Large Scale Quantum Simulation with Qaptiva

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an atos business

Numerical Simulation For Quantum Algorithms

- **Today, only classical computers can run quantum programs (without errors)**

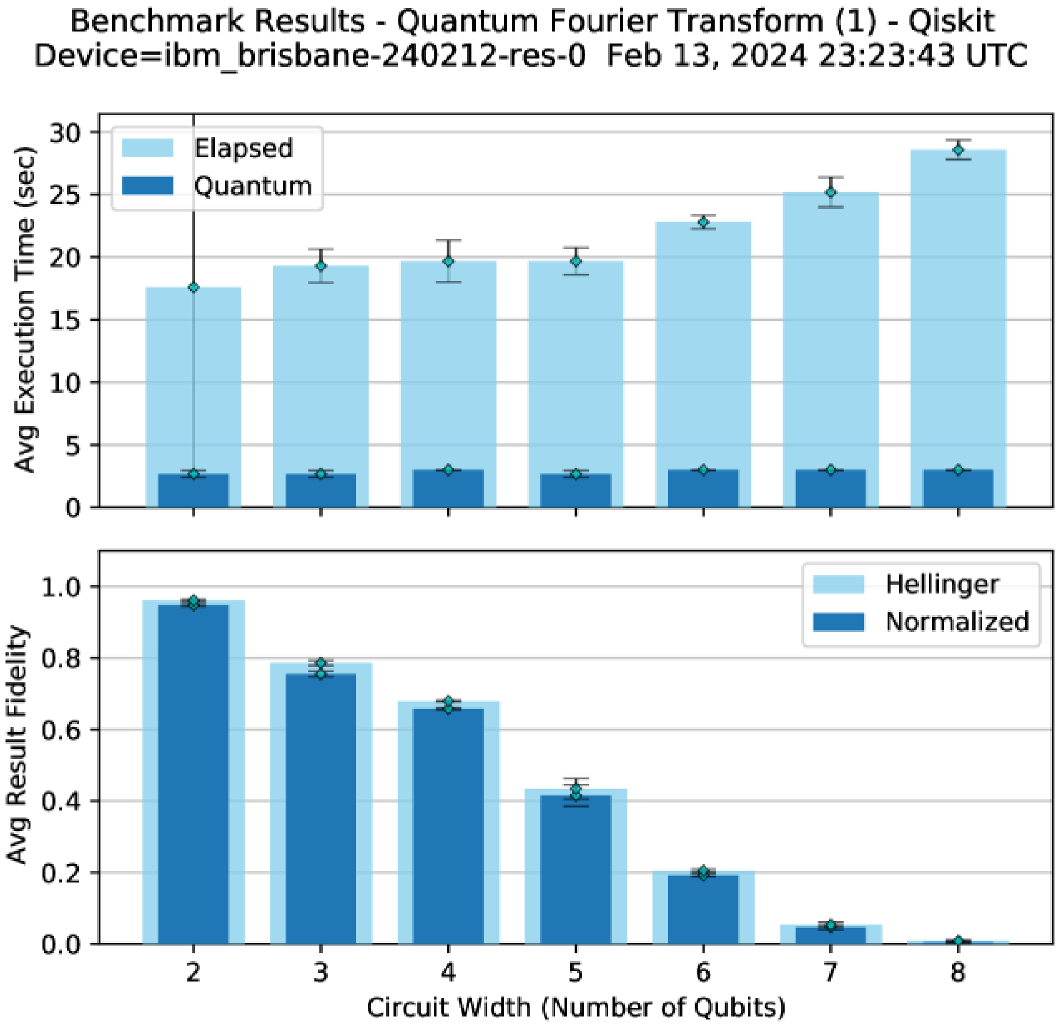
- For gate based computing

$$\psi_{out} = \prod_{k=0}^{N} U_k \, \psi_{in}$$

- For analog computing

$$H(t) = \sum_i \lambda_i(t) H_i$$

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$



https://arxiv.org/html/2402.08985v1

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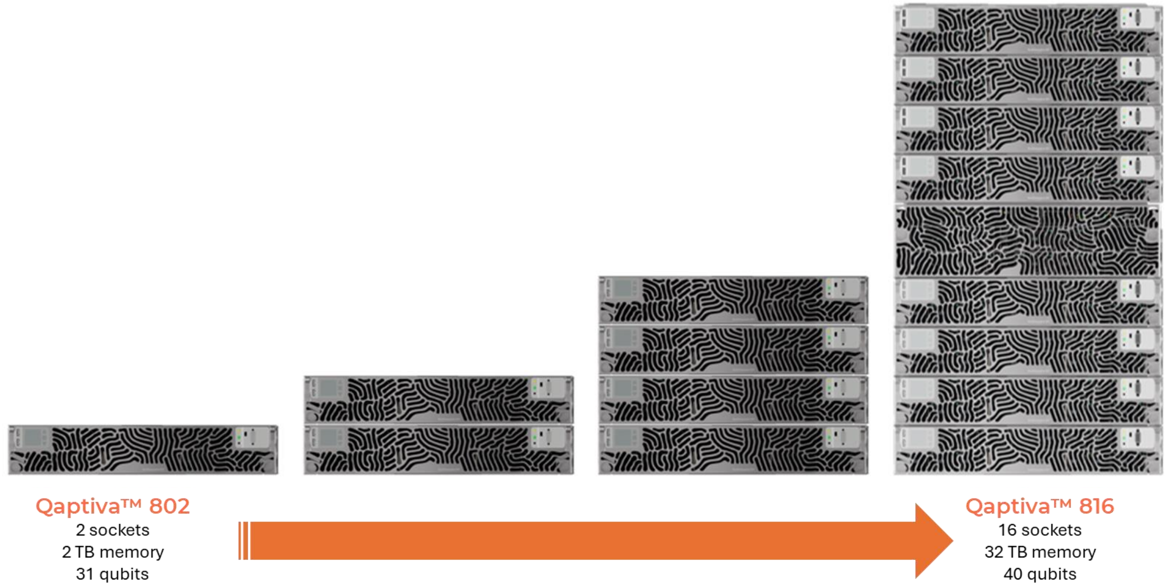
Numerical Simulation with Qaptiva

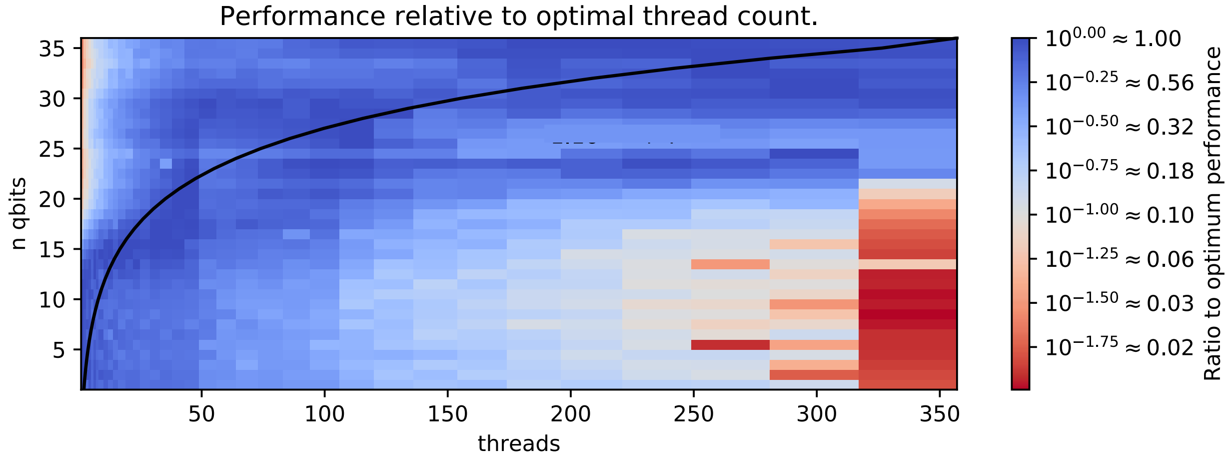
- Programming: no distinction between simulation and quantum hardware:

```
job = circuit.to_job()
qpu = CLinalg()
result = qpu.submit(job)
```

```
qpu2 = IQMqpu()
result2 = qpu2.submit(job)
```

- Simulation on the Qaptiva Appliance - Shared Memory system





- Optimal thread allocation

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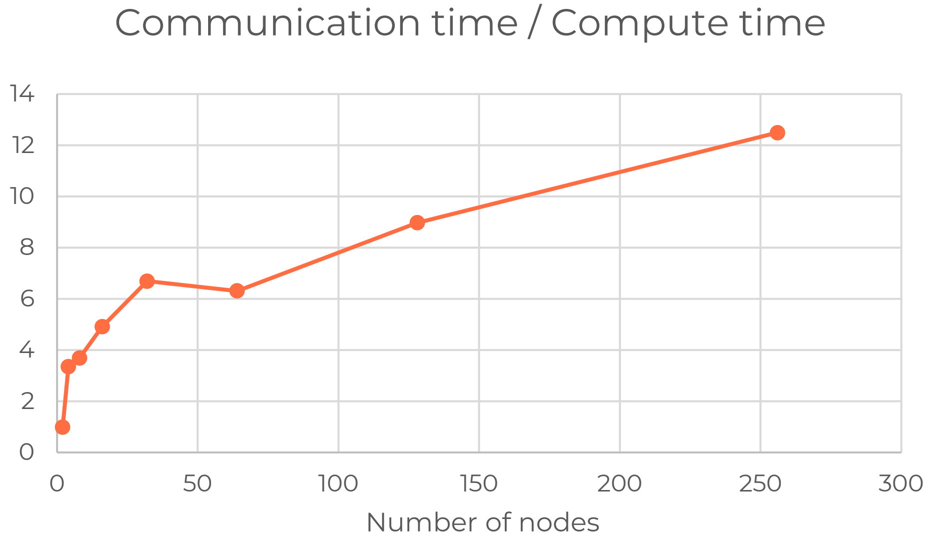
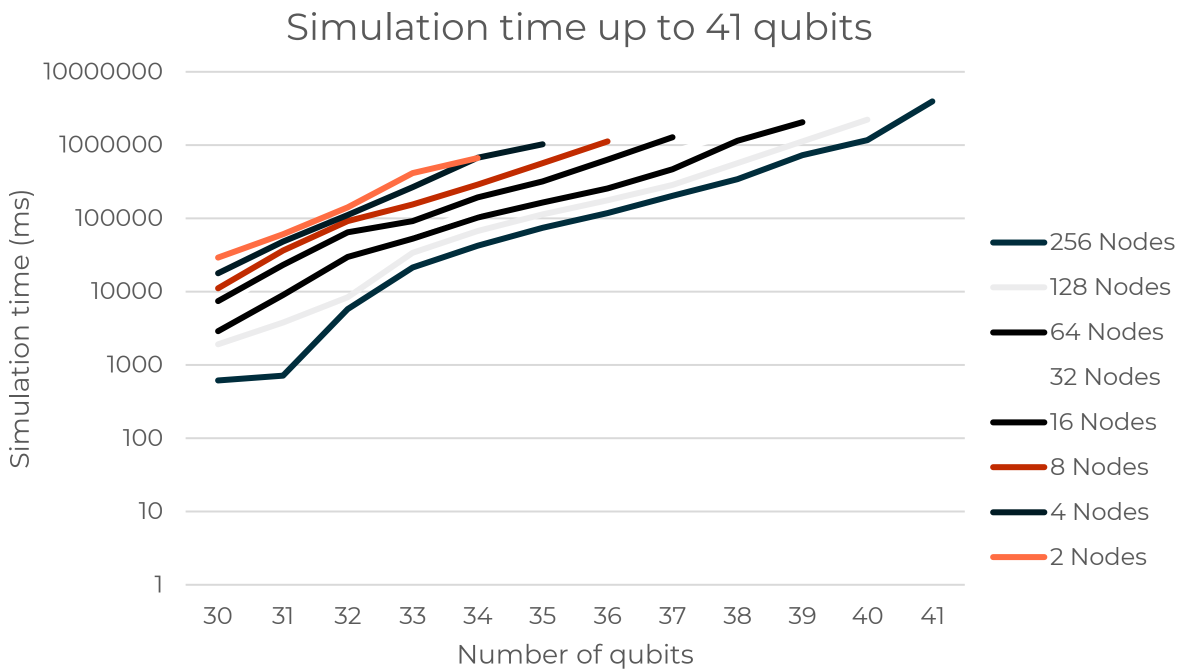
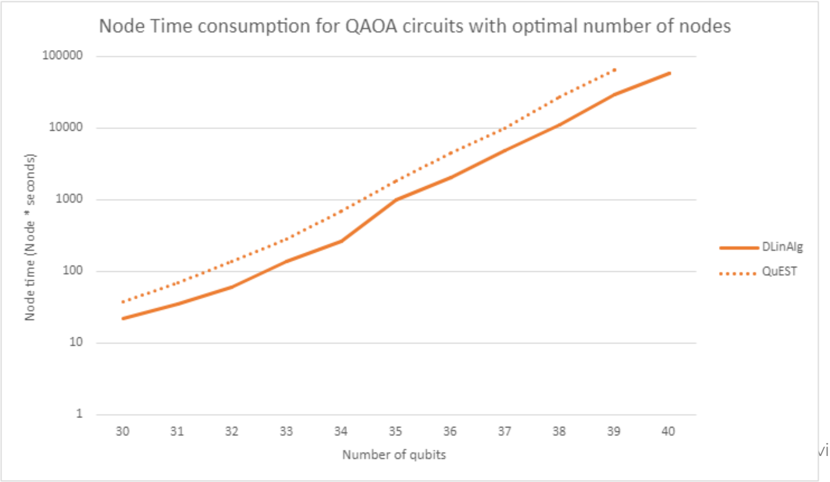
Numerical Simulation with Qaptiva on HPC

- The Qaptiva framework allows to offload simulations to an HPC
- Technical challenge for an MPI simulator: quantum simulation is a nightmare for memory circulation!







Simulating Quantum Noise

- Noise is here for long, so quantum programs must be designed noise-robust
- **Only HPC simulation can simulate noise (efficiently)**
- For gate based computing

  density matrix: $\rho = |\psi\rangle\langle\psi|$

  $$\rho_{out} = U\rho_{in}U^{+}$$

  $$\rho_{out} = \sum_{k_M}\left(E_{k_M}^{(M)} \dots \left(\sum_{k_1} E_{k_1}^{(1)}\rho_{in}E_{k_1}^{(1)\dagger}\right) \dots E_{k_M}^{(M)\dagger}\right)$$

- For analog computing
  - Noise is embedded in the Schrödinger evolution!

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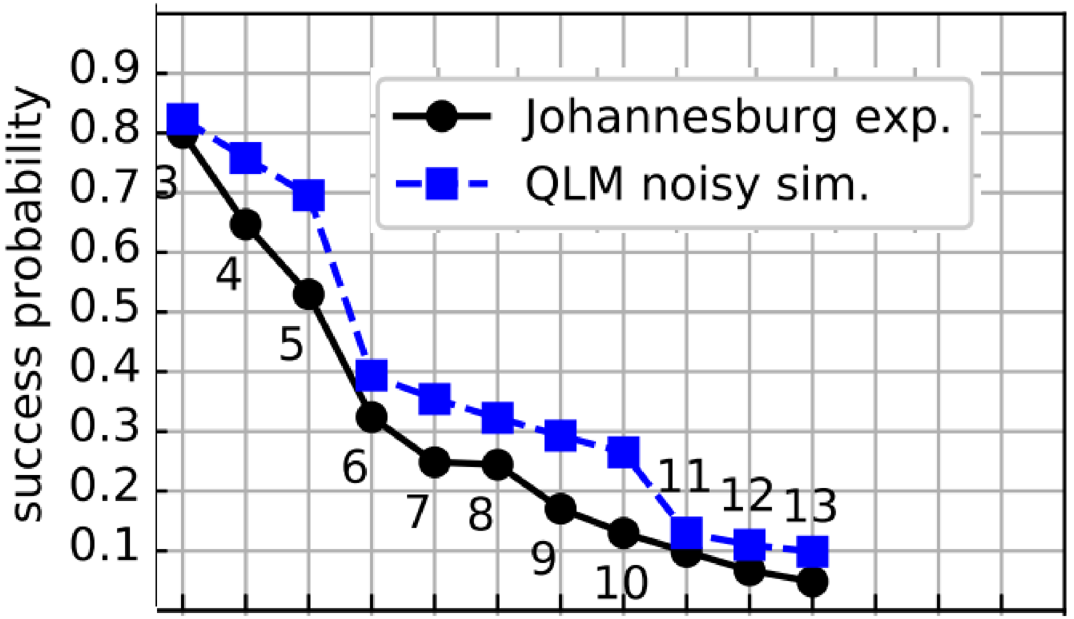
Simulating Quantum Noise with Qaptiva

- Programming interface is the same as QPU/emulators

```
hardware_model = HardwareModel(gates_spec, idle_noise=idle_noise)
qpu = NoisyQProc(hardware_model=hardware_model)
result = qpu.submit_job(job)
```

- 2 types of computation:
  - Deterministic : full computation of the density matrix
  - Stochastic : Monte Carlo sampling



https://arxiv.org/pdf/2005.12874

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Approximate Simulation Techniques

- Memory is the limit. Exact simulation beyond 50 qubits is intractable (128000 nodes!)
- Approximate methods, mostly based on matrix product representations
- Problem: how to control the approximation?

➢ **How to ensure the approximation is within the noise tolerance of a target QPU?**

In quantum computing, classical simulation must be allowed approximation

Help the debate on quantum advantage

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Approximate Simulation in Qaptiva

- Several state-of-the art simulation techniques available
- Most of them are published
- All of them are qualified on representative algorithms

PRX QUANTUM **4,** 020304 (2023)

Density-Matrix Renormalization Group Algorithm for Simulating Quantum Circuits with a Finite Fidelity

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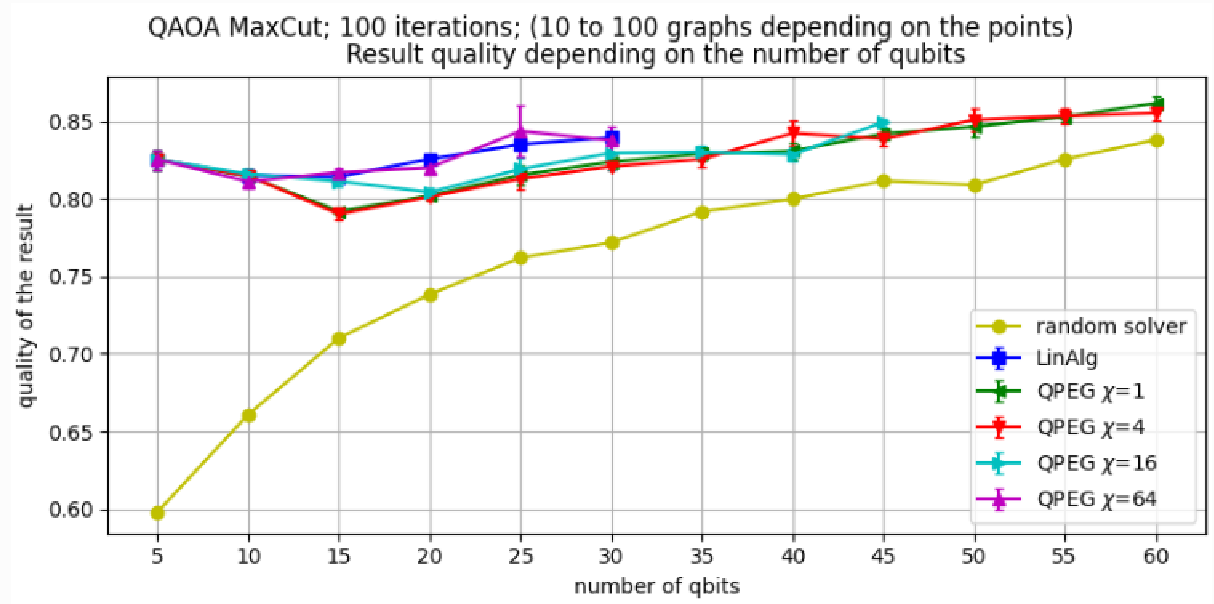

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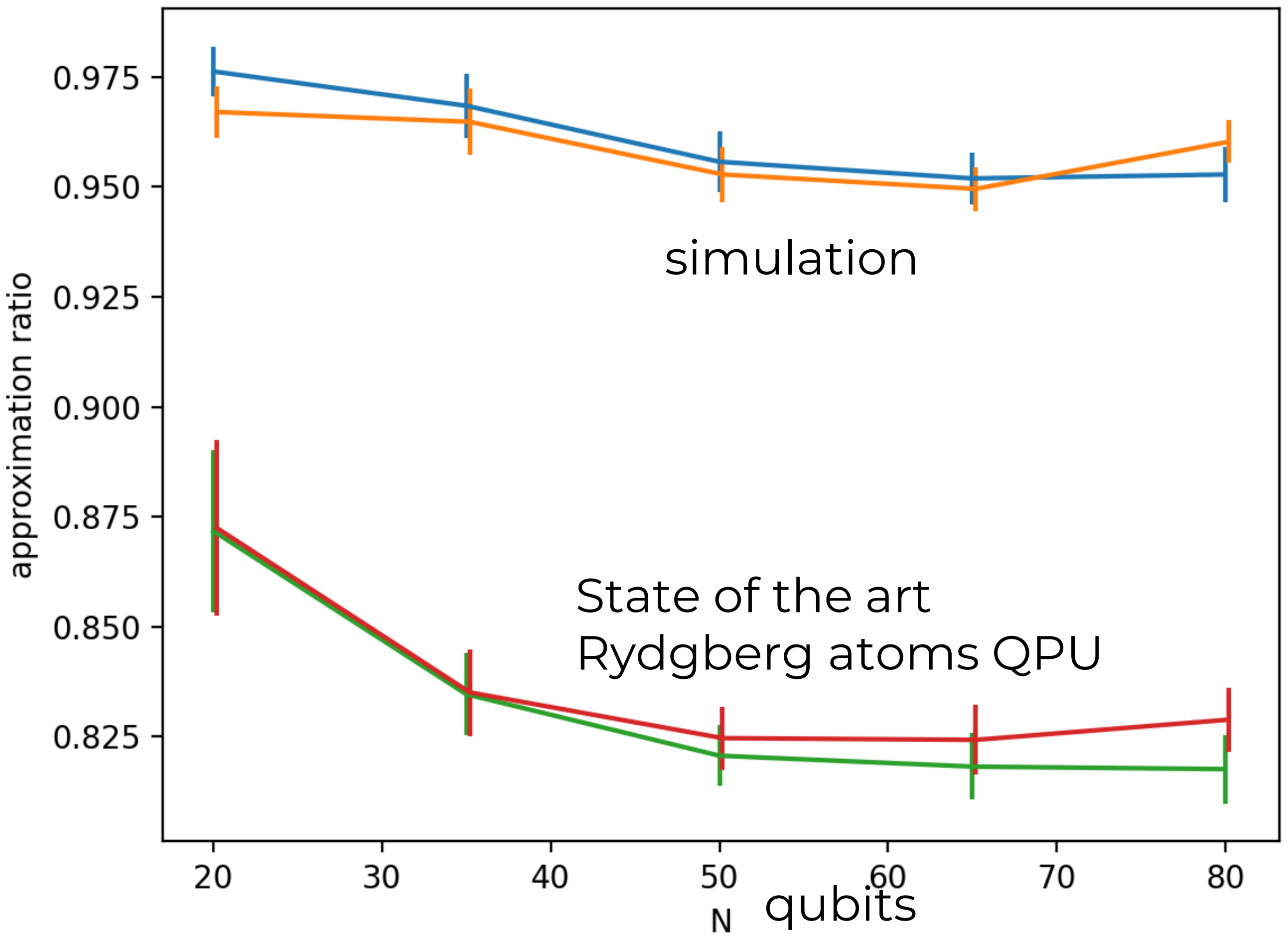
Approximate Simulation and Quantum Advantage



Maximum Independence Set – approximate simulation vs analog device

Simulation time : 3 minutes on 24 cores

Conclusions

- Numerical simulation will remain the reference tool for the design of quantum applications
- Only HPC can provide the capabilities for serious studies
- Approximate simulation to go beyond classical limits and to challenge quantum supremacy
- Qaptiva at the forefront - give it a try: https://myqlm.github.io/

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Questions

Thanks!

For more information, please contact:
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