



Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

Upscaling QC simulators on HPC Systems

M. De Pascale | 15.12.2023 | HPCQC 2023

Upscaling QC Simulators on HPC Systems

Where I'll take you



- Introduce LRZ and QC Team



- Software Portfolio

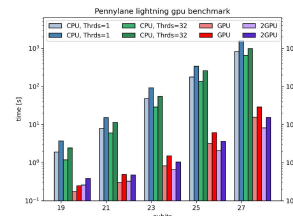


- Deployments



Mentioned

- Deployment results



Upscaling QC Simulators on HPC Systems

Leibniz Supercomputing Center



- Est. 1967
- Supercomputing centre from State of Bavaria
- Provides services to public research institutes (e.g. Munich Universities)
- SuperMUC-NG (40th in top 500 11.2023) - Lenovo
 - 311,000 compute cores
 - Peak perf 26.9 PFlops
 - Intel Xeon Skylake
- AI Cluster
 - 4 NVIDIA DGX A100, 252 CPU cores/node, 80GB/GPU
 - 1 NVIDIA DGX V100, 76 CPU cores/node, 16GB/GPU



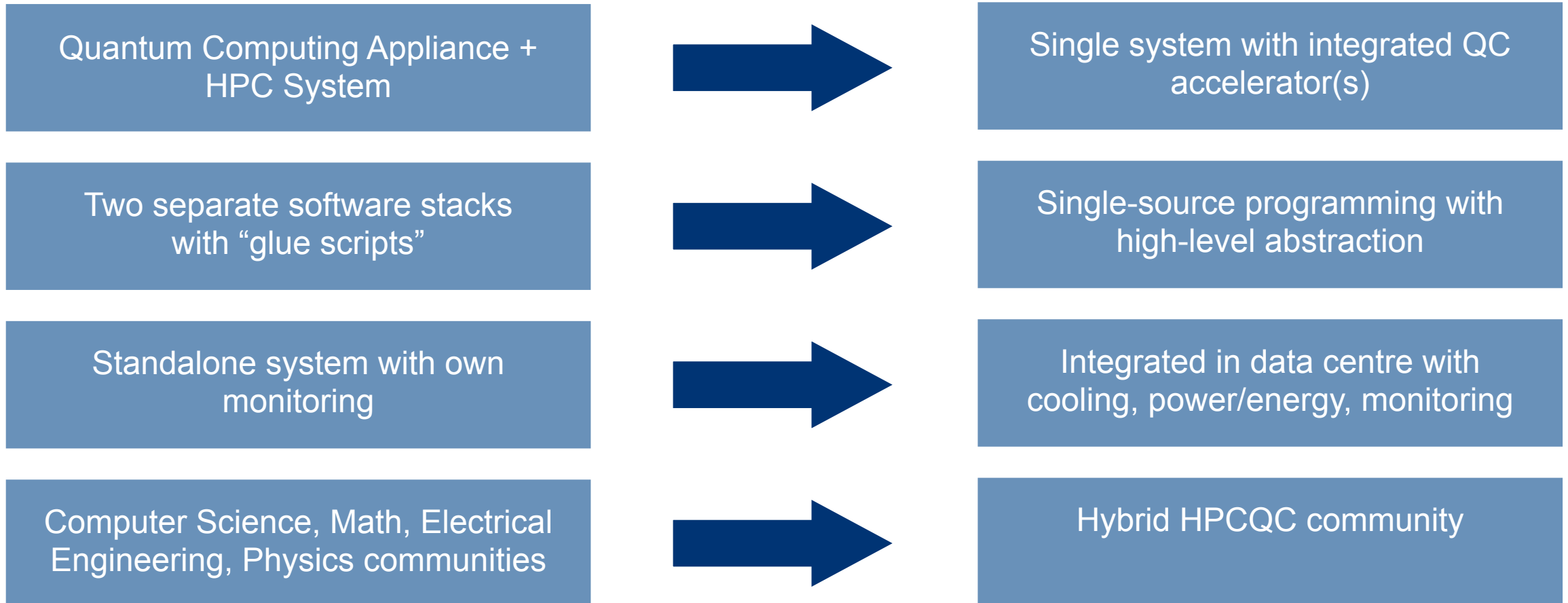
The Quantum Computing and Technologies Department (QCT)



- Established in April 2022
- 30+ people of many nationalities (Africa, Asia, Middle East, Europe, US)
- Four Groups:
 - *Program Development*
 - *Quantum system operations*
 - *Development of the integrated HPCQC software stack*
 - *Establishing services in QC on HPC infrastructure*



HPCQC End goals



Upscaling QC Simulators on HPC Systems

Software Portfolio



Upscaling QC Simulators on HPC Systems

Software Portfolio



Dedicated Quantum Simulator

Upscaling QC Simulators on HPC Systems

Software Portfolio



Dedicated Quantum Simulator

intel/**intel-qs**

High-performance simulator of quantum circuits

intel.

NVIDIA/
cuQuantum



Quantum simulators
/accelerators

Upscaling QC Simulators on HPC Systems

Software Portfolio



Dedicated Quantum Simulator

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Quantum simulators
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nVIDIA
CUDA QUANTUM

Software Development Frameworks

Upscaling QC Simulators on HPC Systems

Software Portfolio



Dedicated Quantum Simulator

intel/intel-qs

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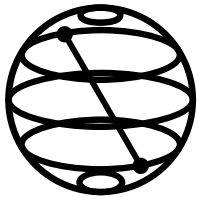
NVIDIA/
cuQuantum



Quantum simulators
/accelerators



PENNYLANE



Qiskit



NVIDIA

CUDA QUANTUM



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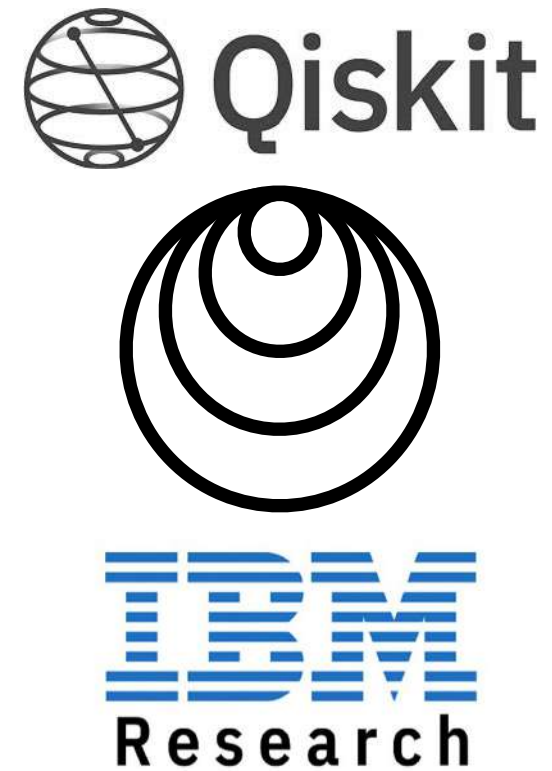
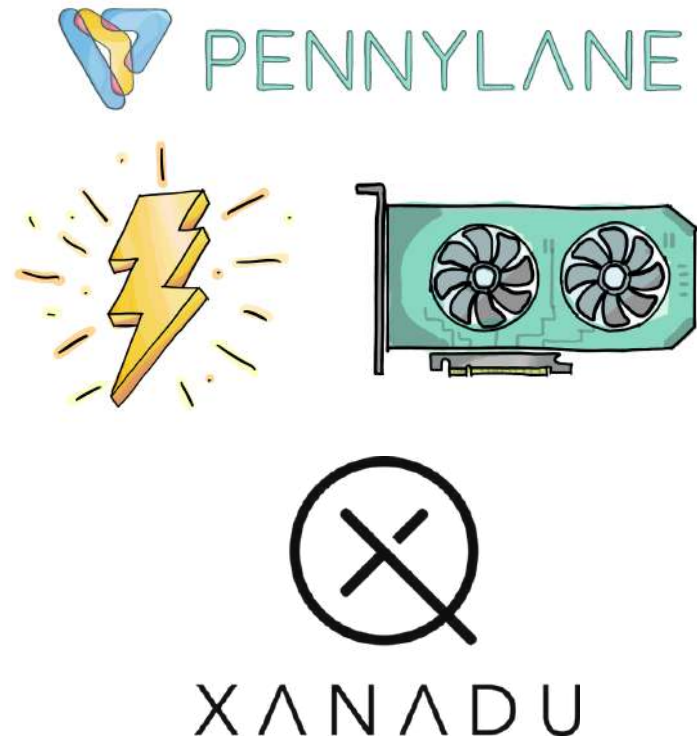
Quantum simulators /accelerators



Software Development Frameworks

Upscaling QC Simulators on HPC Systems

PennyLane and Qiskit

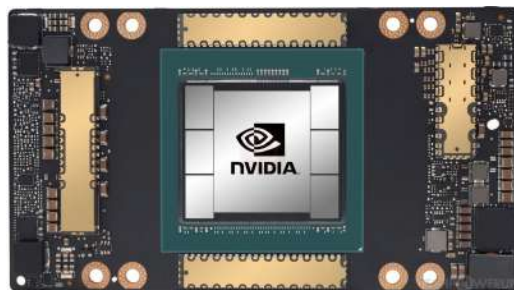


<https://github.com/PennyLaneAI/pennylane-lightning-gpu>

<https://github.com/Qiskit/qiskit-aer>

Upscaling QC Simulators on HPC Systems

Which HW HPC Technologies?



NVIDIA DGX A100 80GB

- 64 cores AMD EPYC 7742
- 8 GPU A100 (Ampere architecture)
- Up to 36 qubits in full state vector simulation



Intel Skylake Xeon

- On flagship cluster SuperMUC-NG
- 311,000+ cores
- 26.9 PFlops

Which SW backend?



NVIDIA
CUQUANTUM

cuStateVec

cuTensorNet



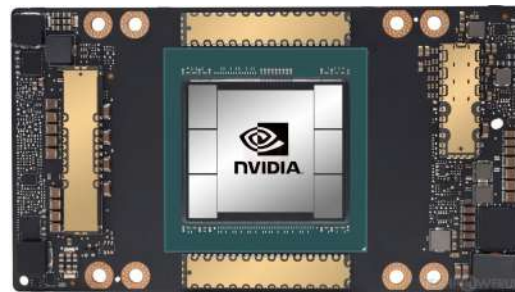
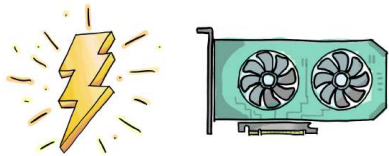
Qiskit



MPI

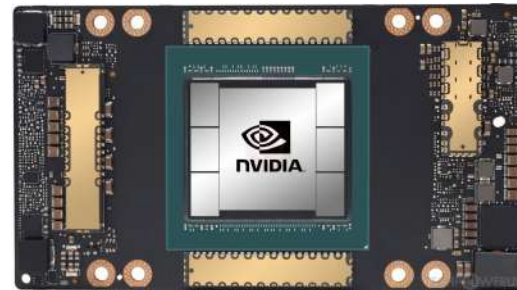
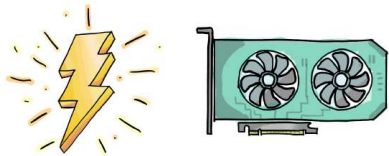
Intel MPI / open MPI

Deployment — PennyLane lightning GPU

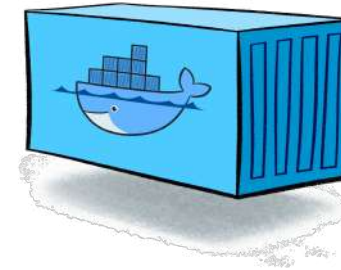


NVIDIA DGX A100 80GB

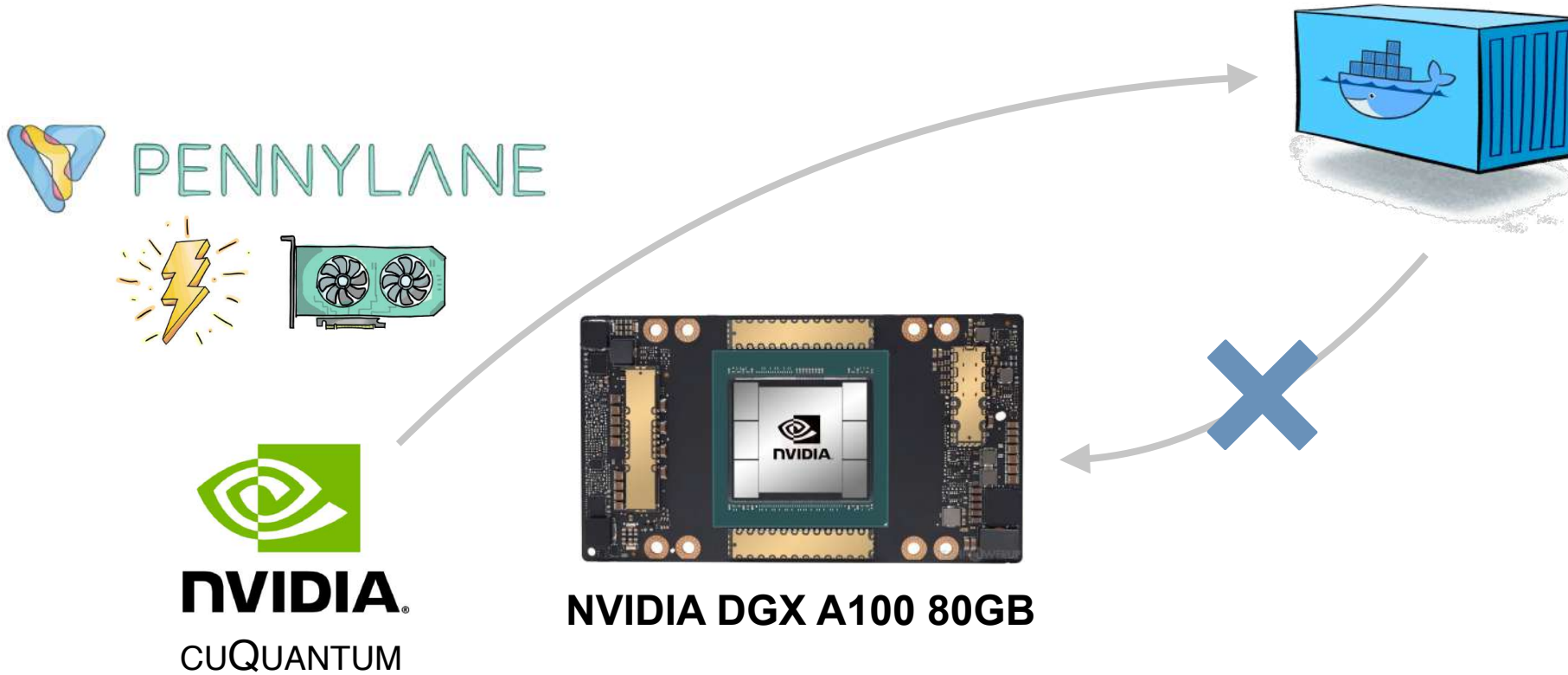
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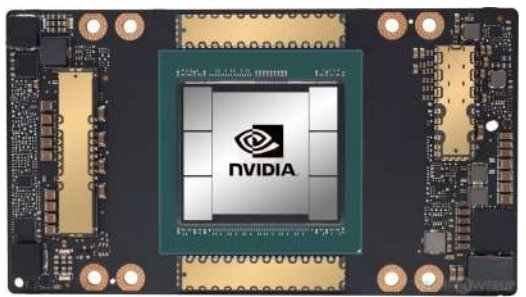
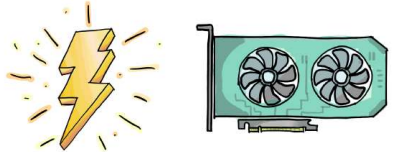
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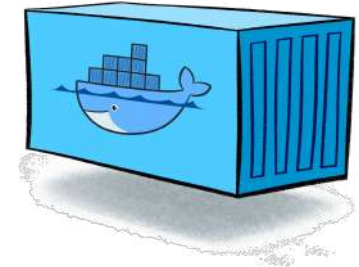
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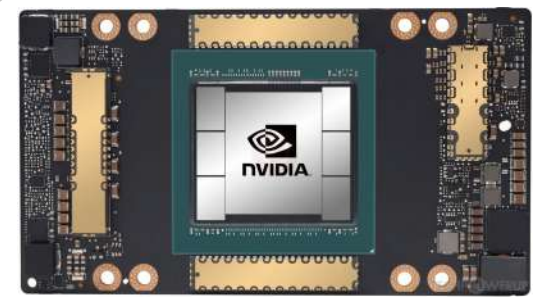
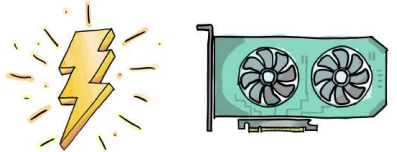
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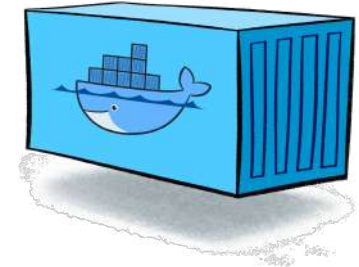
NVIDIA/enroot

A simple yet powerful tool to turn traditional container/OS images into unprivileged sandboxes.

Deployment — PennyLane lightning GPU



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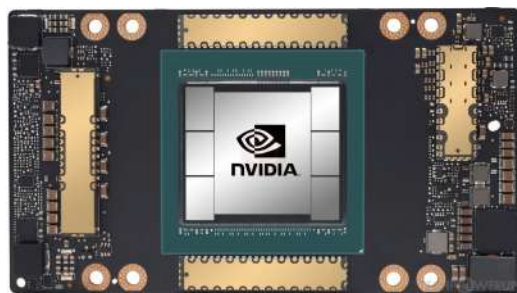
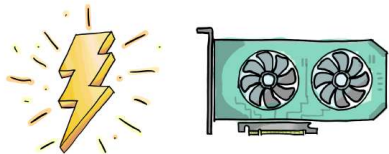


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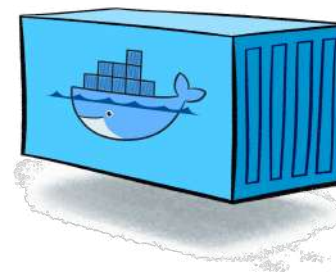
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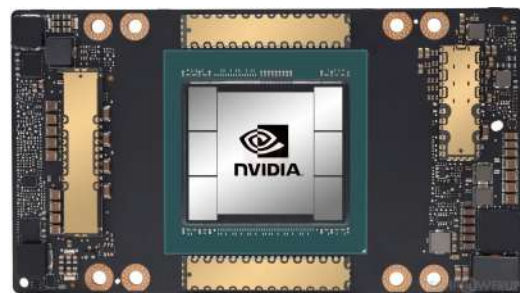
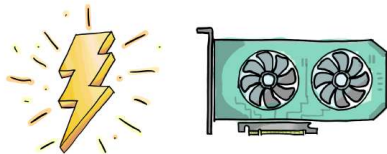
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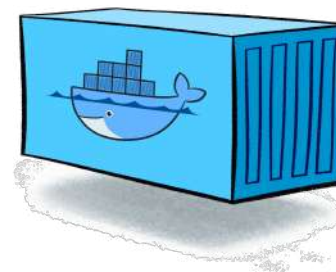


```
pip install \
pennylane-lightning[gpu]
```

Deployment — PennyLane lightning GPU



NVIDIA DGX A100 80GB



NVIDIA/enroot

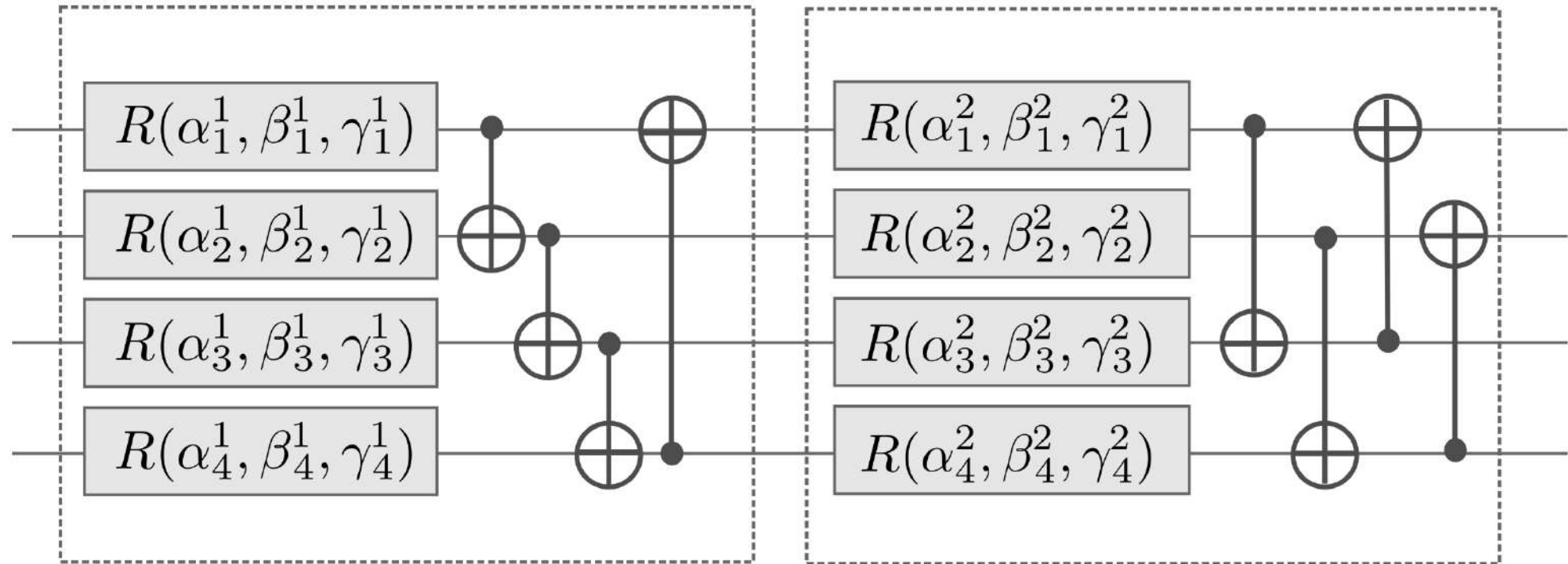
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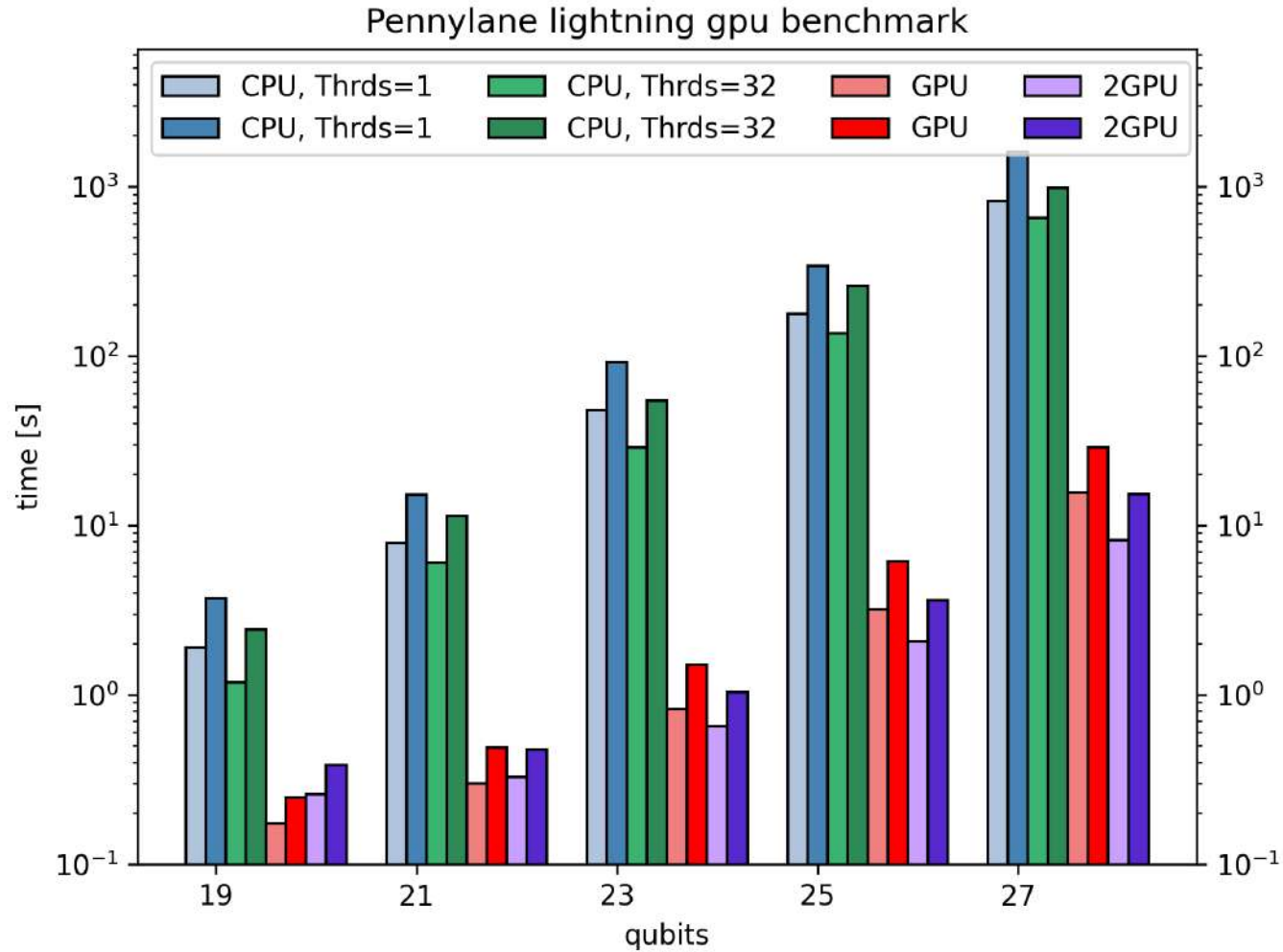
PennyLane lightning GPU — Simulation

- Strongly Entangling Layers Circuit



- One measure of circuit's Jacobian repeated 50 times, no optimisation

PennyLane lightning GPU — Results



Deployment — `qiskit-aer` and MPI support

```
pip install qiskit-aer-mpi
```

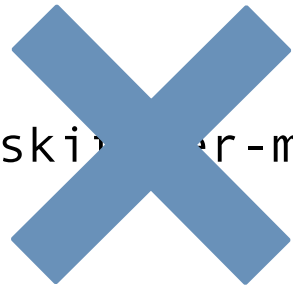


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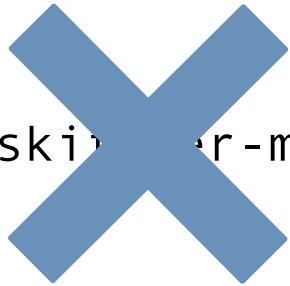


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- MPI support build **from source**
- Dependencies + build chain
 - **openBLAS**
 - **openMPI**
 - **gcc 11.2**



- Developed by NVIDIA
- Only a possible backend as simulator; the NVIDIA cuQuantum
- Possible to use real QPU as backends
- Supports QIR (good since goes towards a standard approach <https://www.qir-alliance.org/>)



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- C++ SDK developed by Quantum Brilliance
- Provides access to different simulator backends
- Quantum kernels can be written in CUDA Quantum