\psi_{01\,01}$	$\psi_{10\,01}$	$\psi_{11\,01}$
$\psi_{00\,10}$	$\psi_{01\,10}$	$\psi_{10\,10}$	$\psi_{11\,10}$
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JUQCS-G

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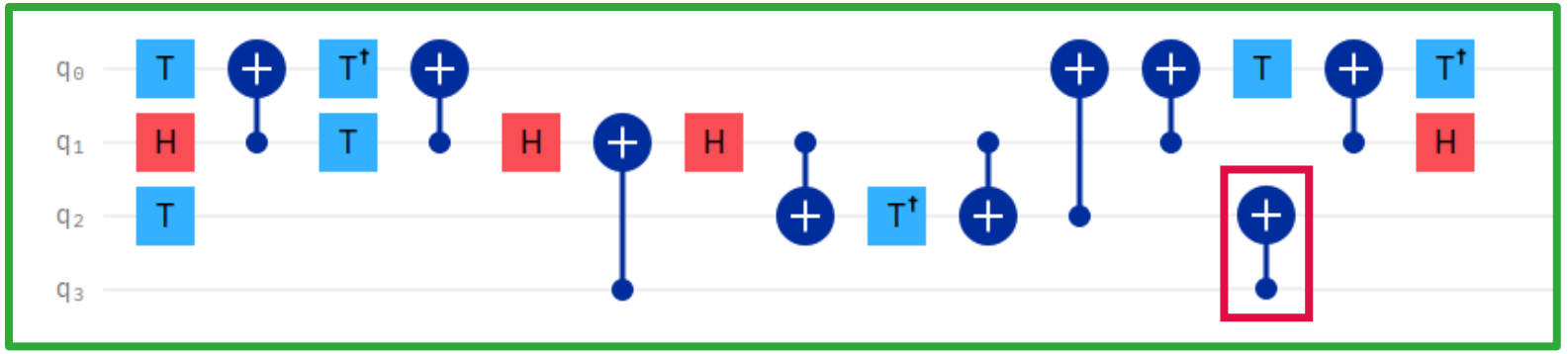

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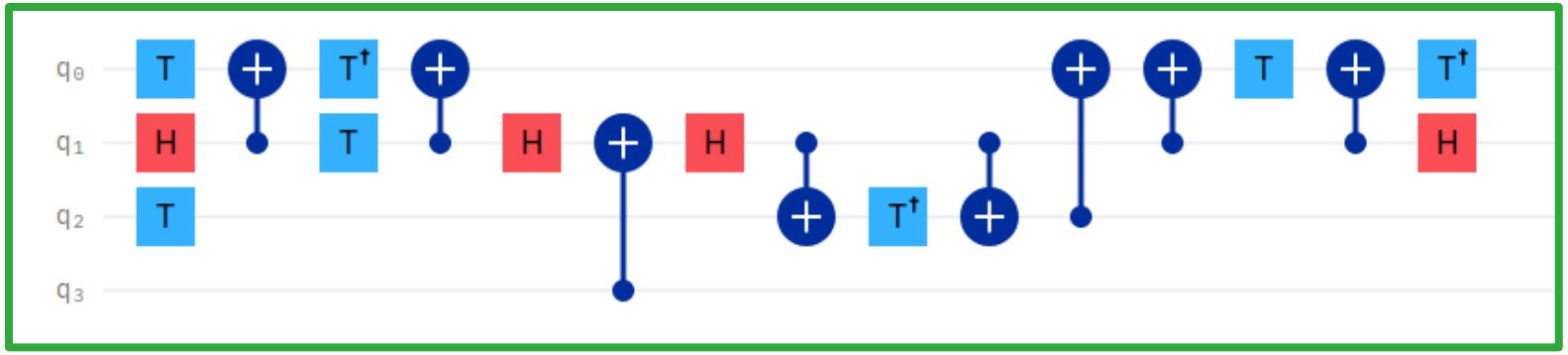

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$$\begin{matrix} \text{GPU0} & \text{GPU1} & \text{GPU2} & \text{GPU3} \\ \begin{pmatrix} \psi_{00\,00} \\ \psi_{00\,01} \\ \psi_{00\,10} \\ \psi_{00\,11} \end{pmatrix} & \begin{pmatrix} \psi_{01\,00} \\ \psi_{01\,01} \\ \psi_{01\,10} \\ \psi_{01\,11} \end{pmatrix} & \begin{pmatrix} \psi_{10\,00} \\ \psi_{10\,01} \\ \psi_{10\,10} \\ \psi_{10\,11} \end{pmatrix} & \begin{pmatrix} \psi_{11\,00} \\ \psi_{11\,01} \\ \psi_{11\,10} \\ \psi_{11\,11} \end{pmatrix} \end{matrix}$$

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- For benchmarking: MPI transfer whenever coefficients on different GPUs are combined

JUQCS-G

Running on JUWELS Booster

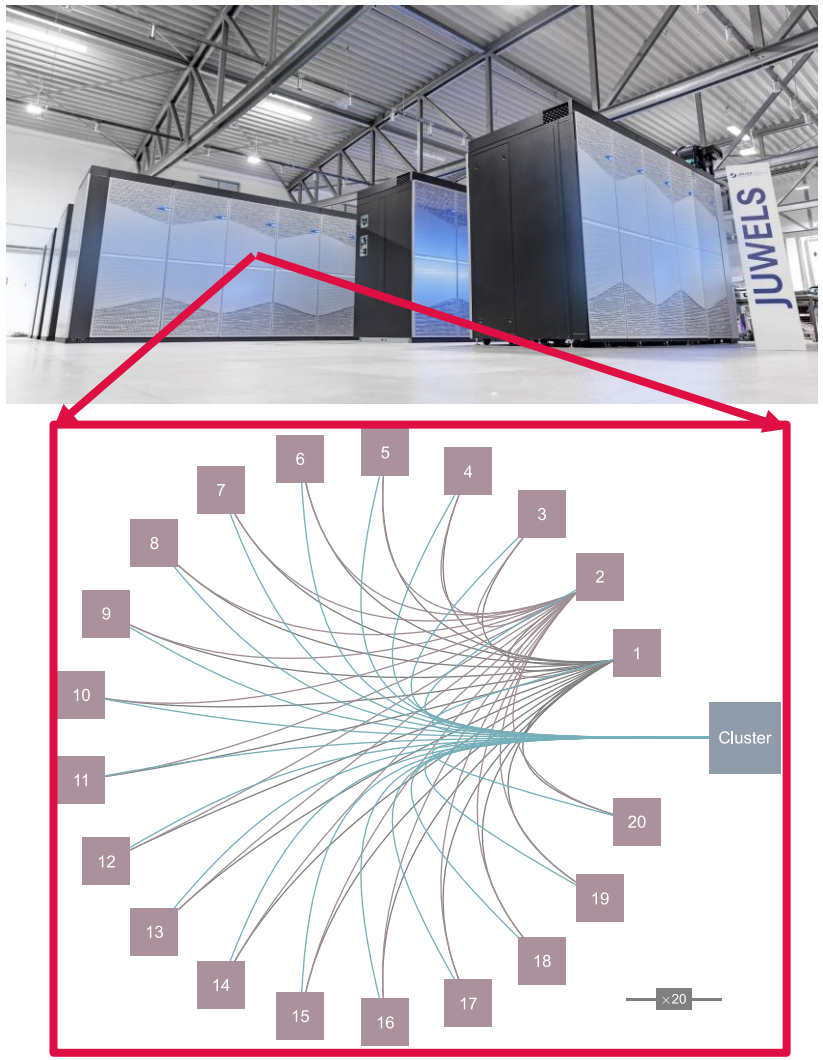
JUQCS-G

Running on JUWELS Booster

- 936 Compute nodes

JUQCS-G

Running on JUWELS Booster



- 936 Compute nodes
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JUQCS-G

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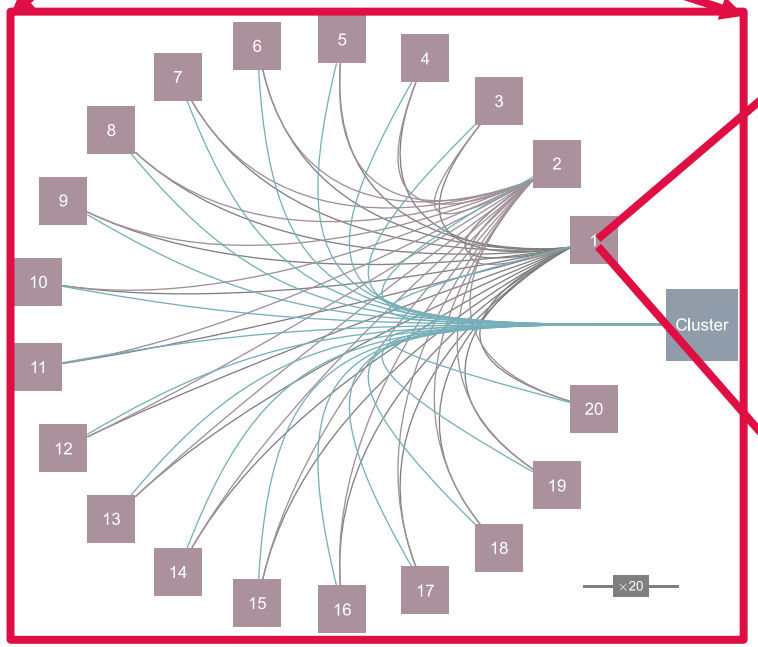

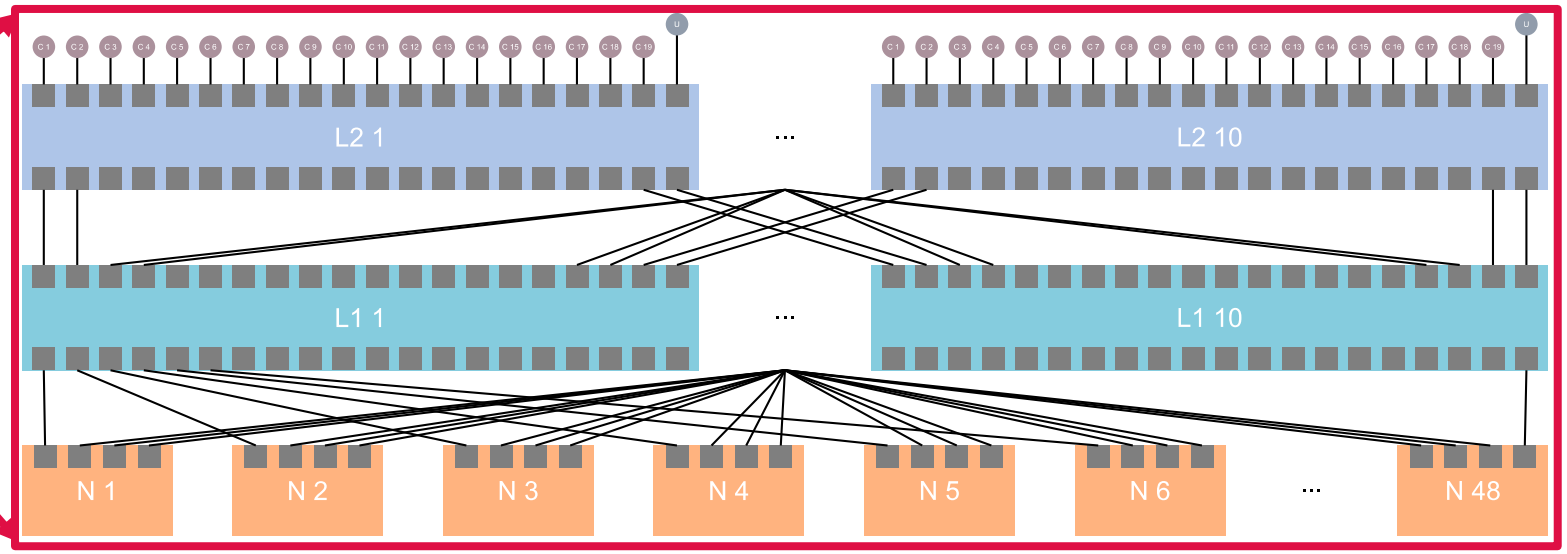

JUQCS-G

Running on JUWELS Booster

- 936 Compute nodes
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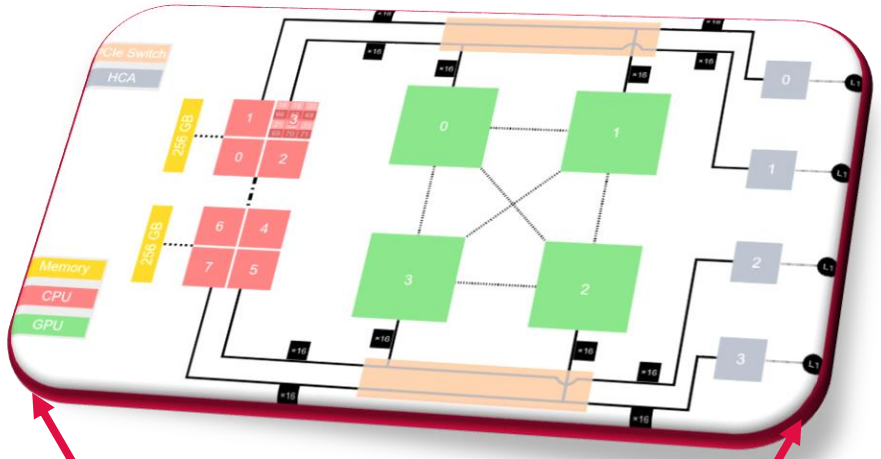
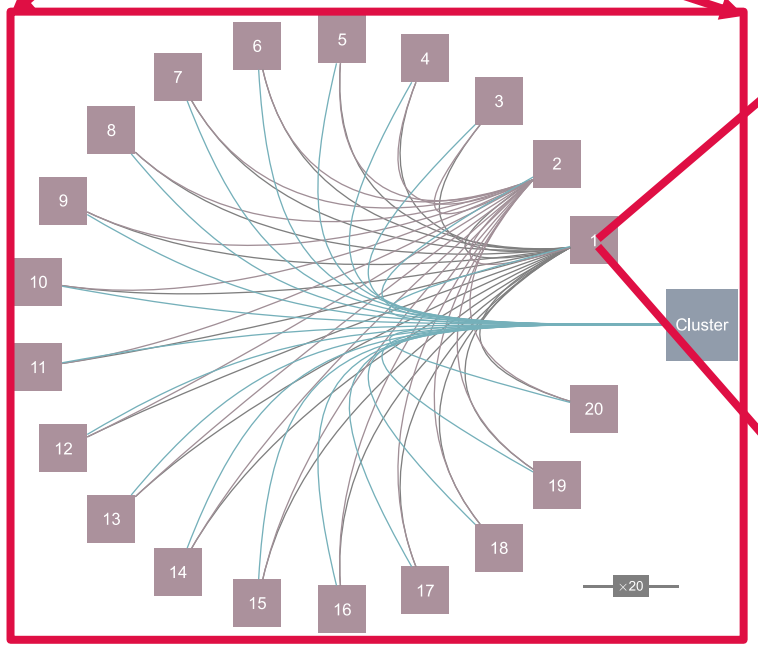
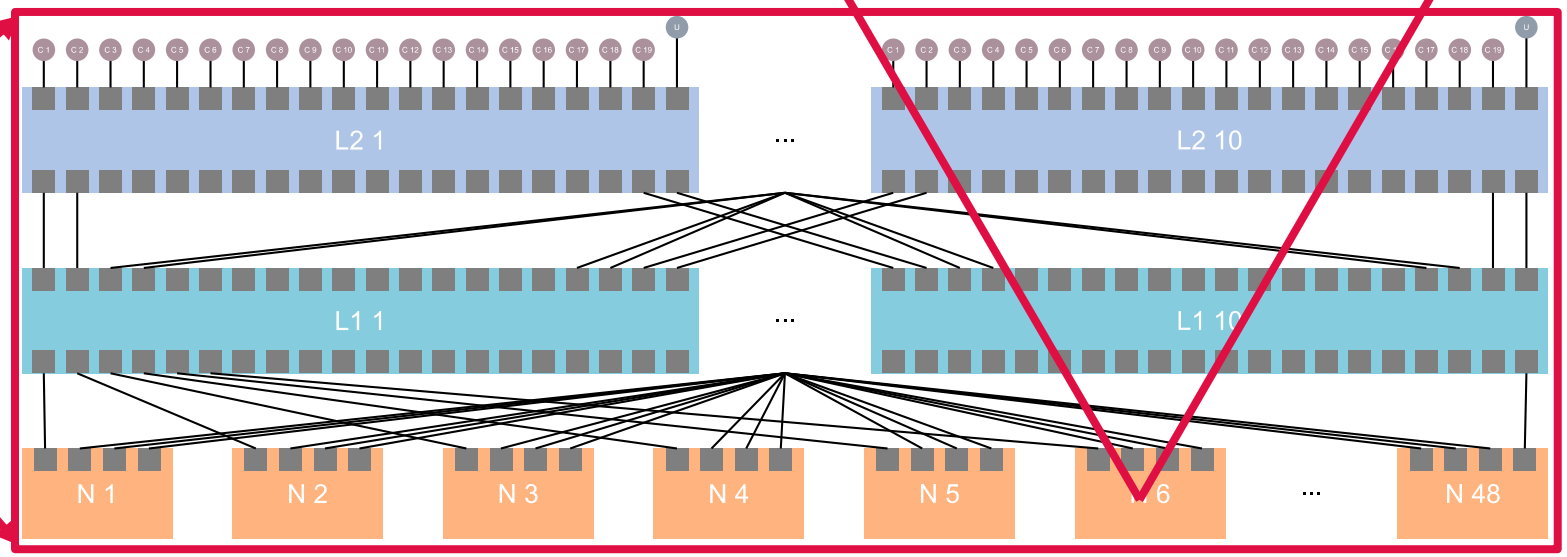
4 A100 GPUs per node





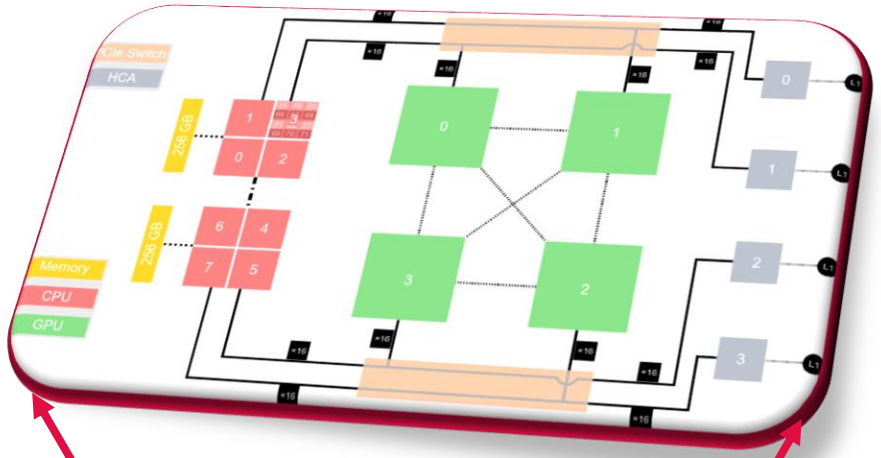


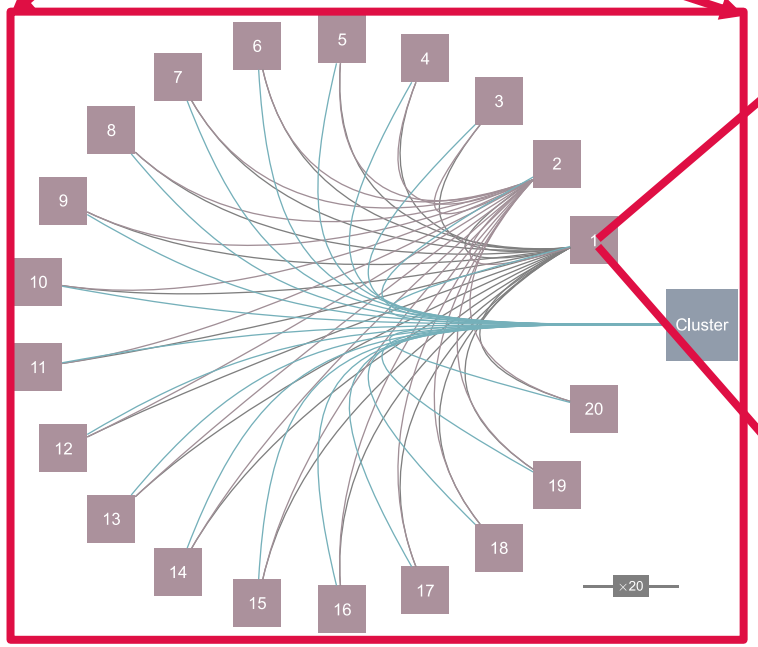
JUQCS-G

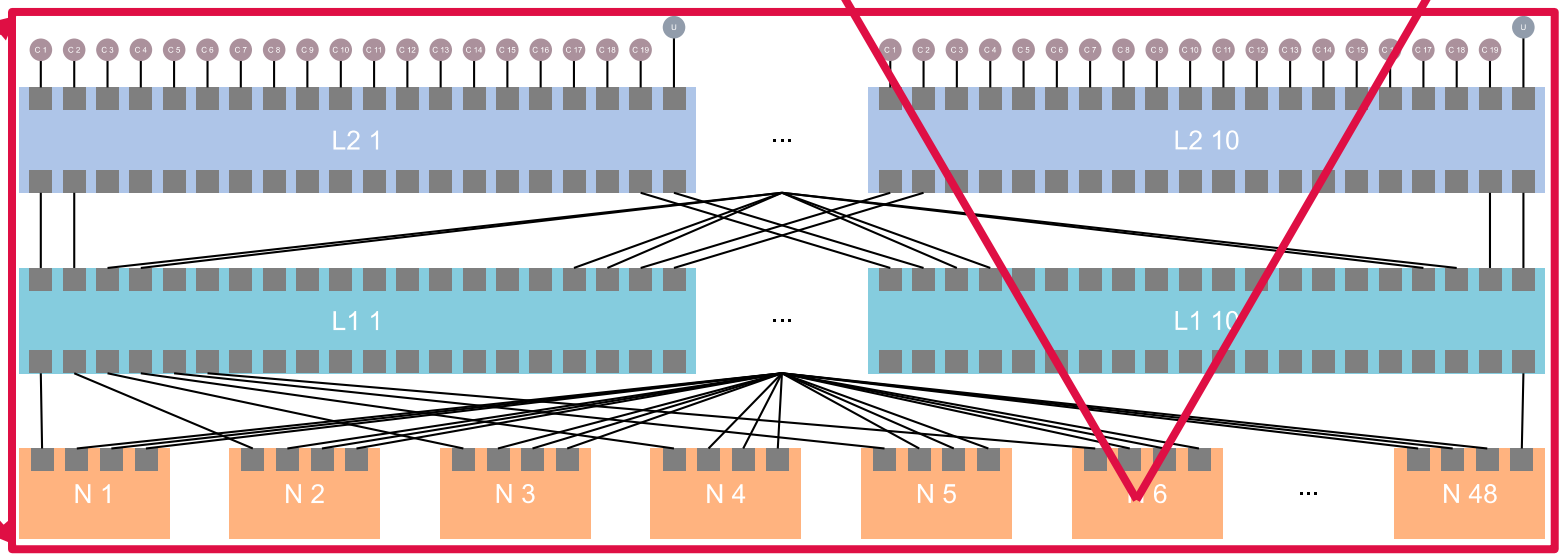
Running on JUWELS Booster

- 936 Compute nodes
- DragonFly+ Topology
- 3744 NVIDIA A100 GPUs

4 A100 GPUs per node







JUQCS-G

Running on JUWELS Booster

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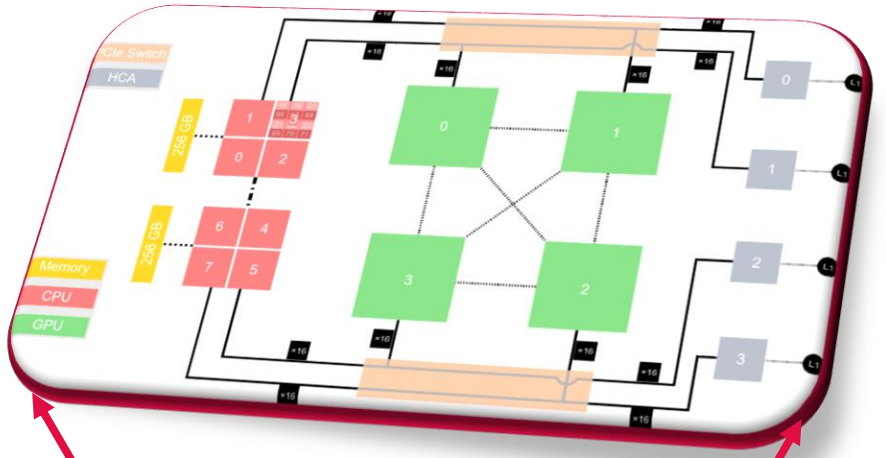
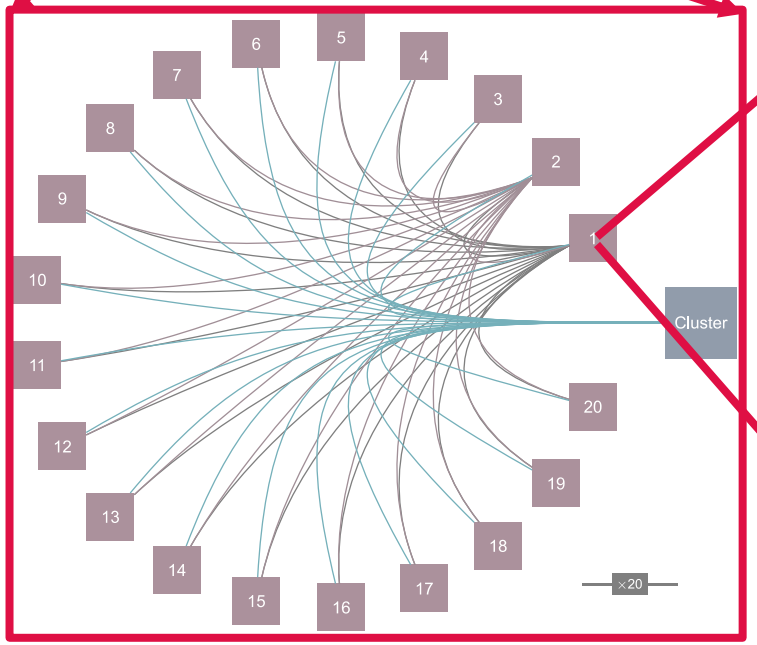
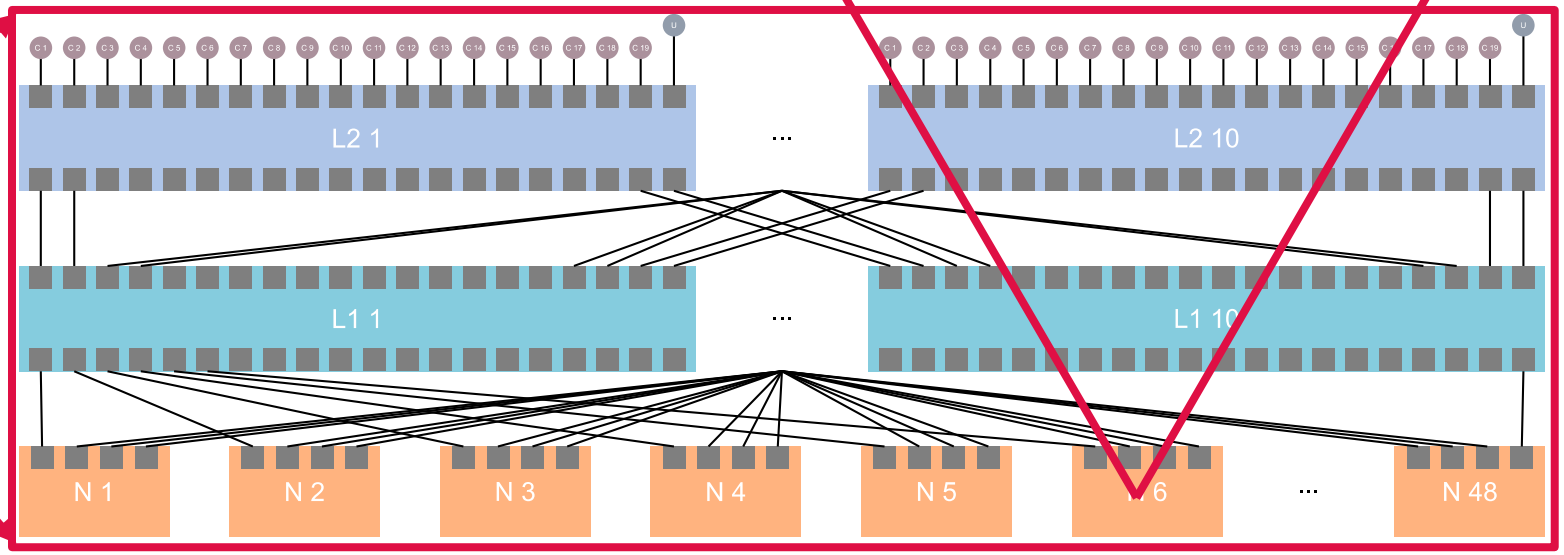
- 3744 NVIDIA A100 GPUs
- 73 PFLOP/s

4 A100 GPUs per node







JUQCS-G

Running on JUWELS Booster

Top500 Nov-2020:

- #1 Europe
- #7 World
- #3 Green500

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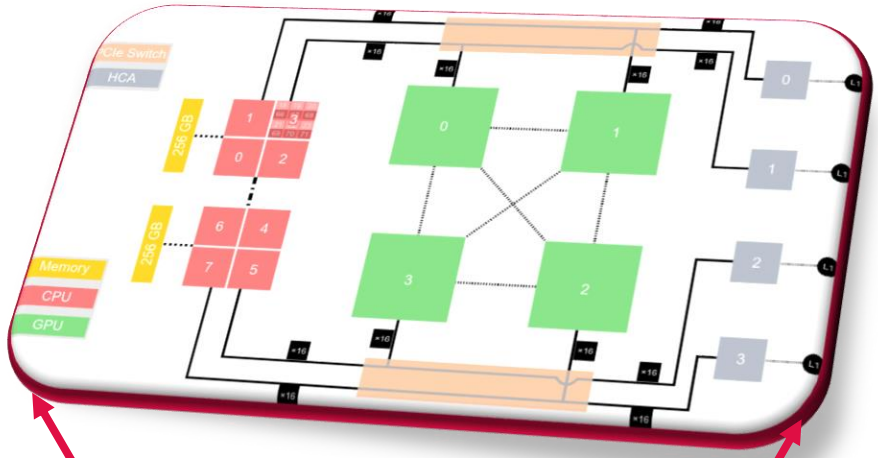

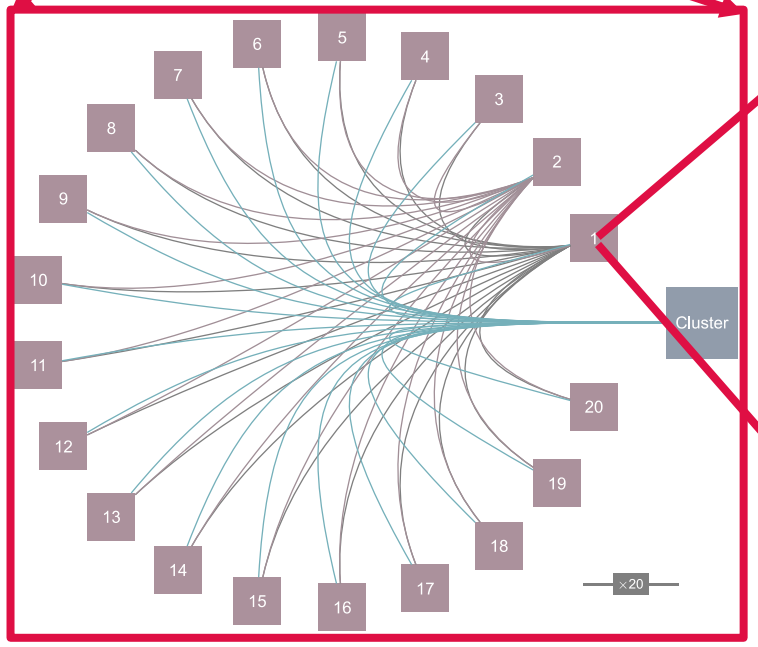

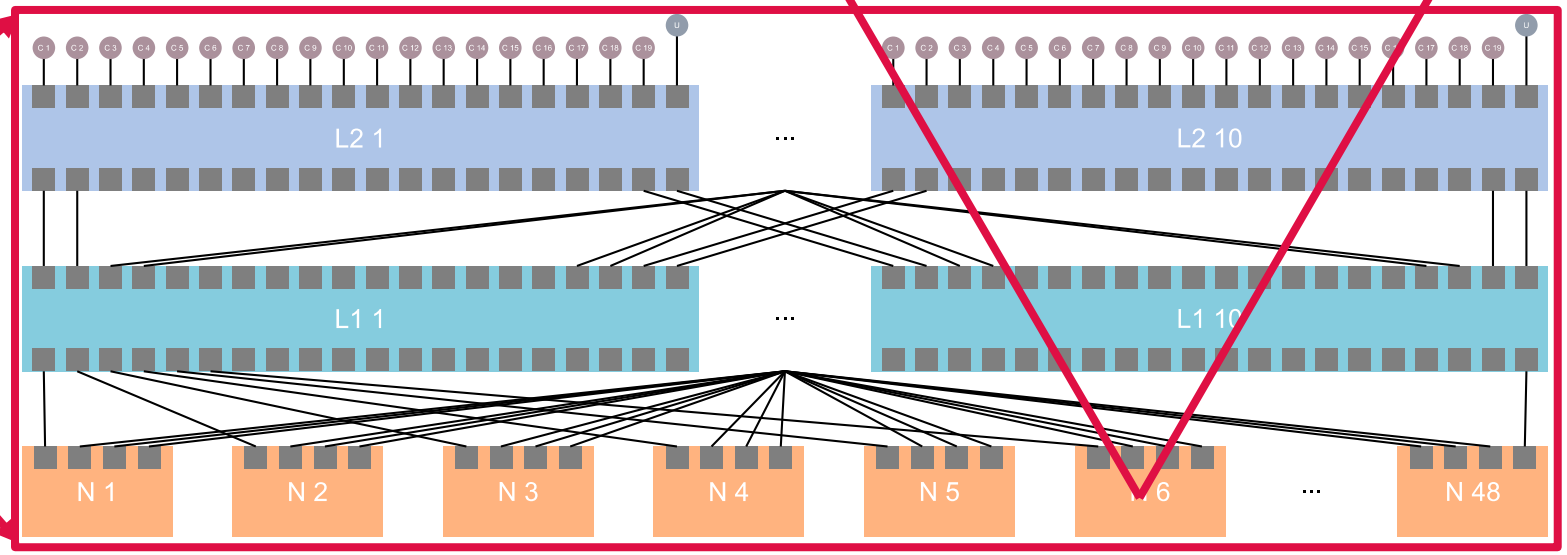

JUQCS-G

Why we can use it to benchmark GPU clusters like JUWELS Booster

JUQCS-G

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- **Memory-intensive:**
  - For 40 qubits: $2^{40}\ \psi's$ = 16 TiB memory

JUQCS-G

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  - Global gates need transfer of **one half** of all memory
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JUQCS-G

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JUQCS-G

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QPU = Quantum Processing Unit

JUQCS-G

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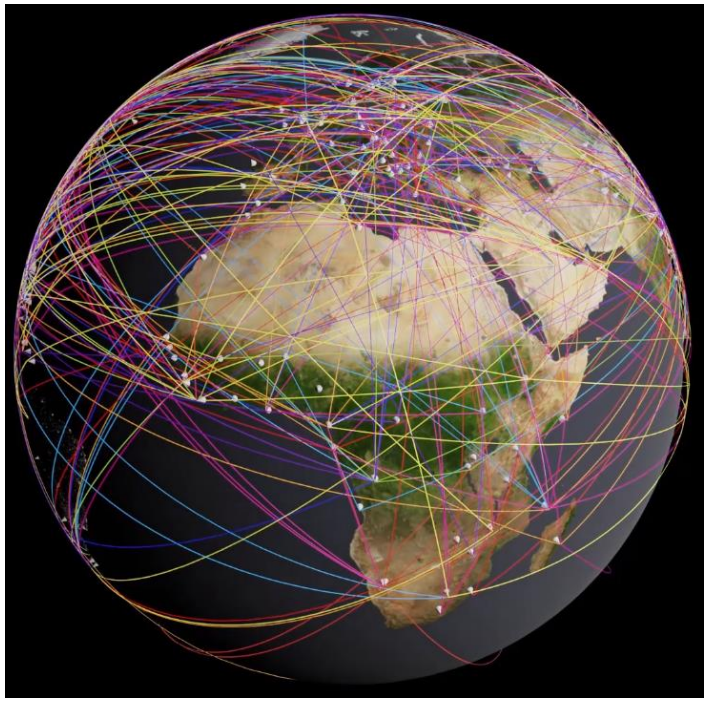
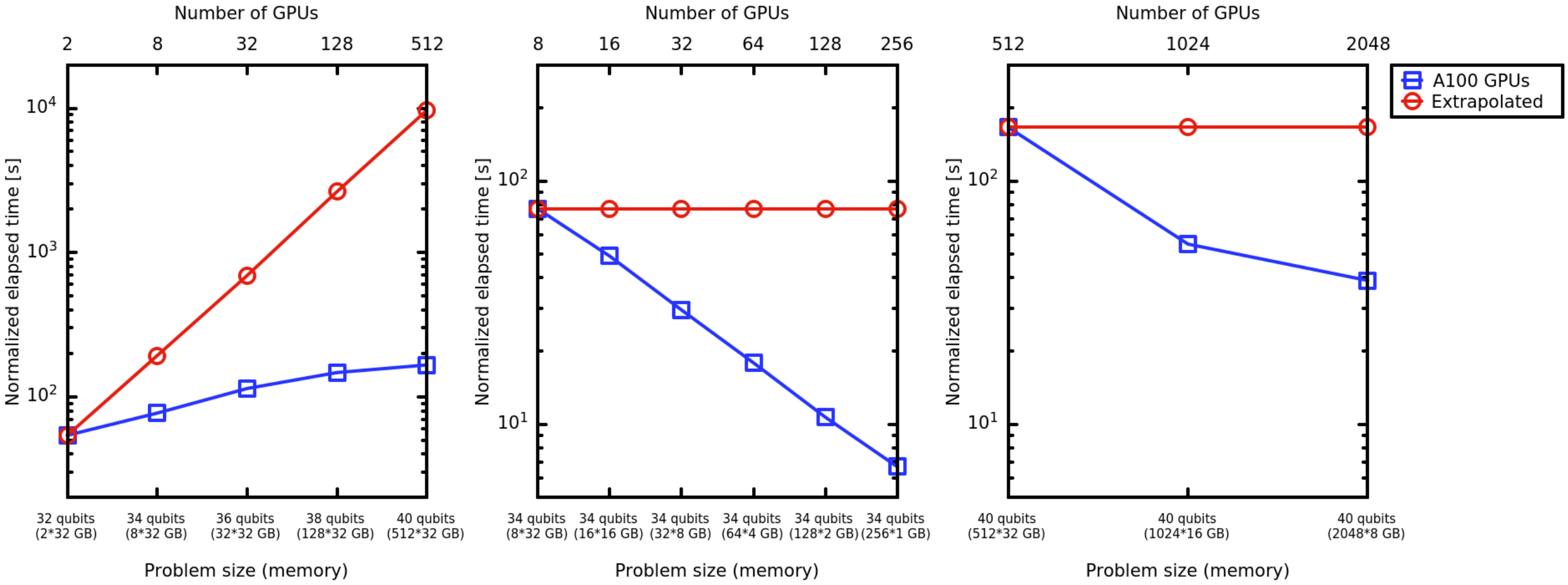
Application:

Solve airplane scheduling problems using the **Q**uantum **A**pproximate **O**ptimization **A**lgorithm



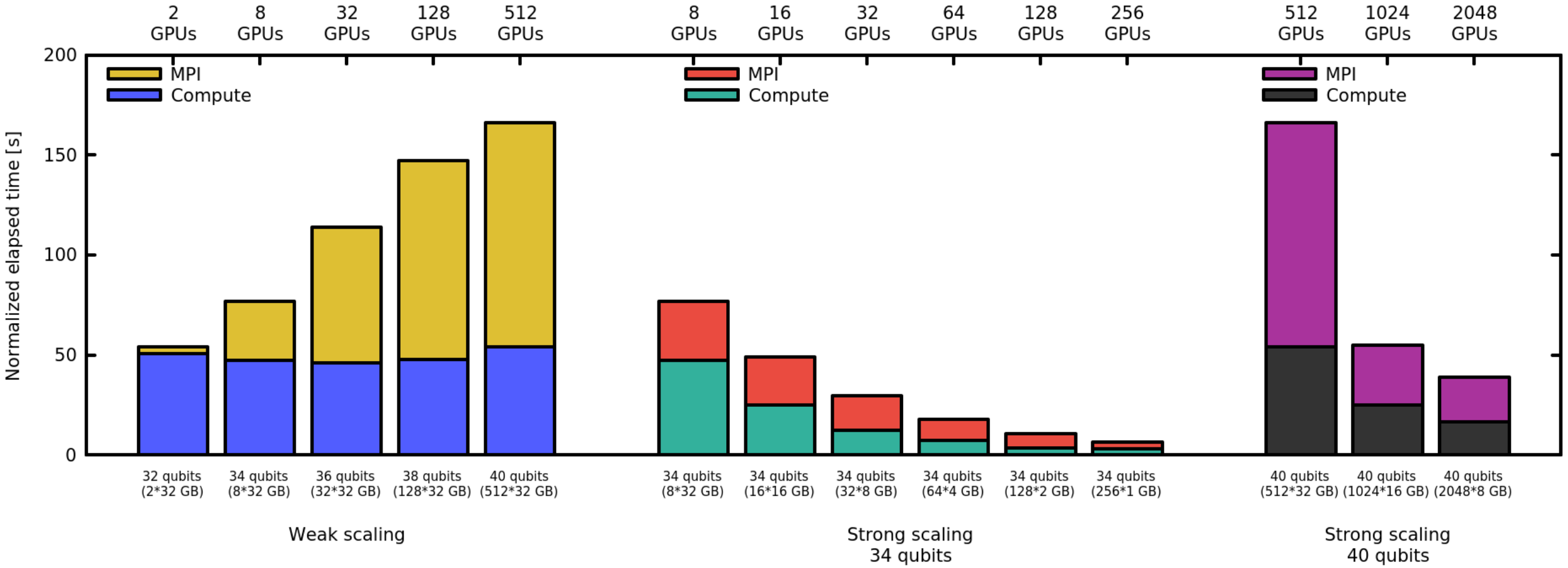
JUQCS-G

Weak and strong scaling results



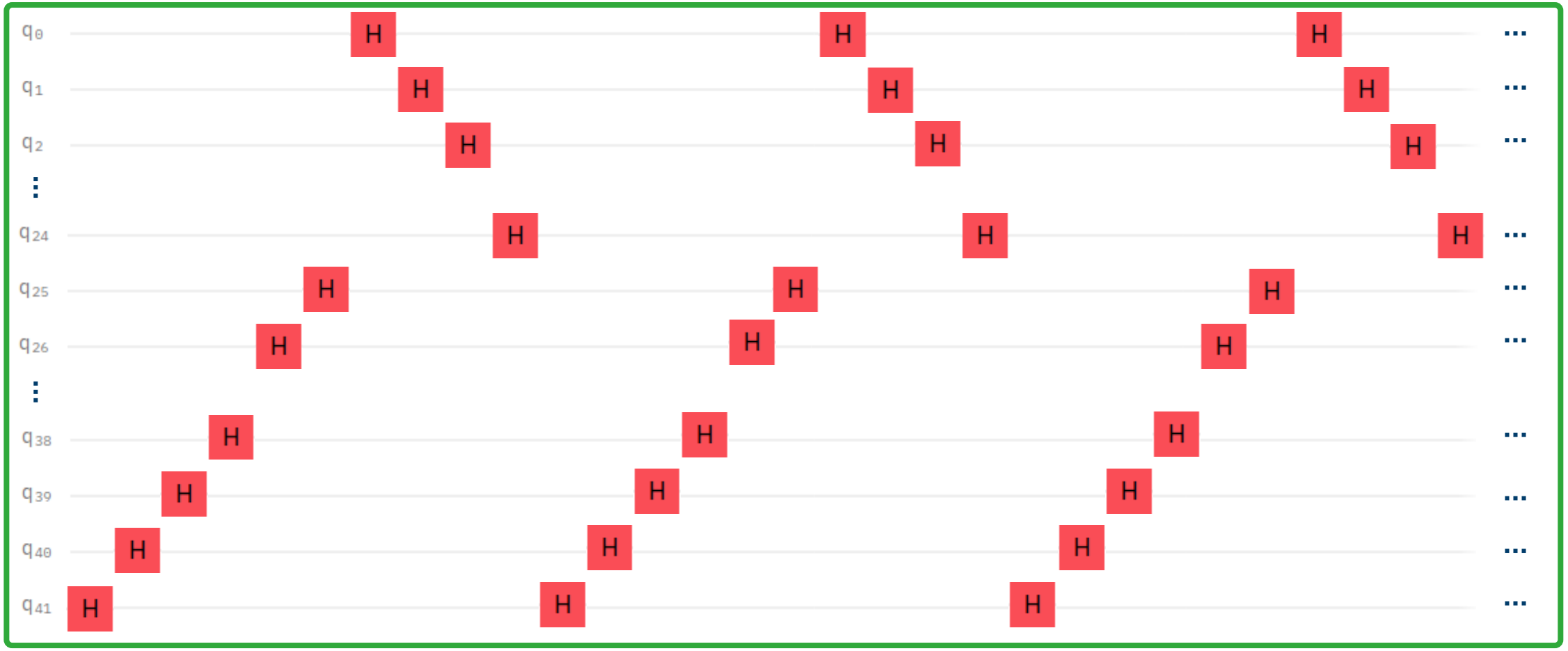
JUQCS-G

Weak and strong scaling results: MPI vs. Compute Time



JUQCS-G

Weak and strong scaling results: Hadamard benchmark circuits



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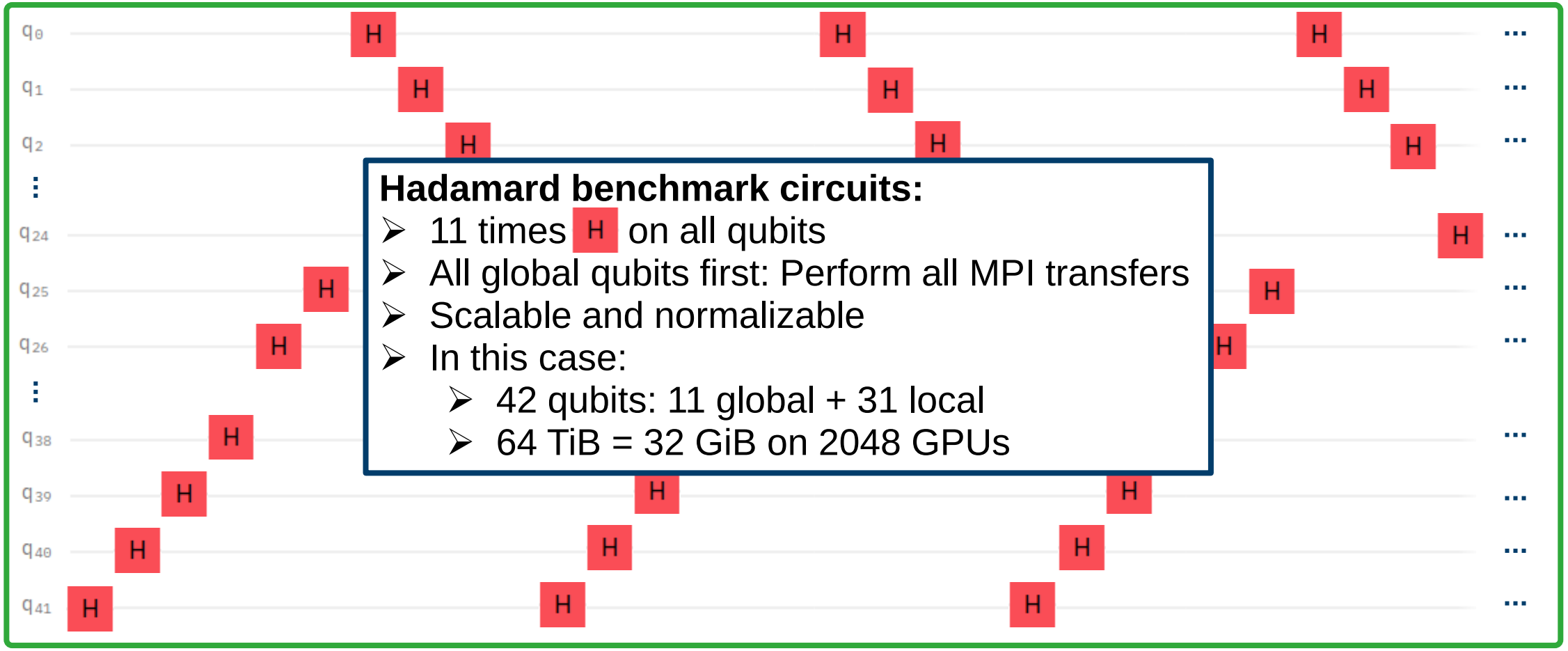
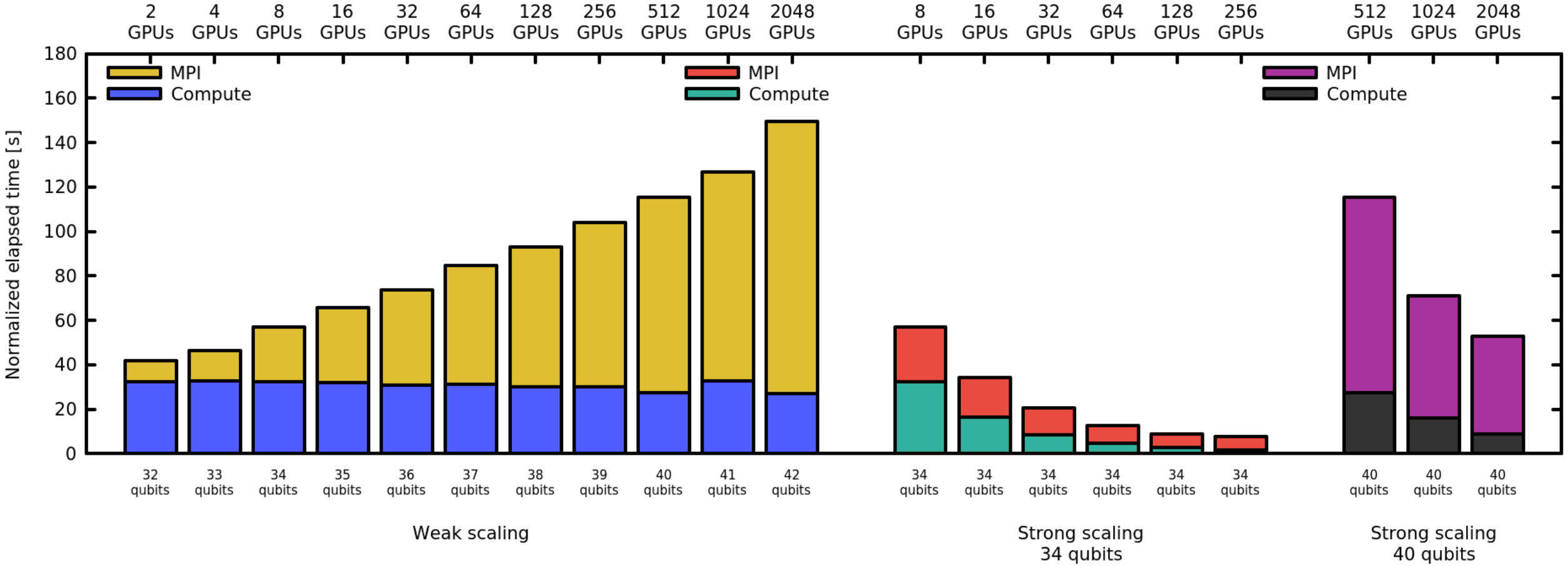


Hadamard benchmark circuits:

- 11 times H on all qubits
- All global qubits first: Perform all MPI transfers
- Scalable and normalizable
- In this case:
  - 42 qubits: 11 global + 31 local
  - 64 TiB = 32 GiB on 2048 GPUs

JUQCS-G

Weak and strong scaling results: Hadamard benchmark circuits



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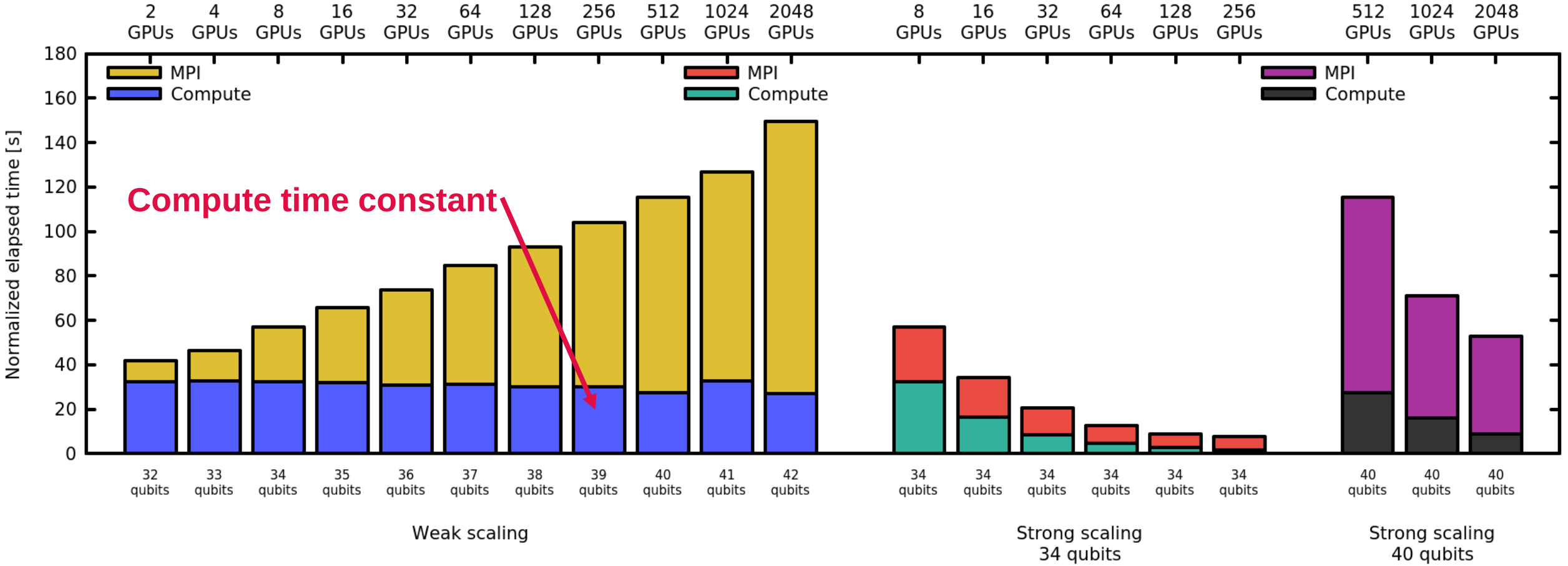

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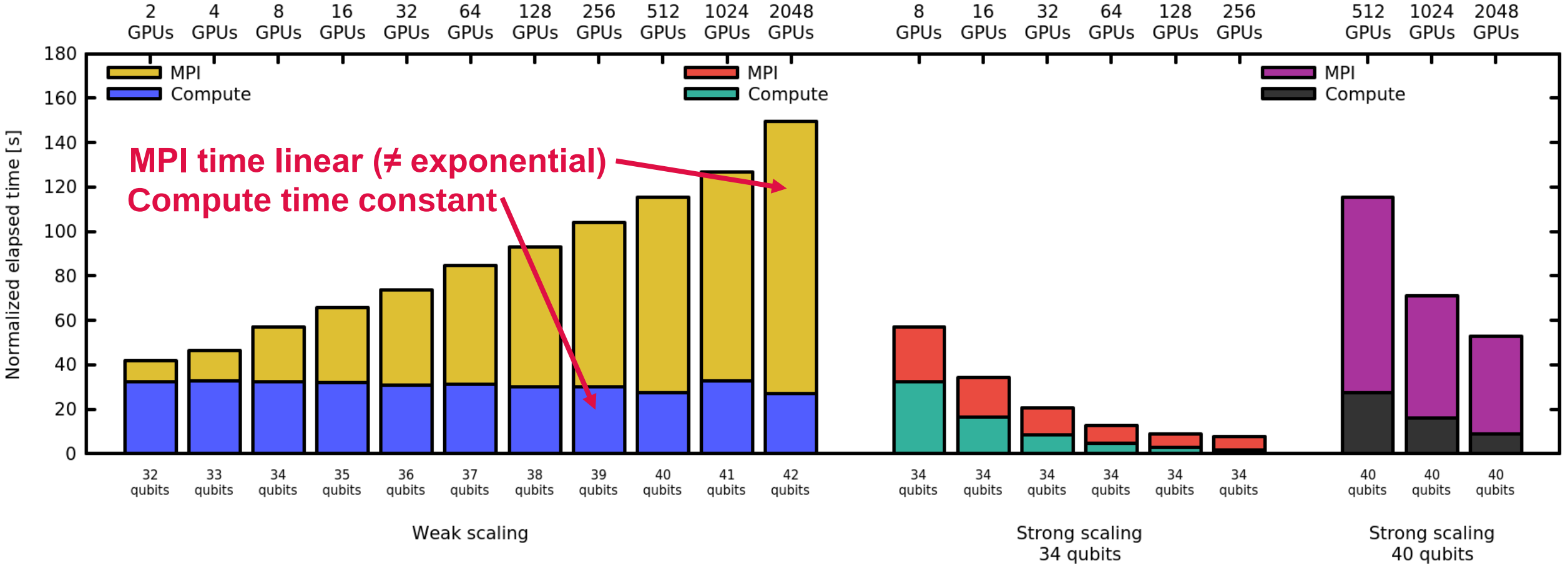

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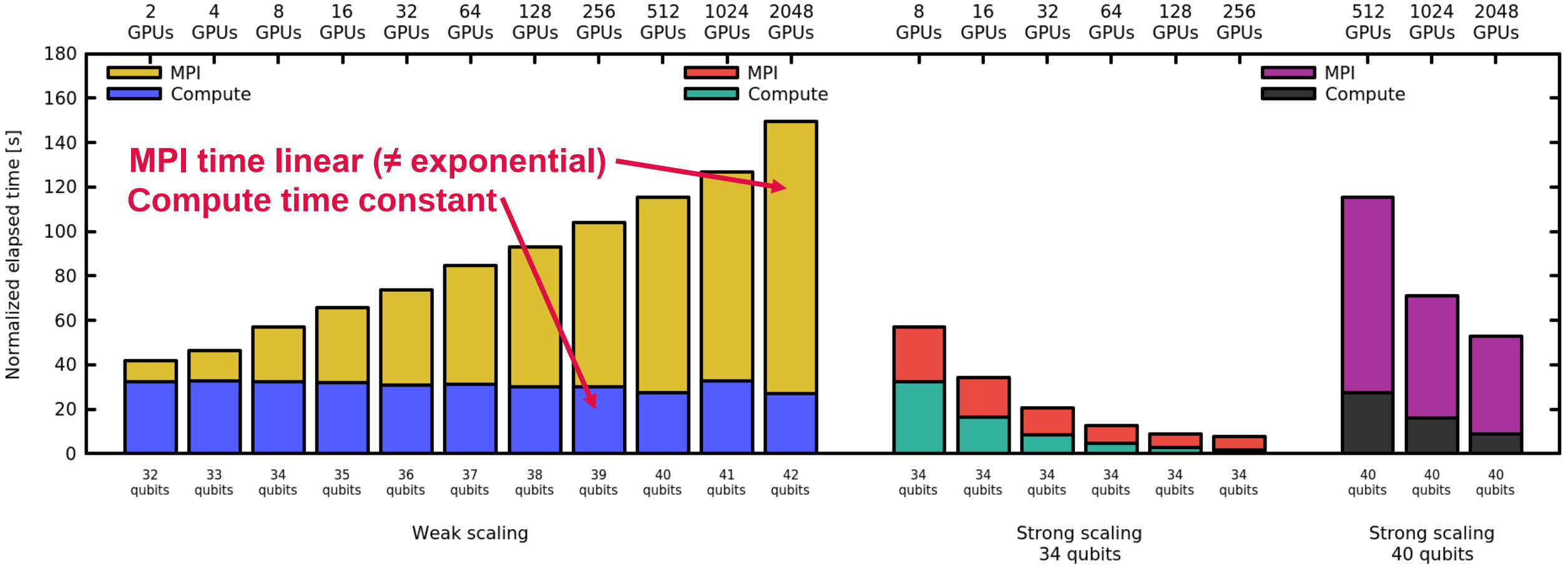

➢ **Speedup** (compute time per node)**:** JUWELS Cluster → JUWELS GPUs (**NVIDIA V100**): 10

JUQCS-G

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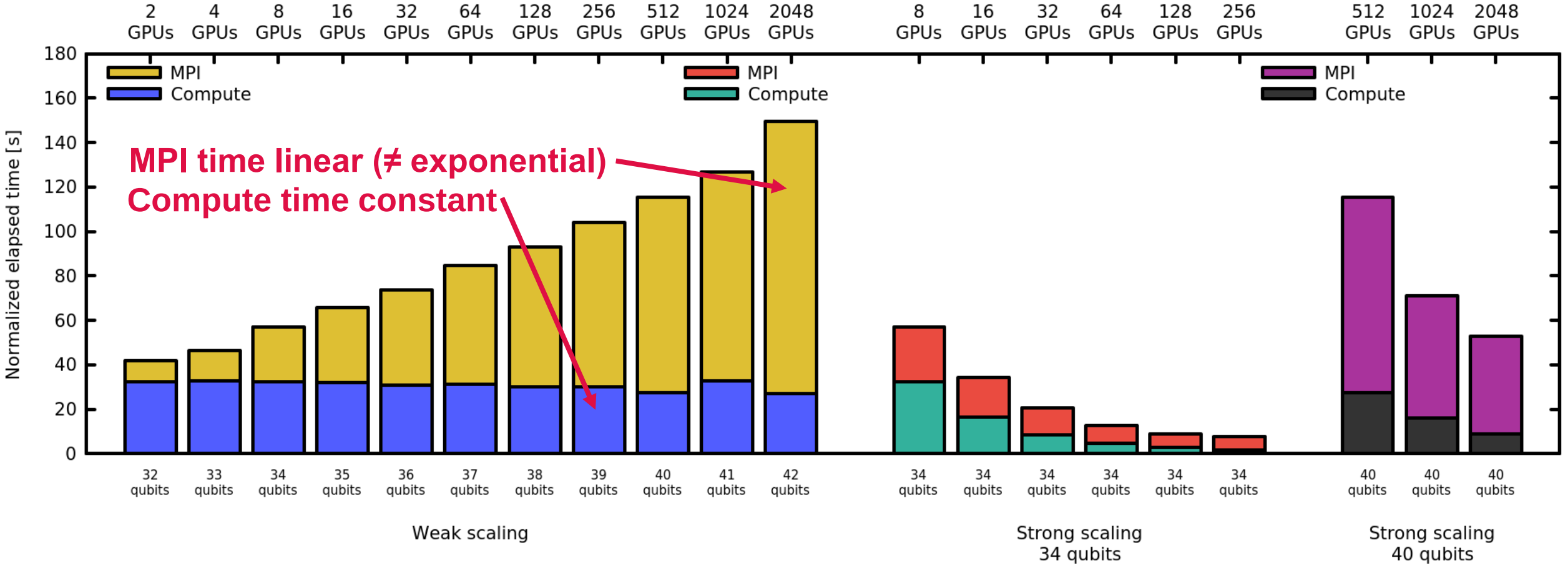

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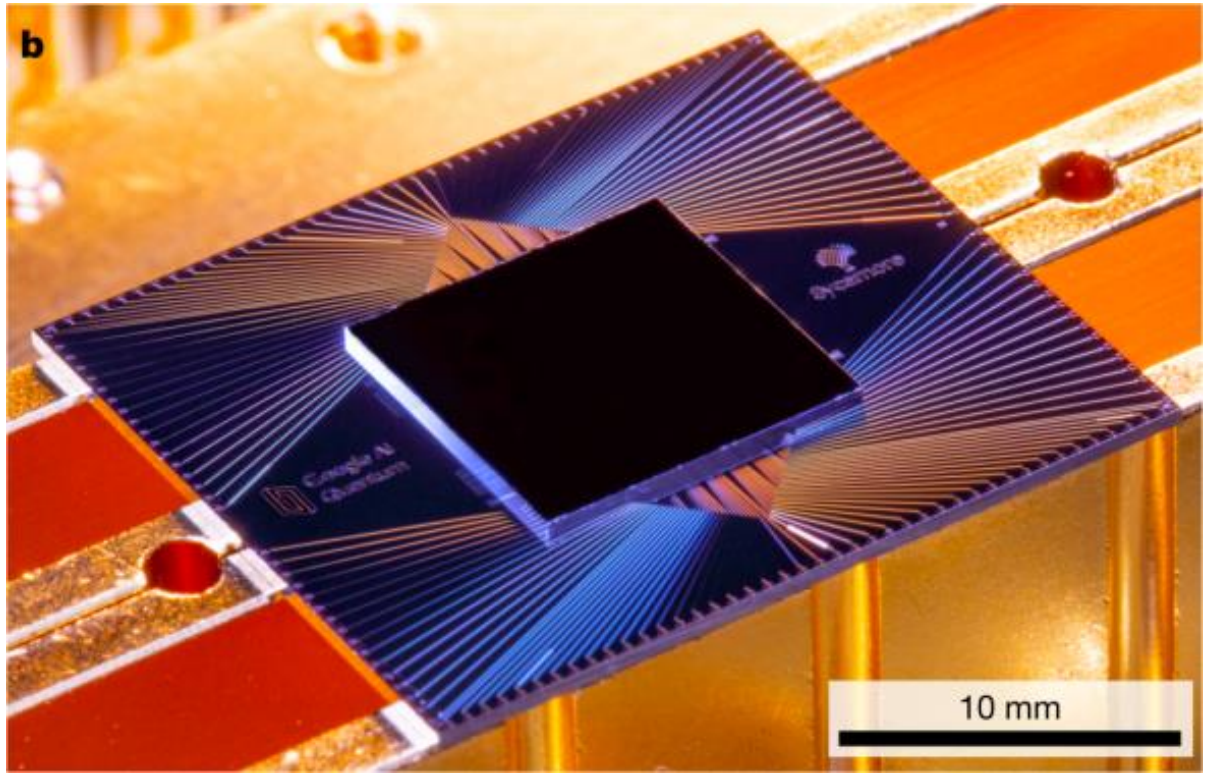
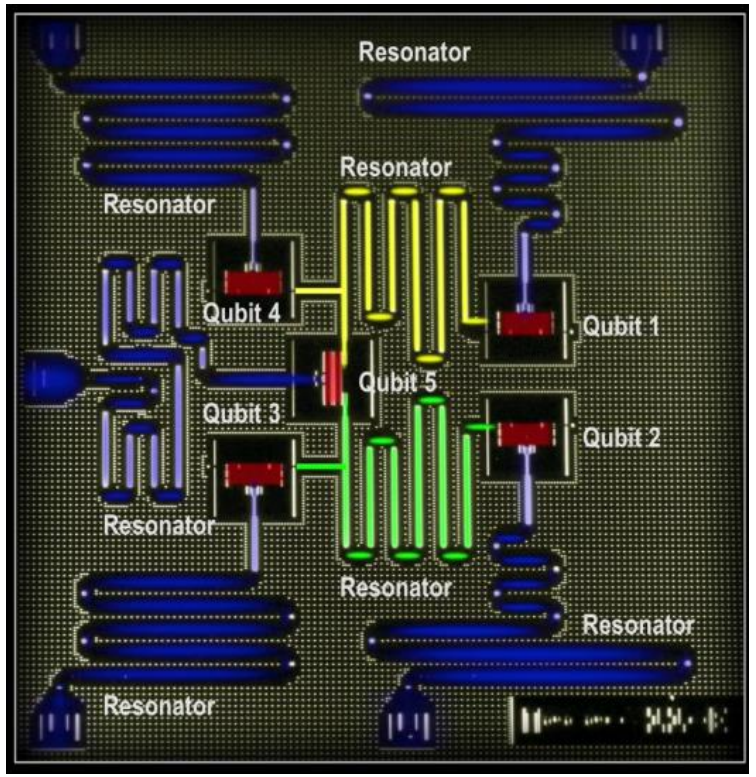
- **Speedup** (compute time per node)**:** JUWELS GPUs → JUWELS Booster (**NVIDIA A100**): 2 – 3

JUQMES: QUANTUM MASTER EQUATION SIMULATOR

Simulating physical realizations of quantum computers on GPUs

CUDA+OpenACC MPI C++





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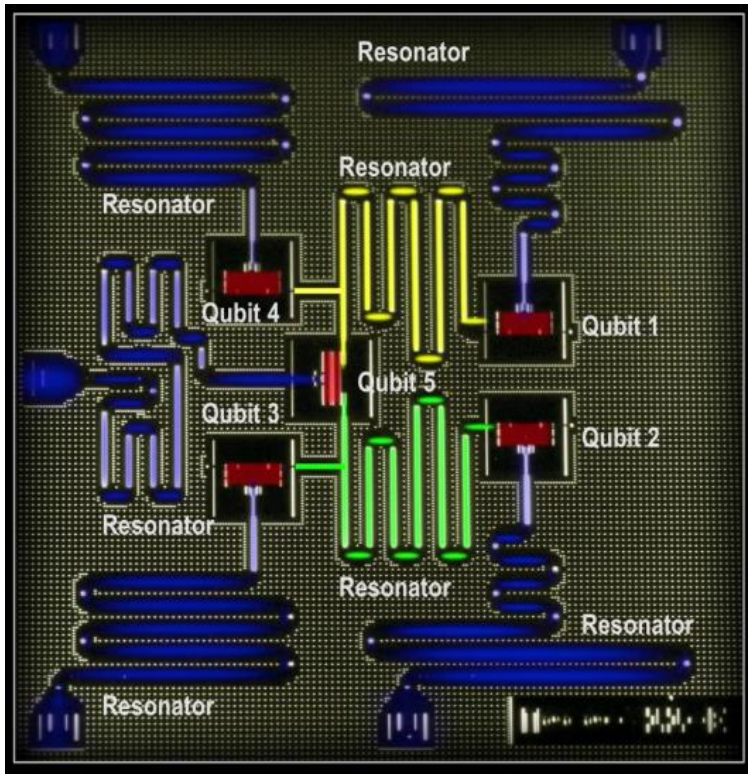
$$\frac{\partial}{\partial t}|\psi\rangle = -iH|\psi\rangle \quad \text{or} \quad \frac{\partial}{\partial t}\rho = -i[H,\rho] + \mathcal{D}[\rho] = \mathcal{L}[\rho]$$



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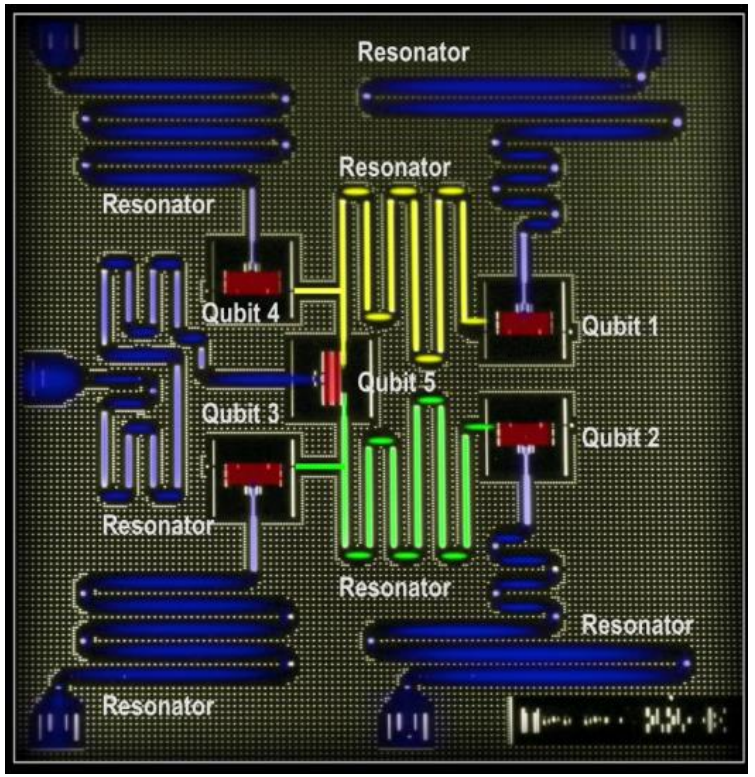

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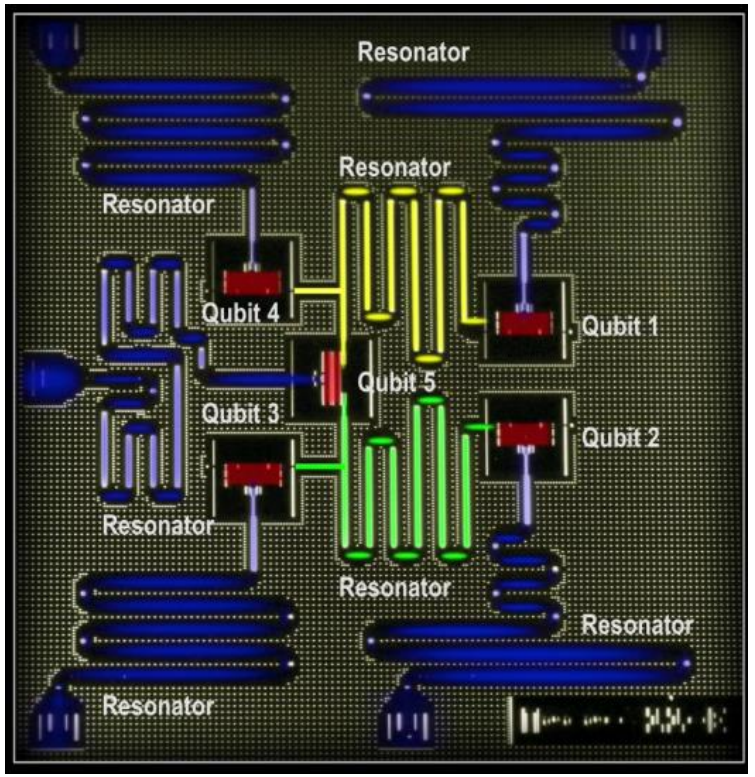
- Similar SPMV updates **but:**
  - Many updates per time step

$$\rho(t+\tau) = e^{\mathcal{L}(t+\tau/2)}\rho(t)$$



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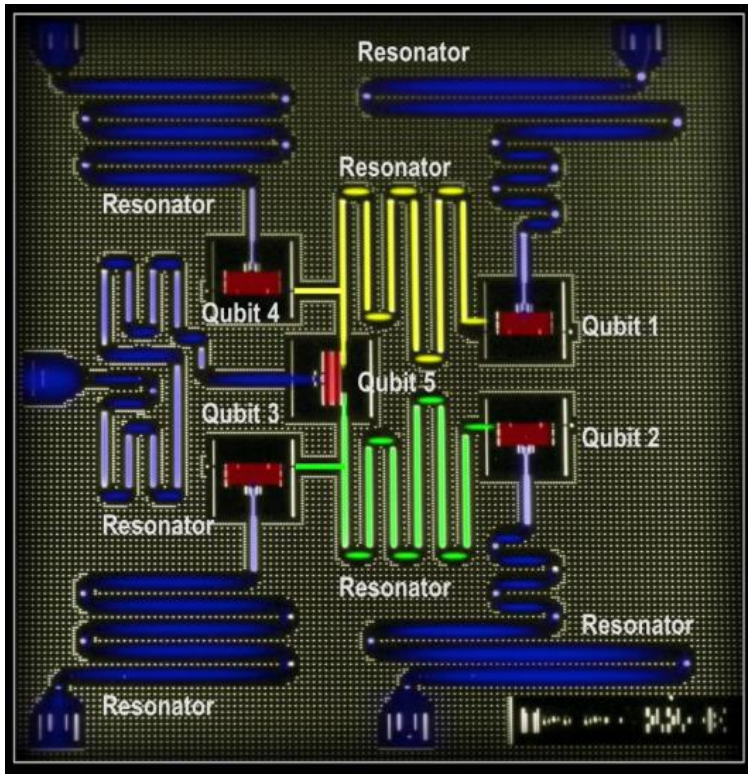

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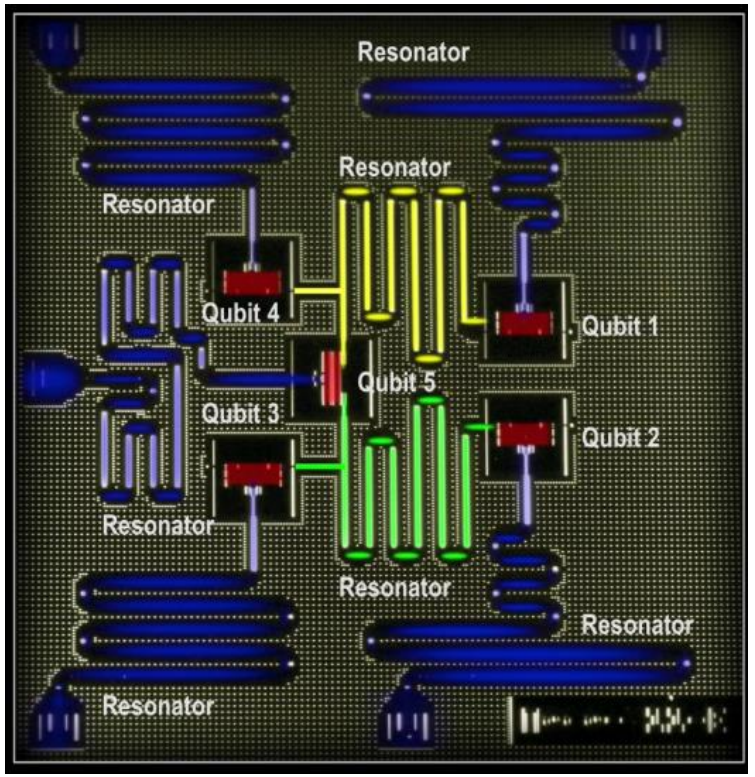

JUQMES: QUANTUM MASTER EQUATION SIMULATOR

Simulating physical realizations of quantum computers on GPUs **CUDA+OpenACC MPI C++**

- Physical realization: Solve Schrödinger / Master Equation

$$\frac{\partial}{\partial t}|\psi\rangle = -iH|\psi\rangle \quad \text{or} \quad \frac{\partial}{\partial t}\rho = -i[H,\rho] + \mathcal{D}[\rho] = \mathcal{L}[\rho]$$

- Similar SPMV updates **but:**
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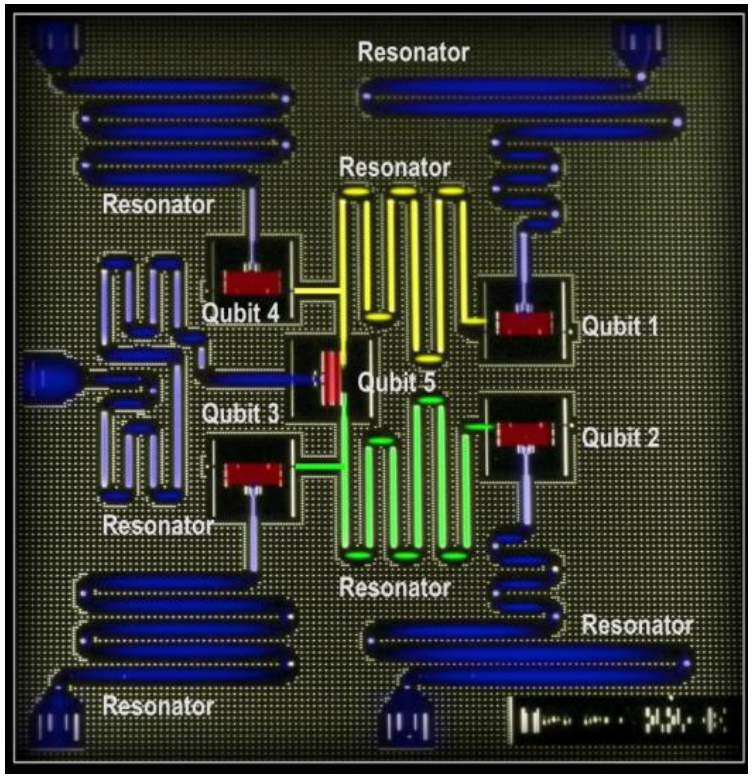

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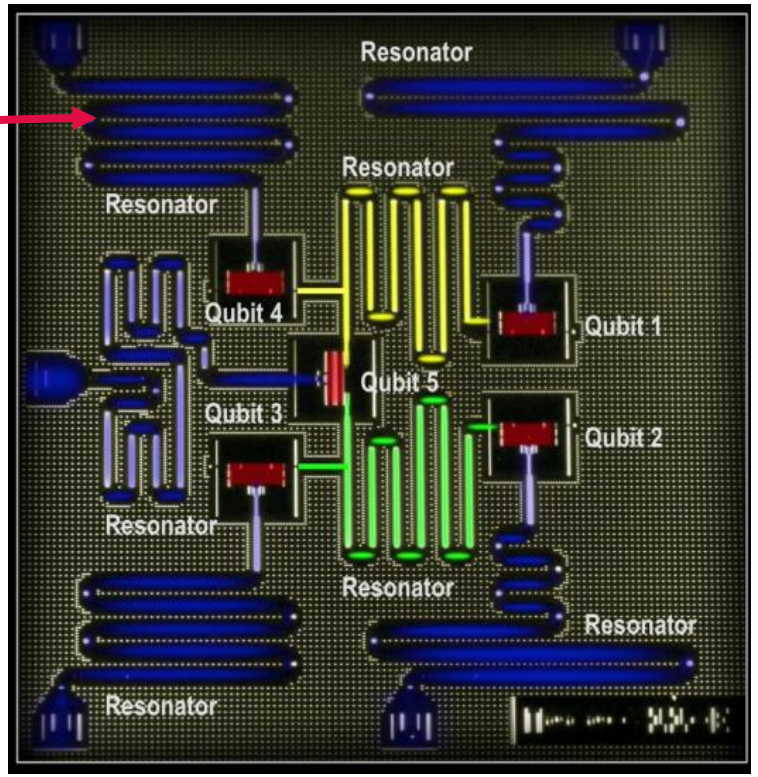

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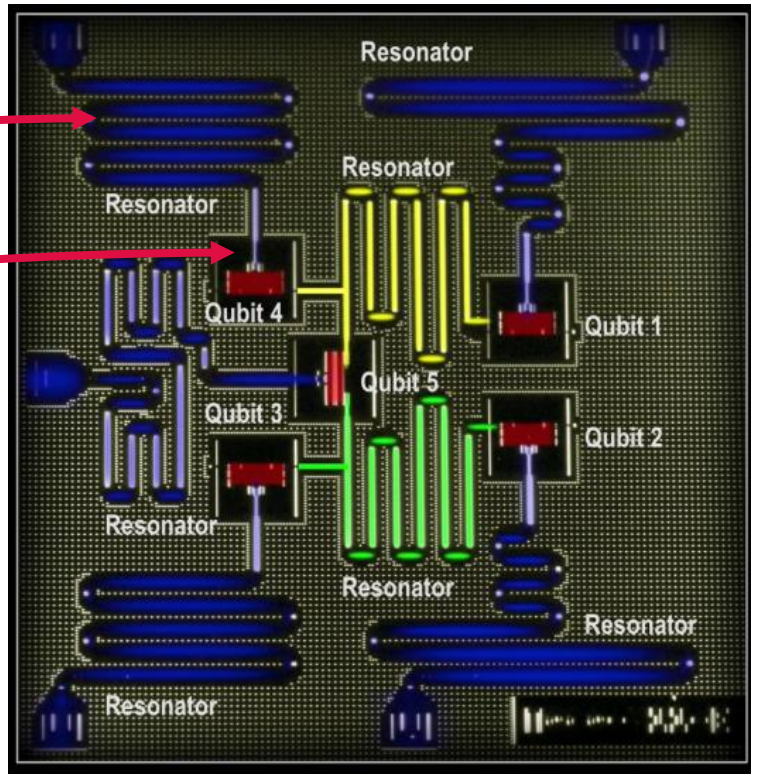

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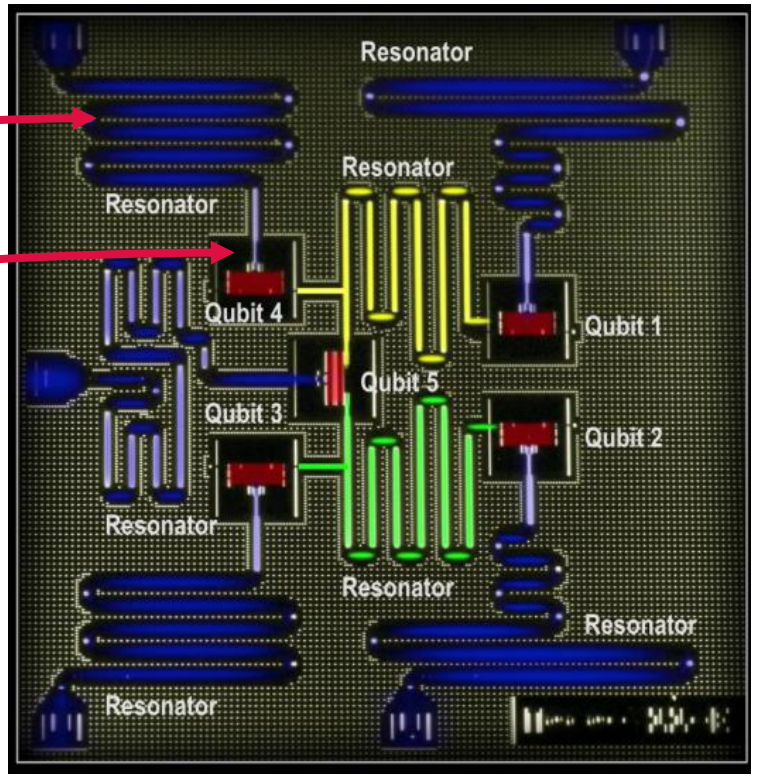

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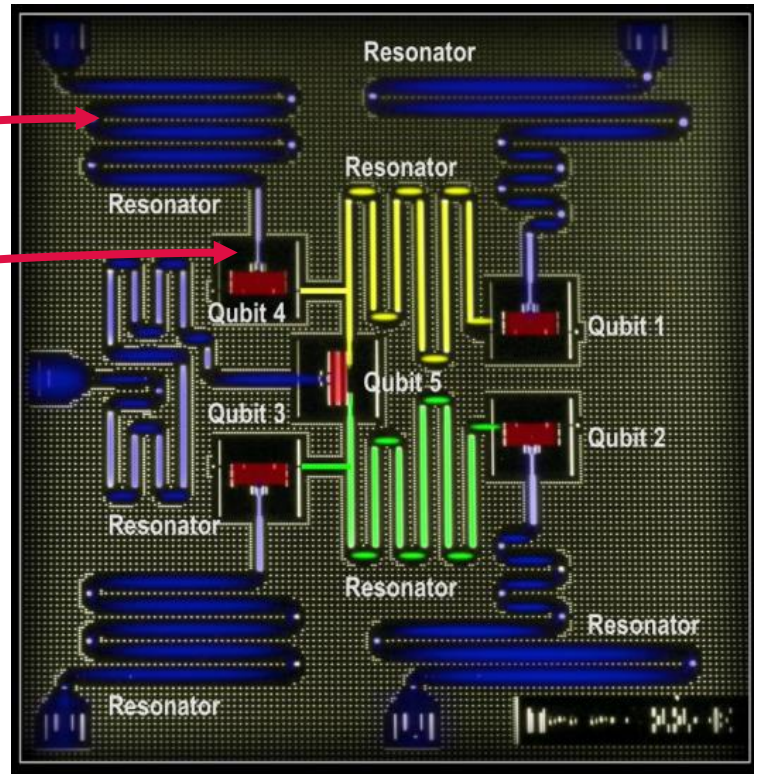

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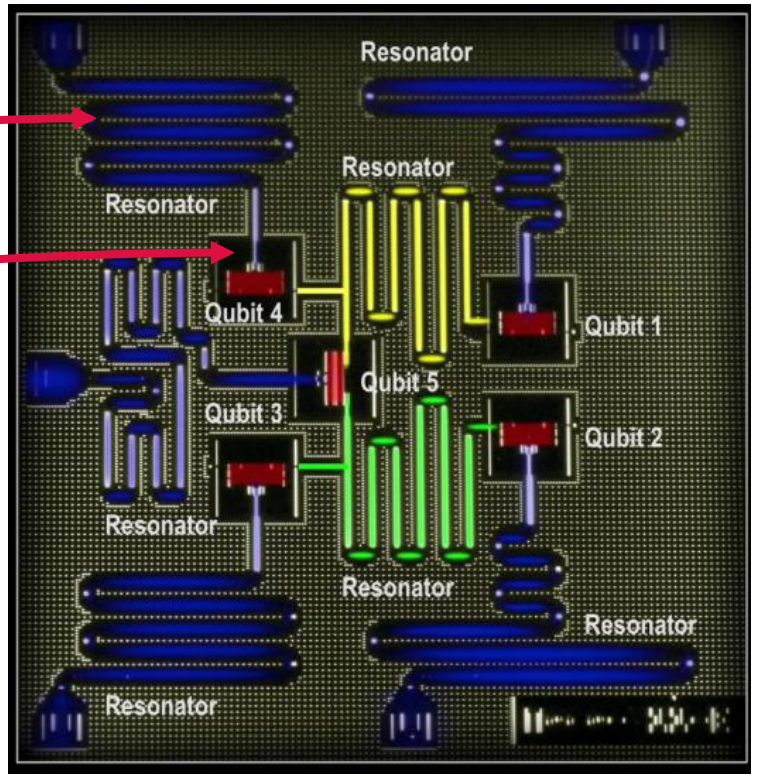

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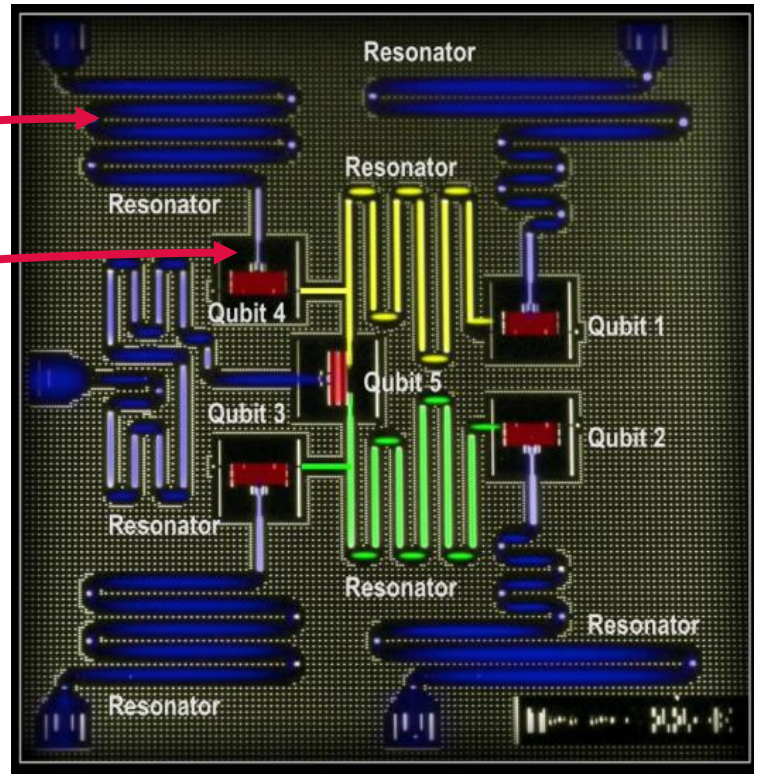

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→ Useful to measure single-GPU performance

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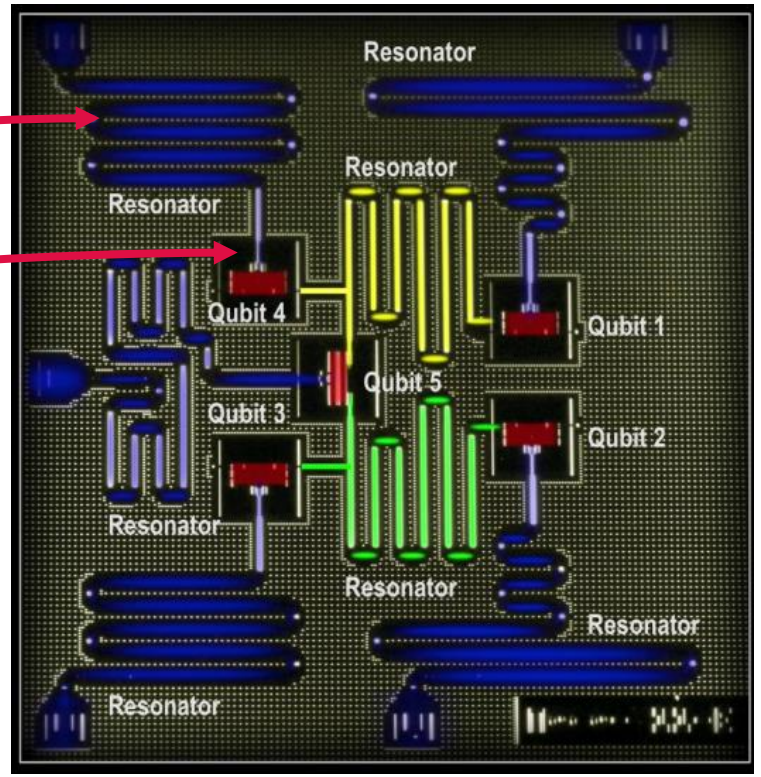

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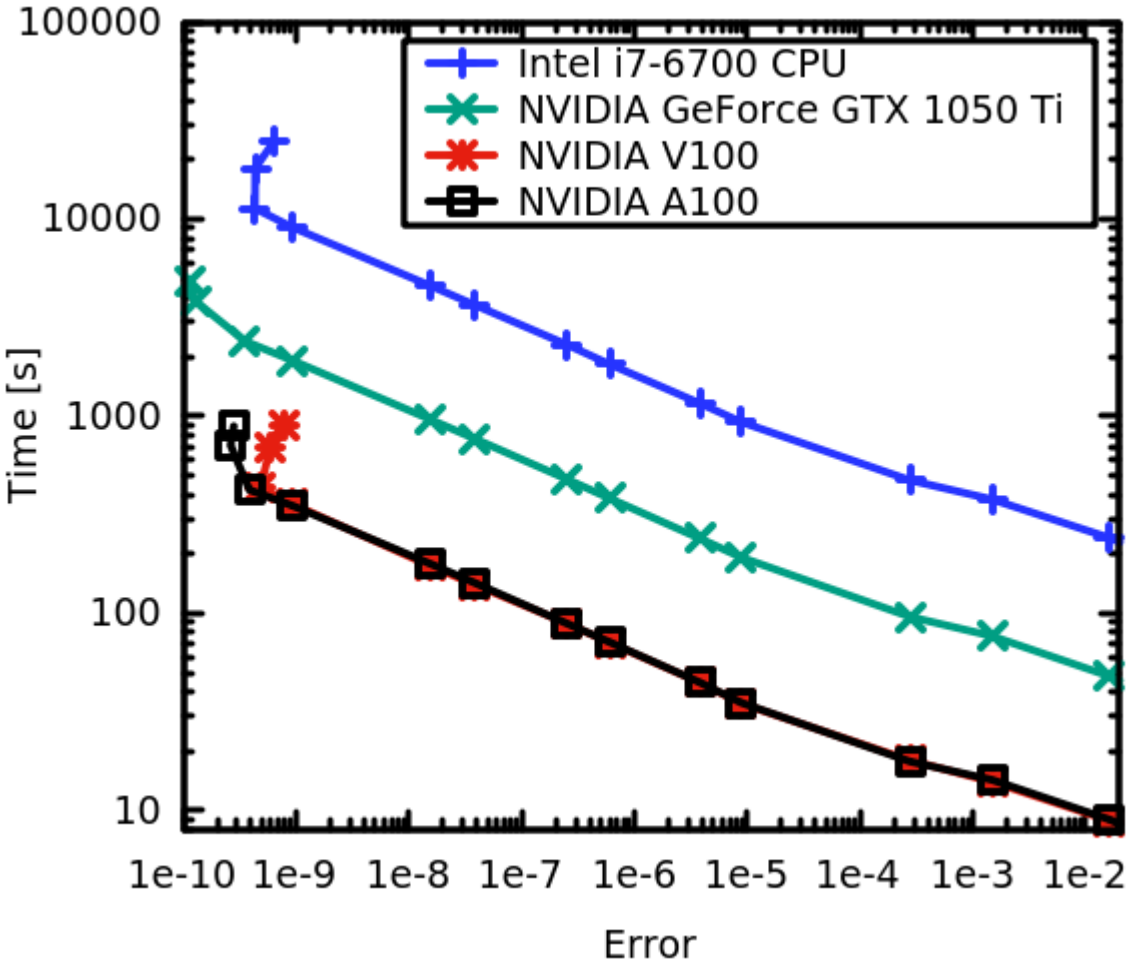

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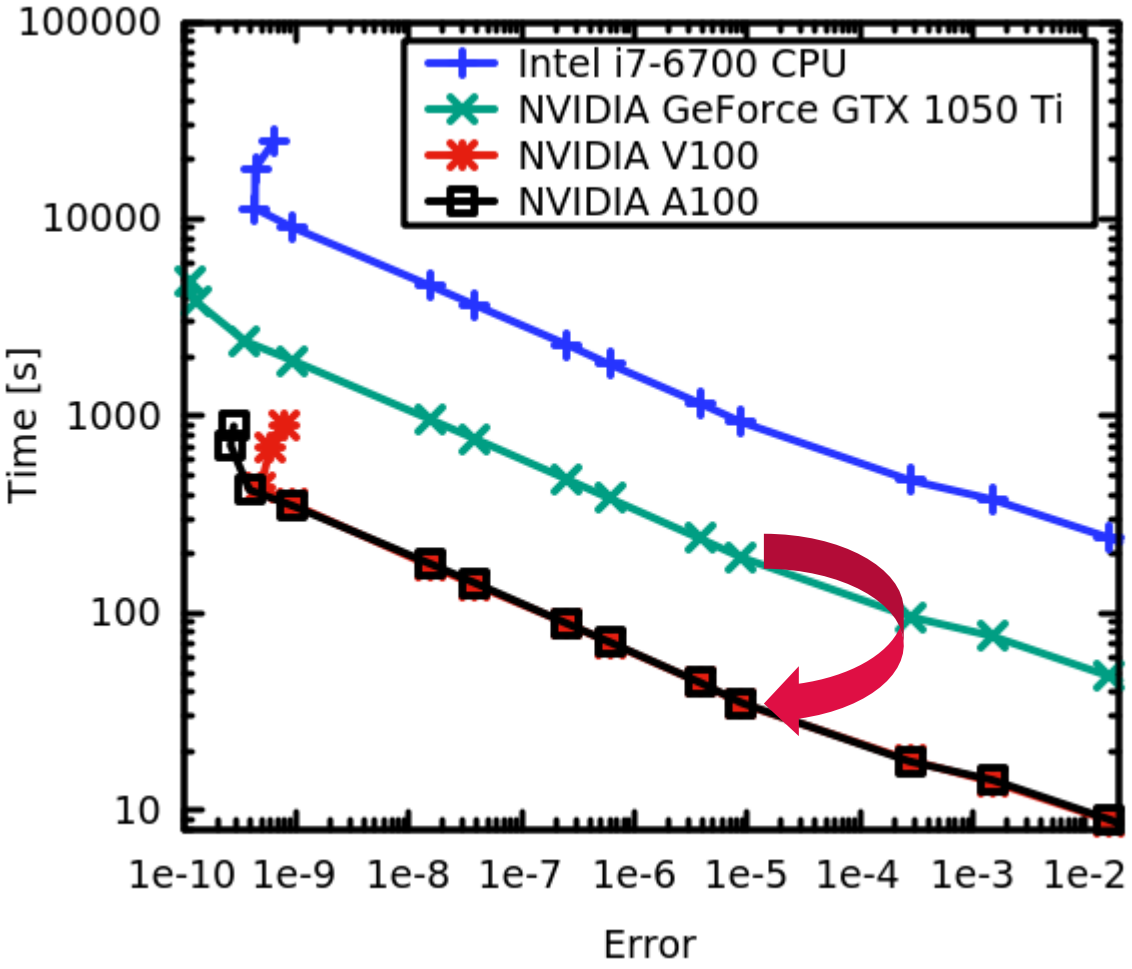

Bottleneck kernels profit from **Tensor Cores**

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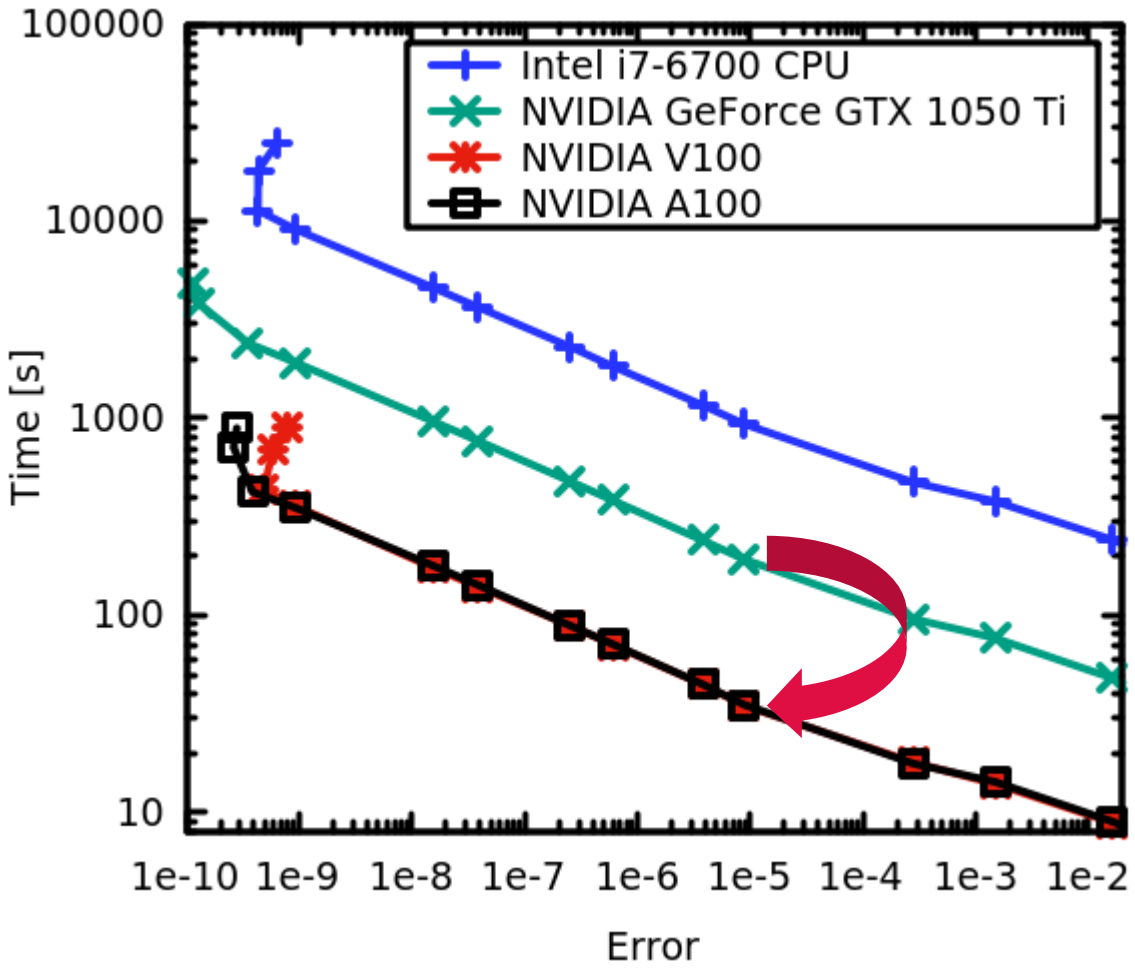

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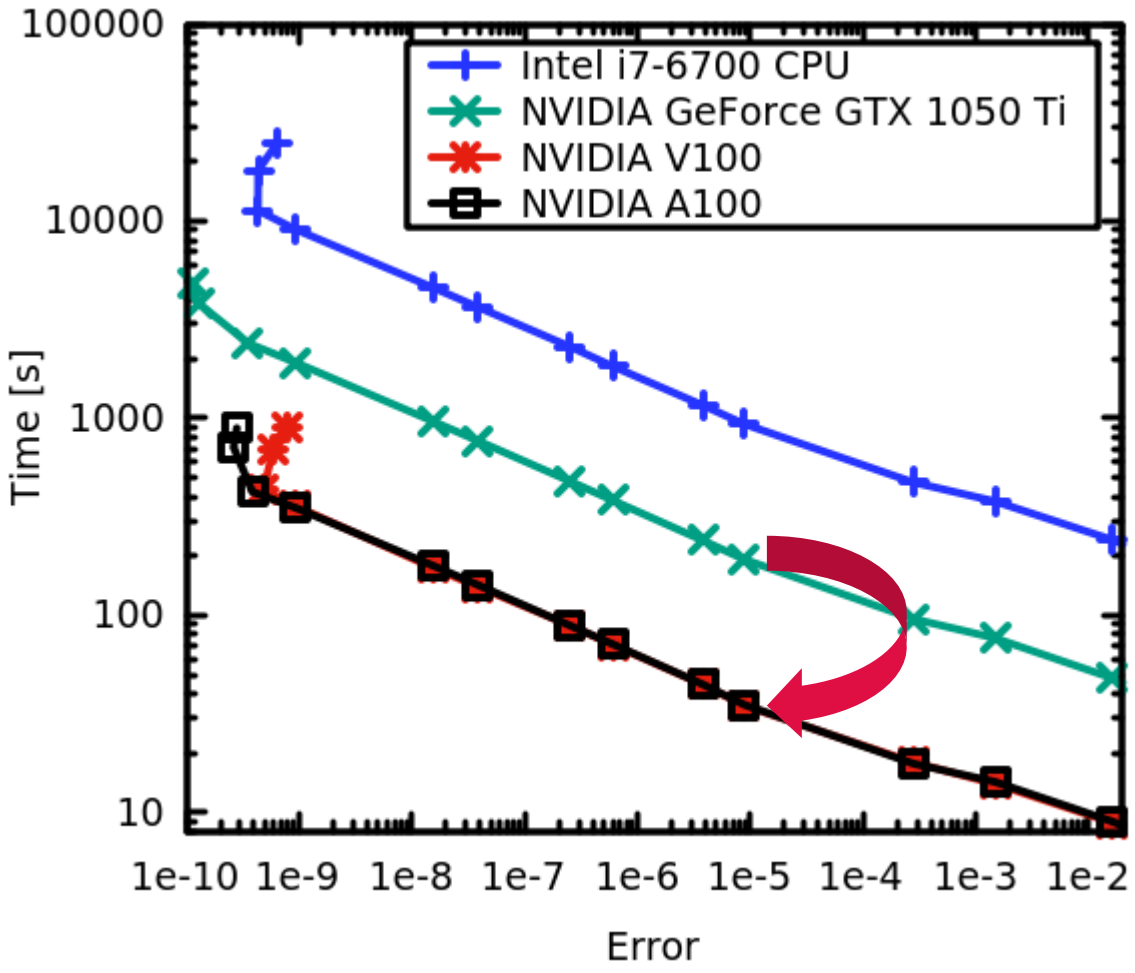

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→ **2-component updates**

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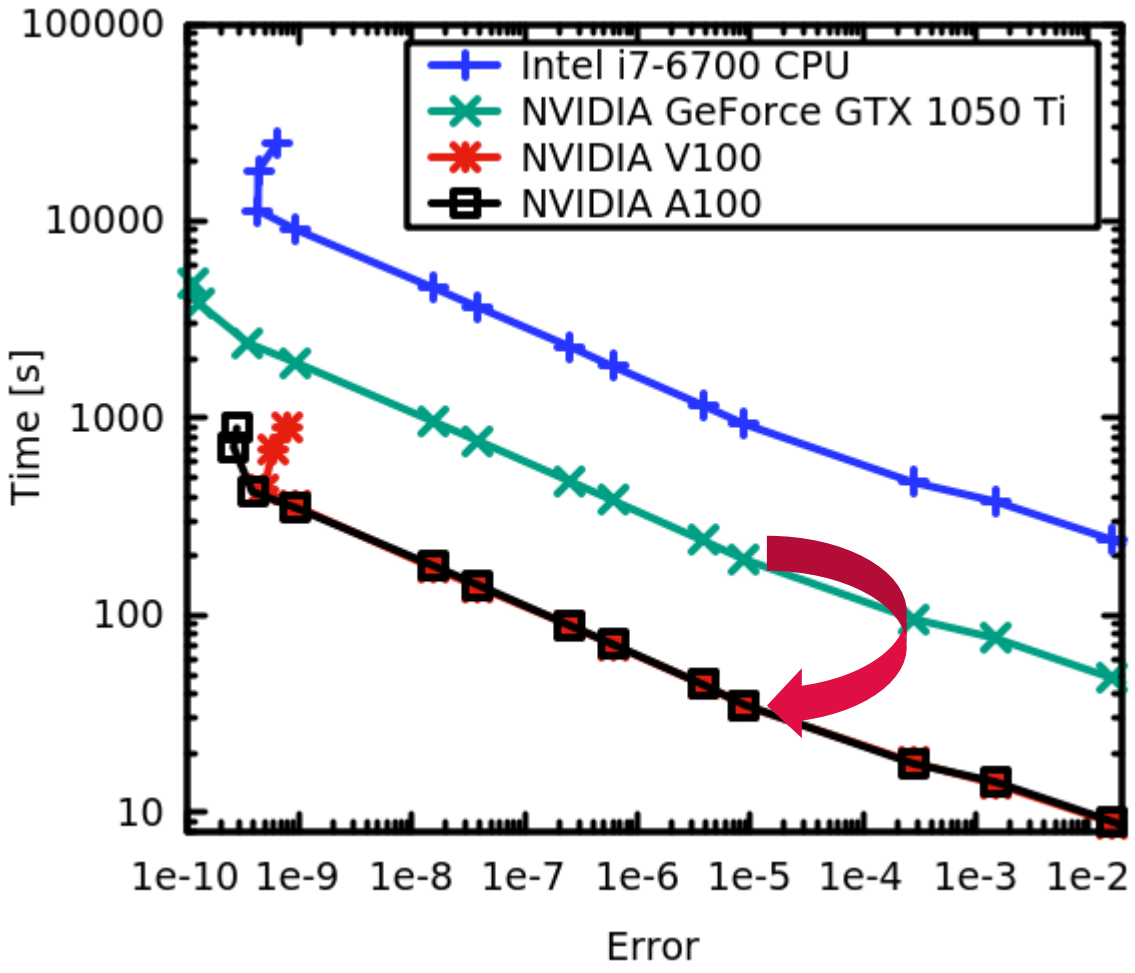

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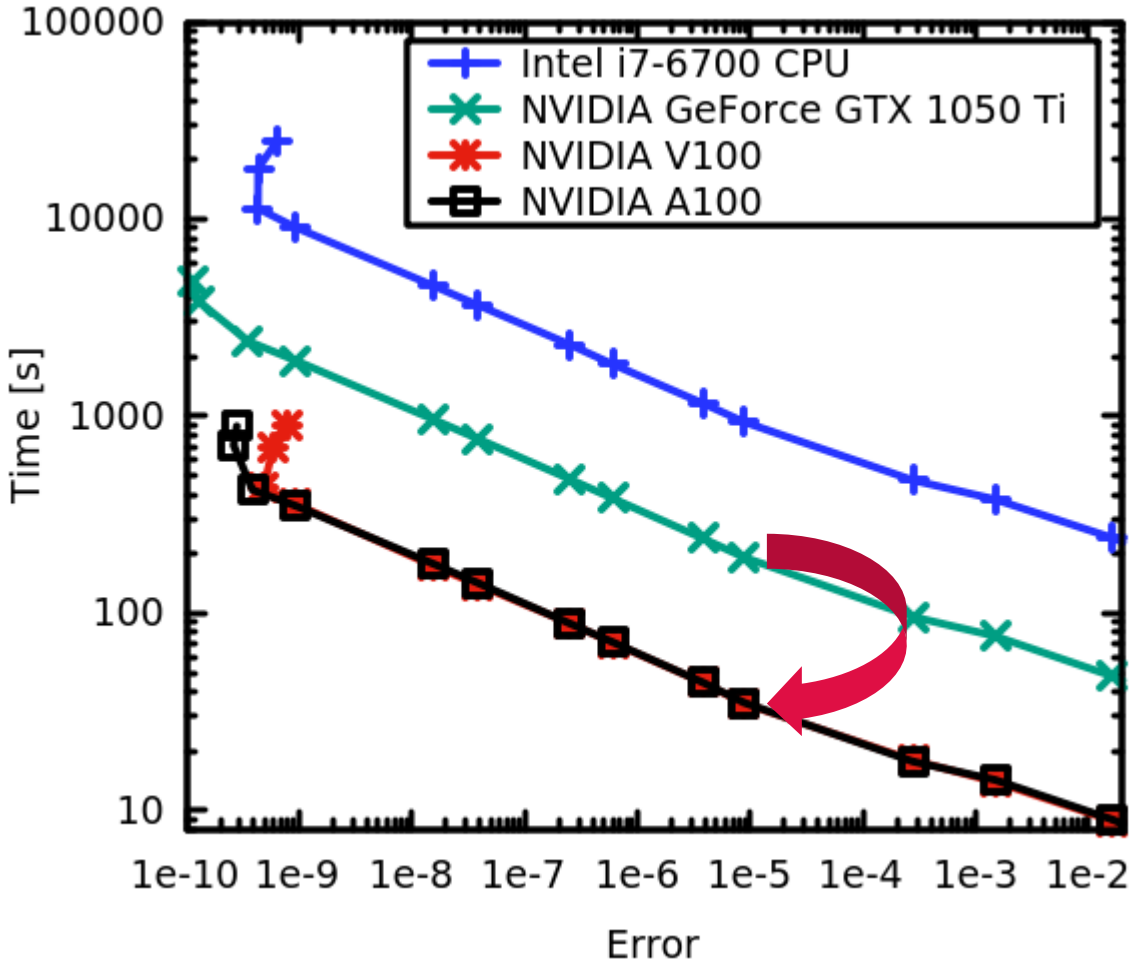

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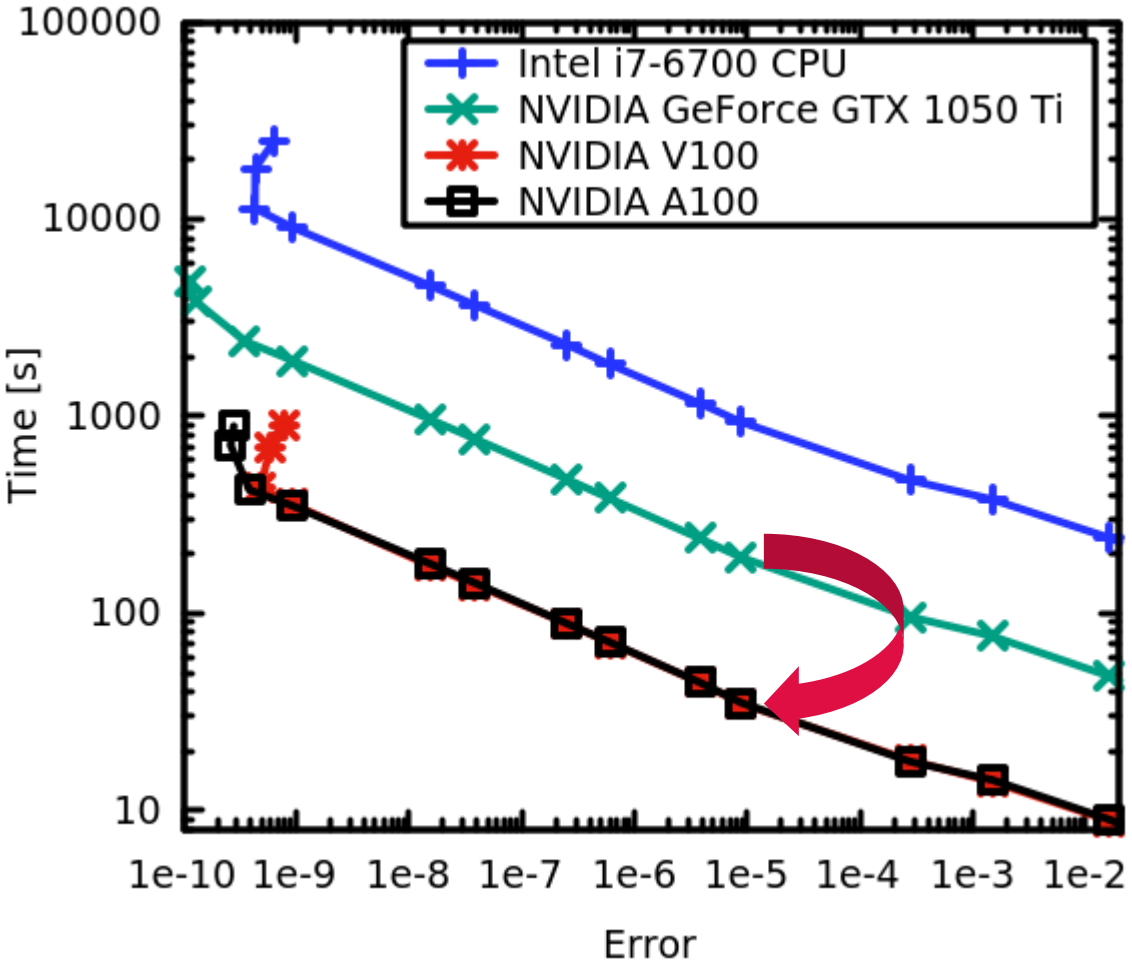

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Small system with **M=4** and **K=100**

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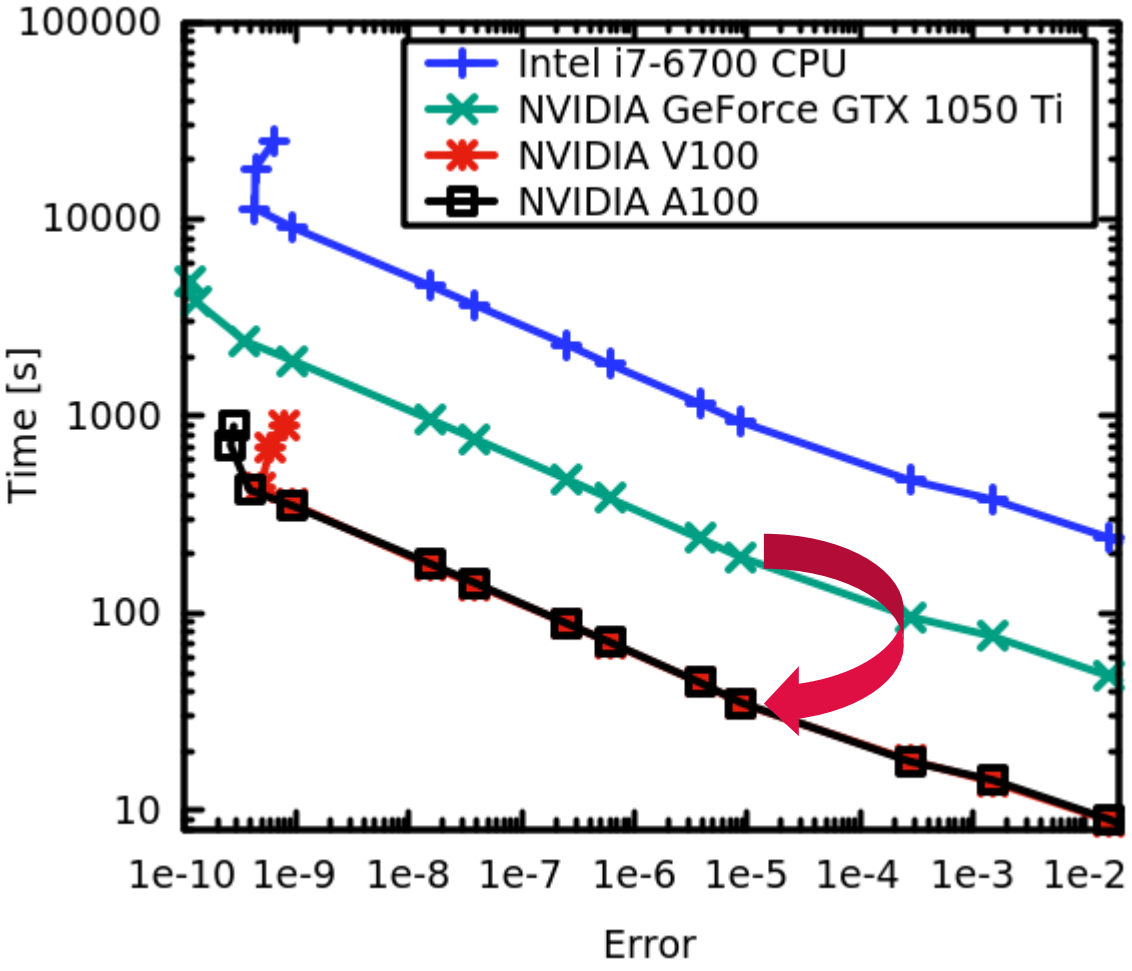

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→ **M-component updates**

Small system with **M=4** and **K=100**

→ Similar performance for **V100** and **A100**

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Simulating physical realizations of quantum computers on GPUs

CUDA+OpenACC MPI C++

Realistic system with **M=12** and **K=400**

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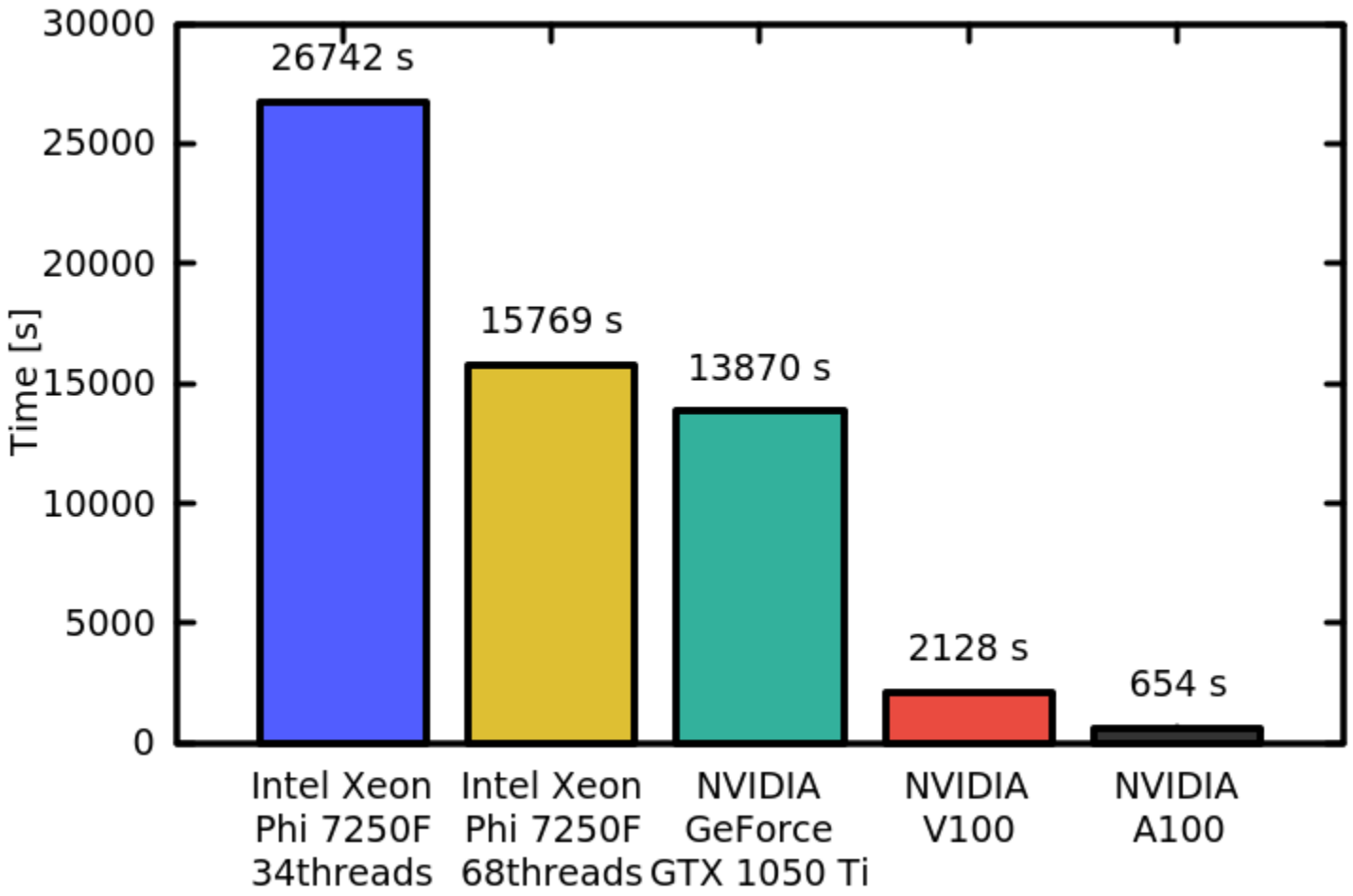

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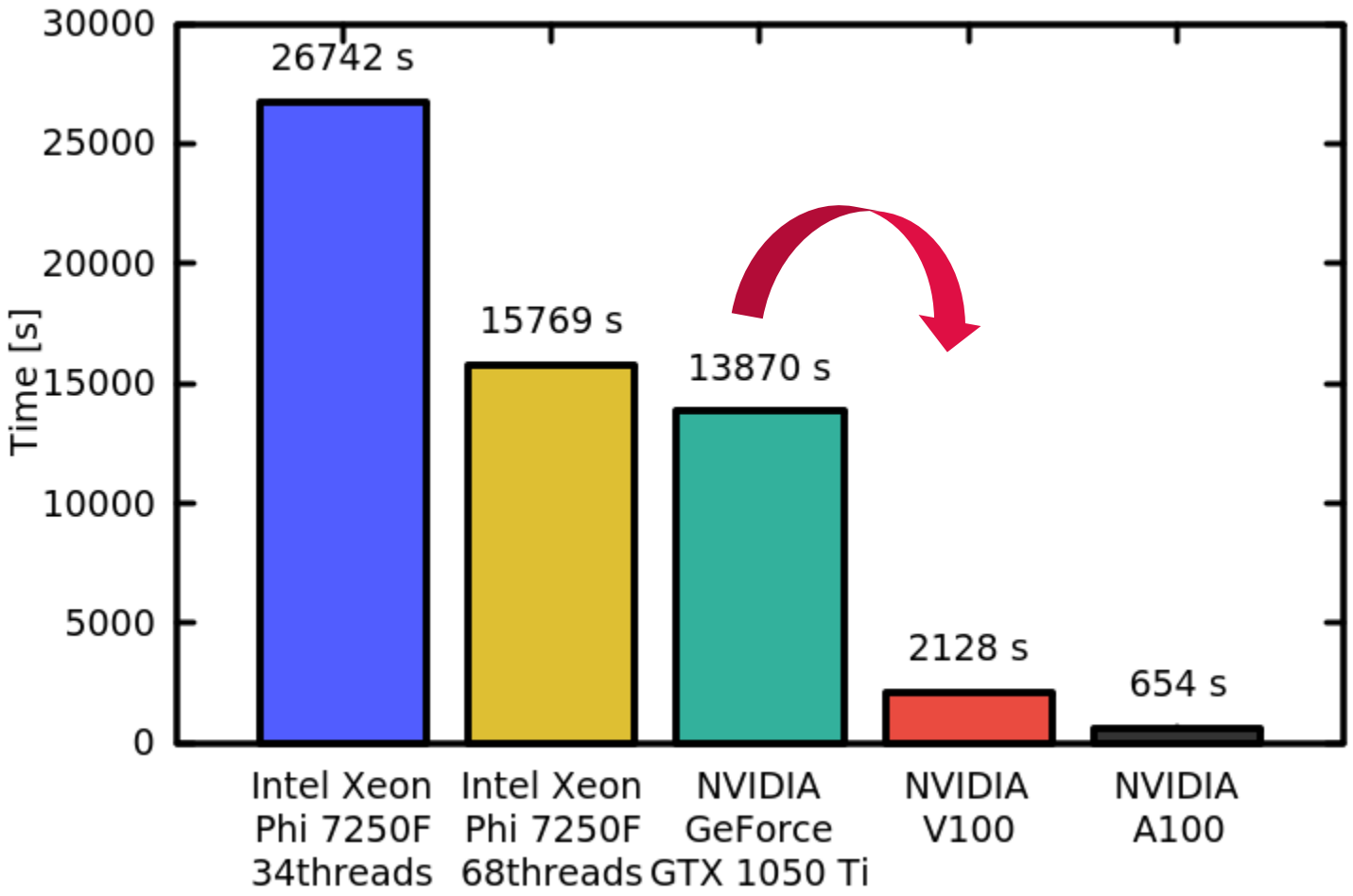
→ Similar speedup until **V100**



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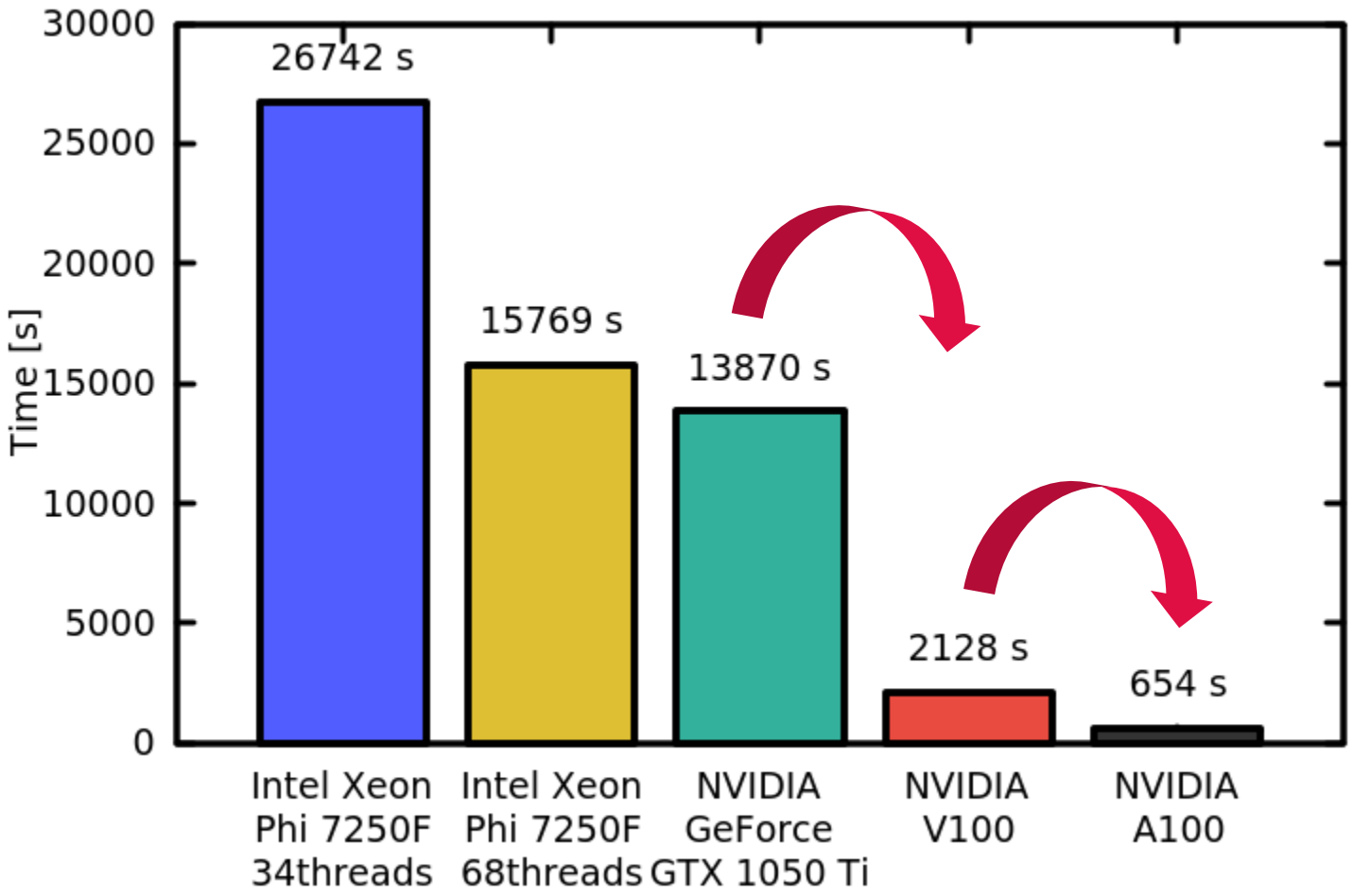

→ Similar speedup until **V100**

→ Further speedup from **V100** to **A100**

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  - Memory-, network-, and computation-intensive

SUMMARY

- All QC simulations are composed of

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THANK YOU FOR YOUR ATTENTION

- More information and references:
  - **MPI communication scheme:** De Raedt et al., Comp. Phys. Commun. 176, 121 (2007)
  - **Benchmarking gate-based quantum computers:** Michielsen et al., Comp. Phys. Commun. 220, 44 (2017)
  - **JUQCS:** De Raedt et al., Comp. Phys. Commun. 237, 41 (2019)
  - **Quantum supremacy with JUQCS:** Arute et al., Nature 574, 505 (2019)
  - **Benchmarking supercomputers with JUQCS:** Willsch et al., NIC Series 50, 255 (2020)
  - **GPU-accelerated simulations of QA and the QAOA:** Willsch et al., preprint available on arXiv (2021)

Q & A

What are the fundamental tensor operations in all simulations of this kind?

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For each k_0 in steps of 2, for each k_1, m_0, m_1

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→ **In-place double complex 2D SPMV updates**

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- **Our custom CUDA kernels were faster**

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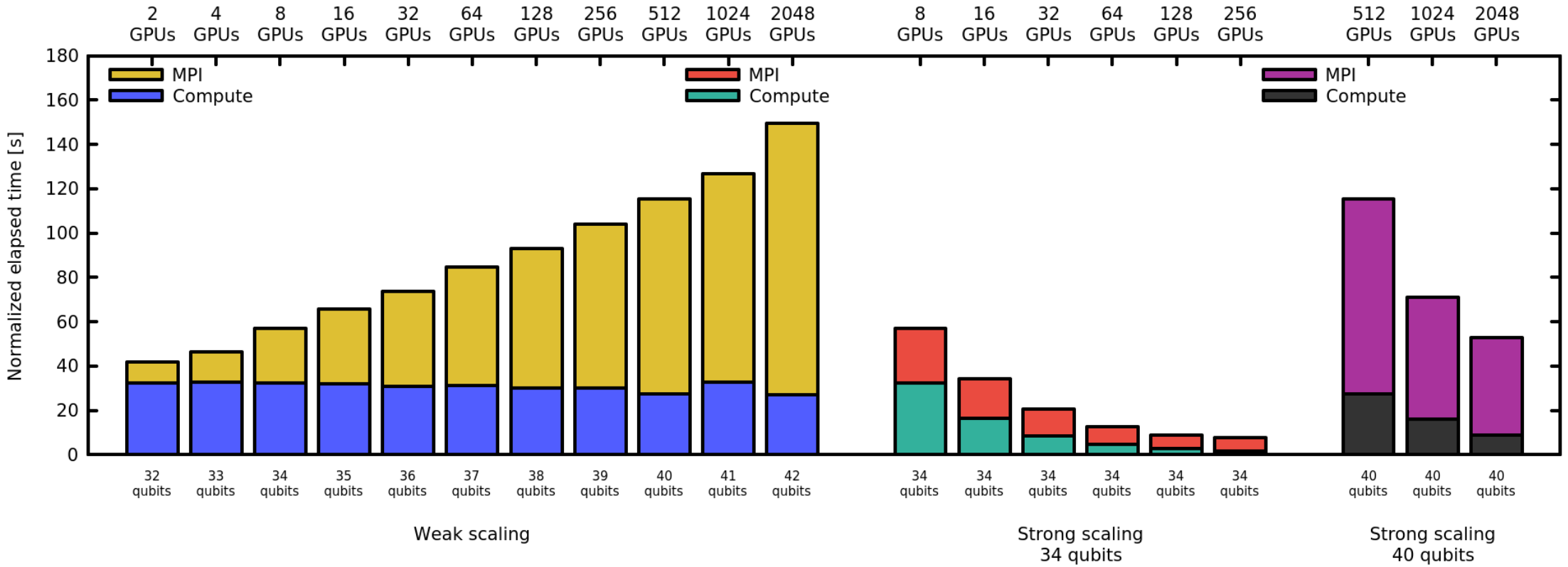

Q & A

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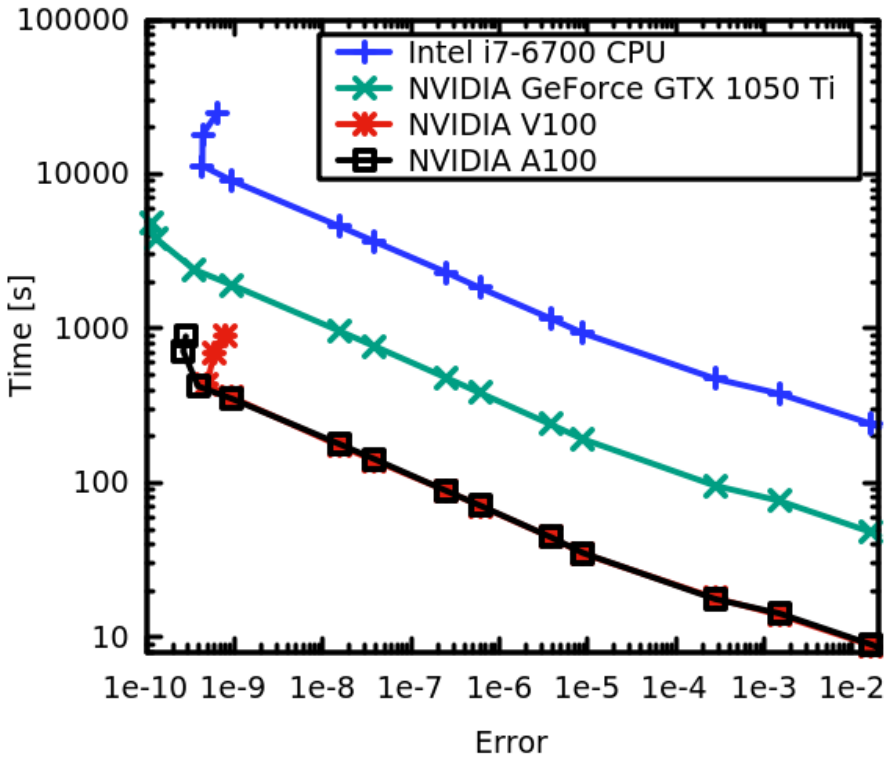

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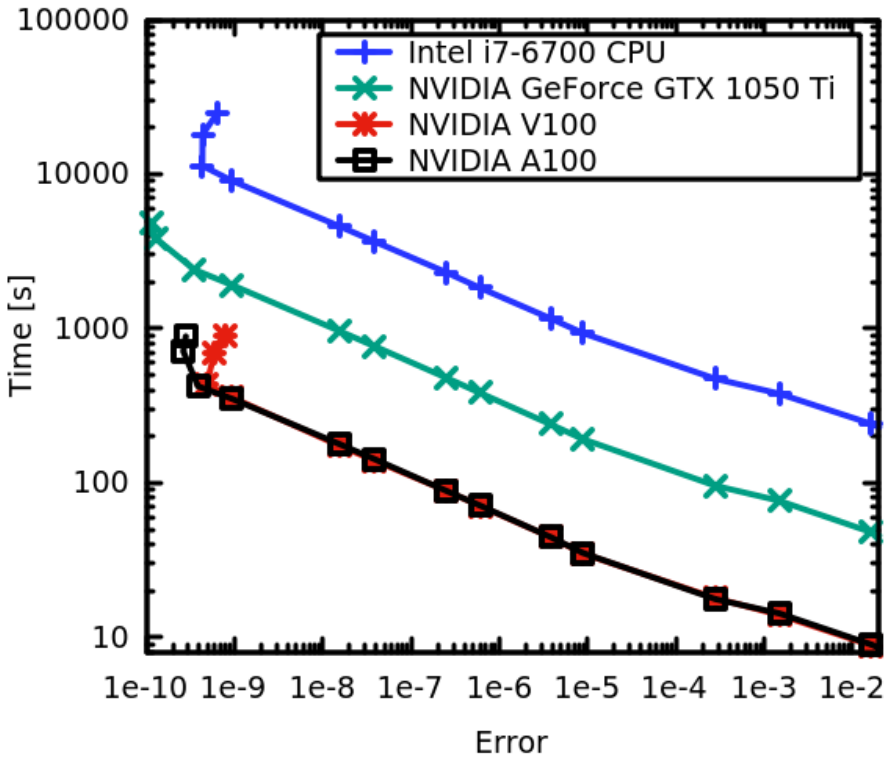

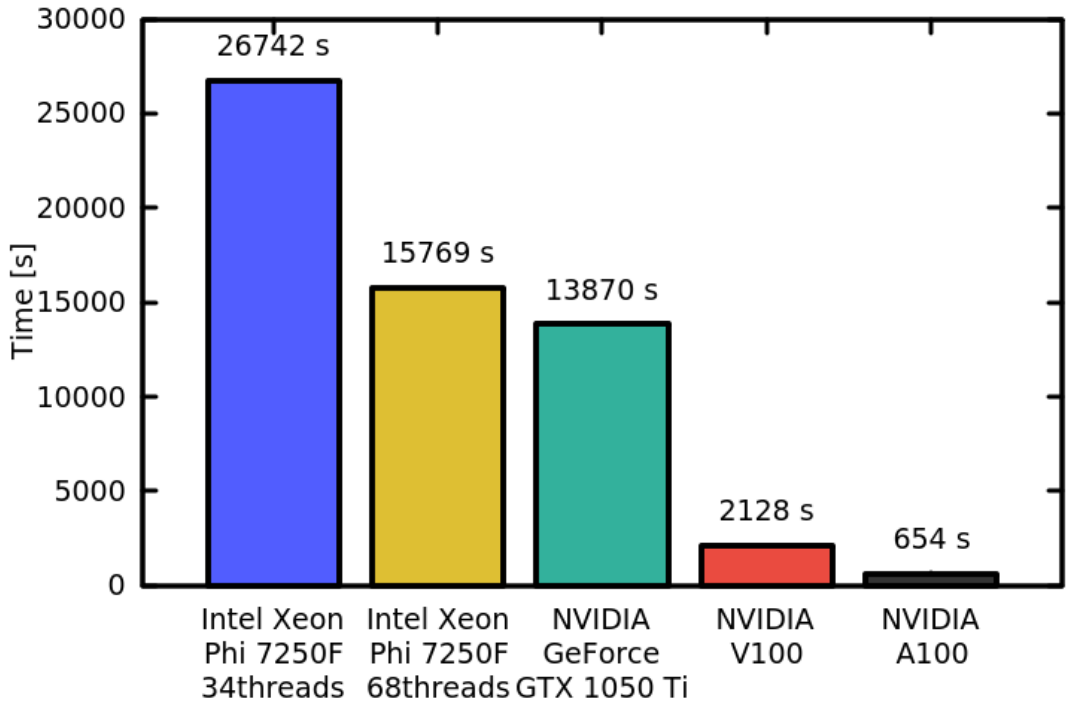

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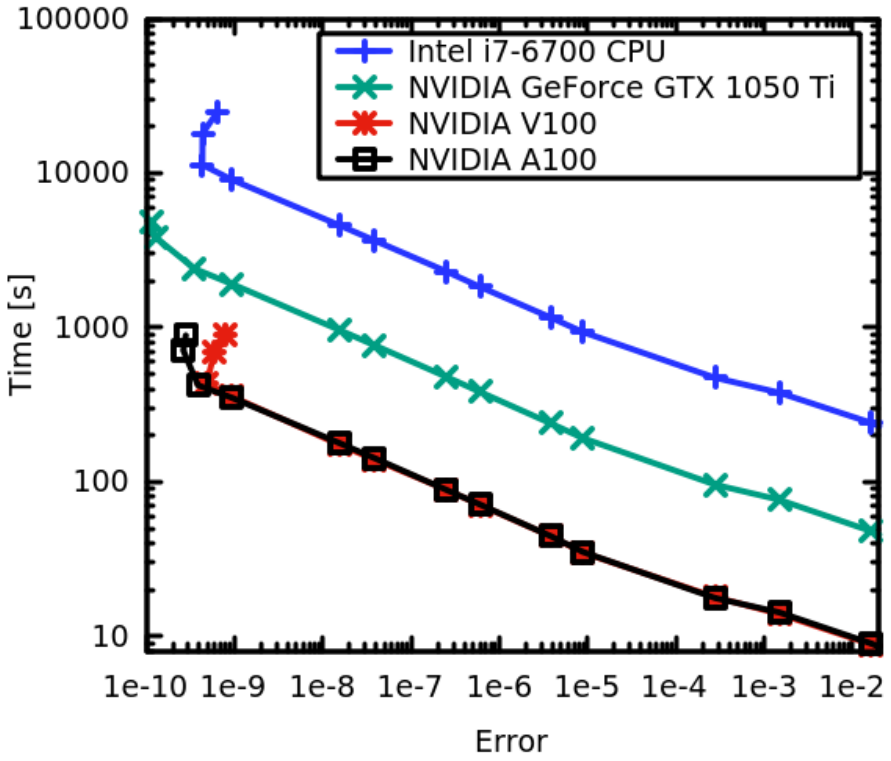

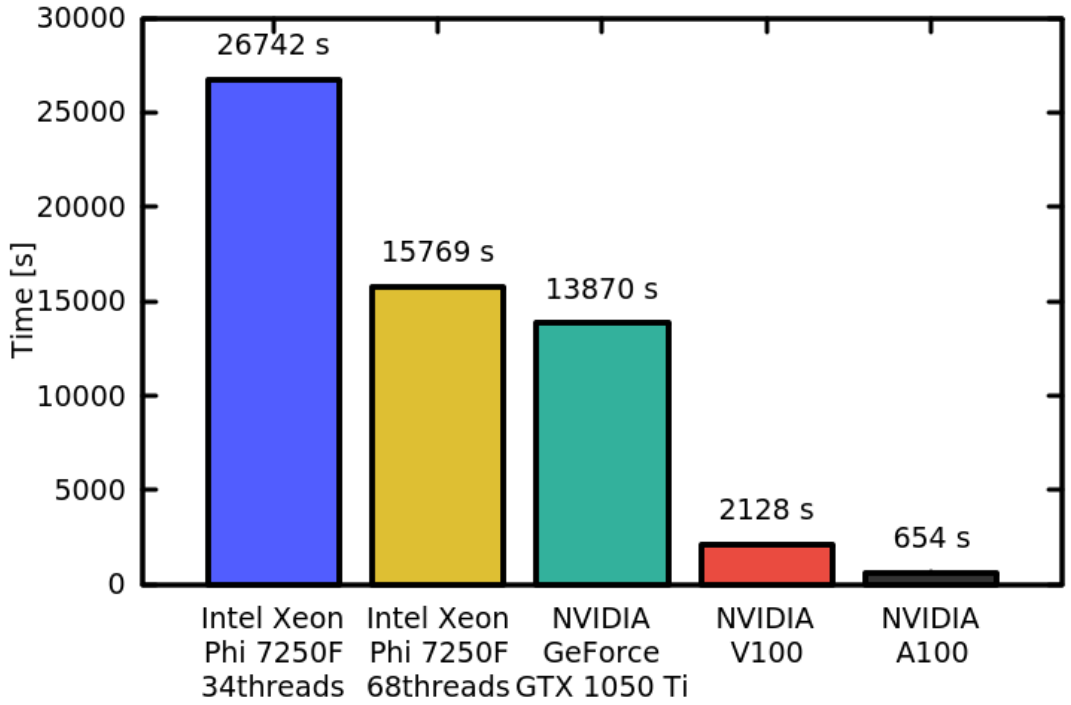

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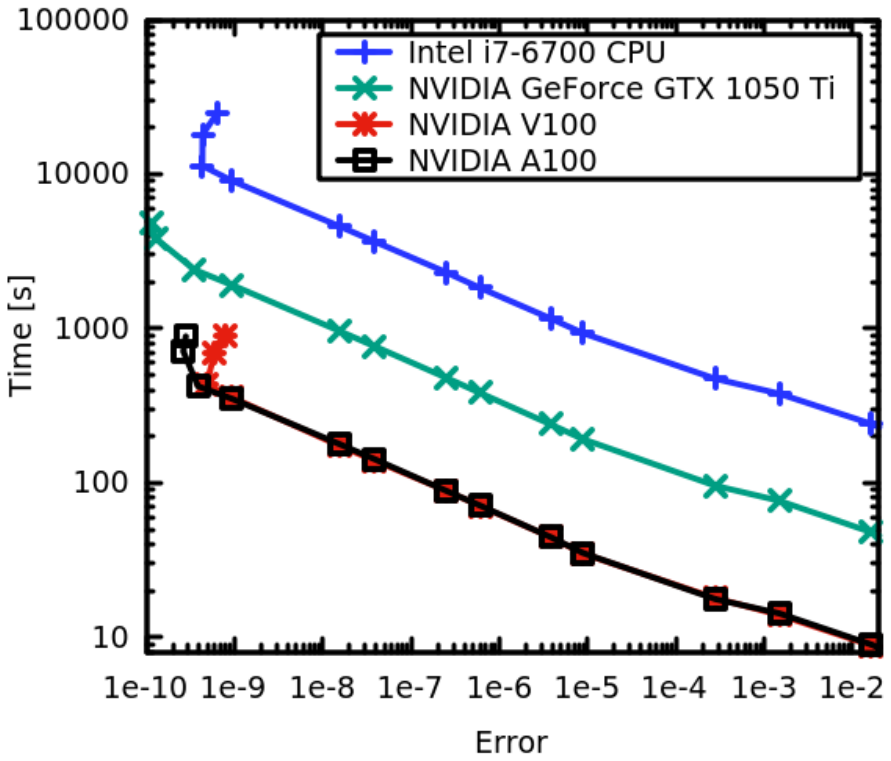

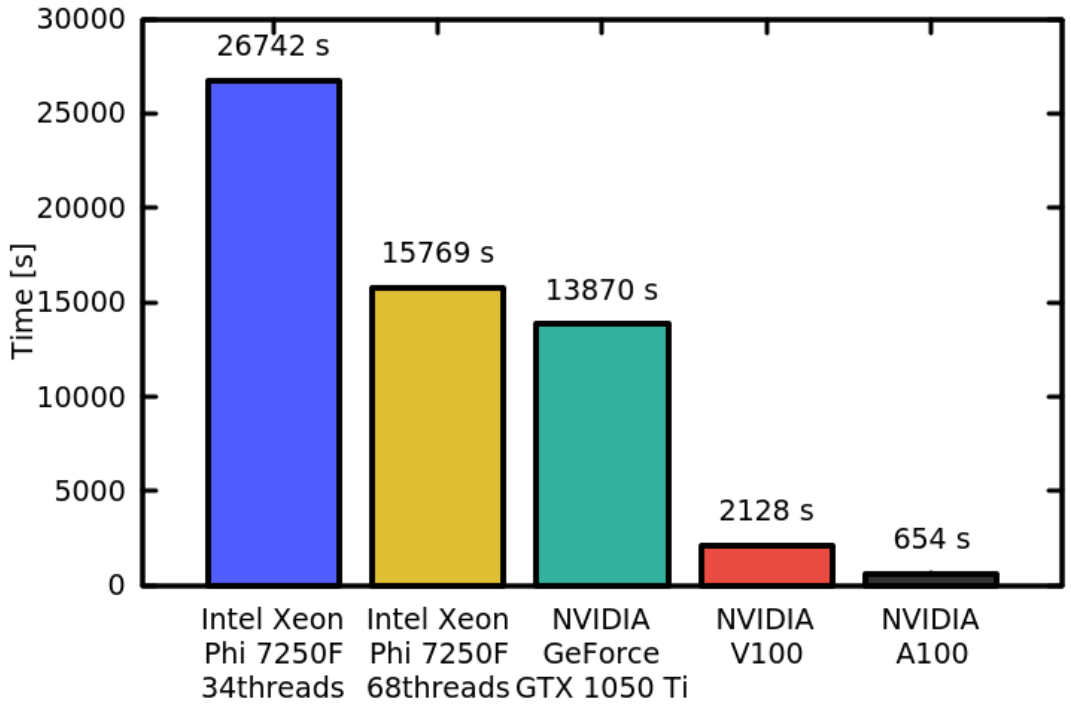

Small system with **M=4** and **K=100**

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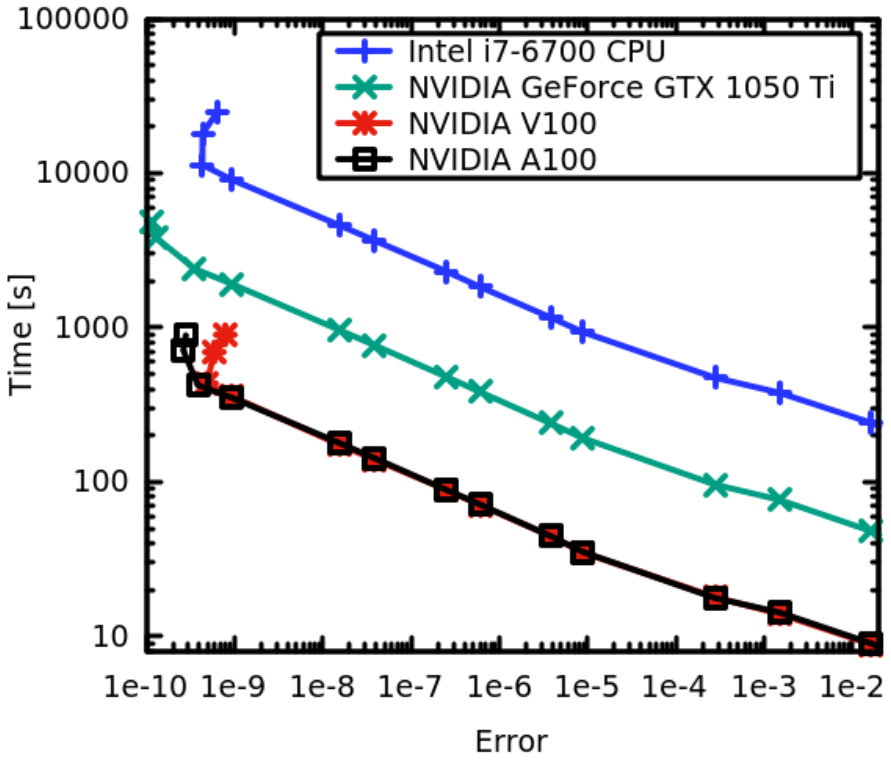

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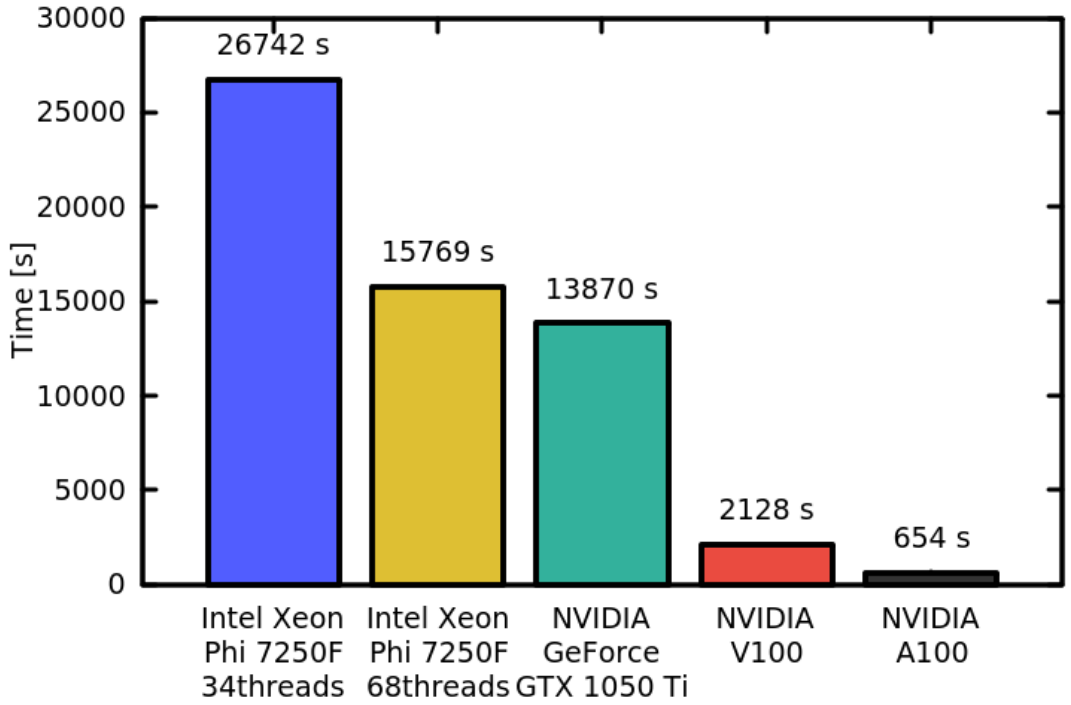

Realistic system with **M=12** and **K=400**