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QUANTUM ALGORITHMS
AND ARCHITECTURES FOR
DOMAIN SCIENCE
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An Early Investigation of the Quantum Linear Solver for Scientific Applications

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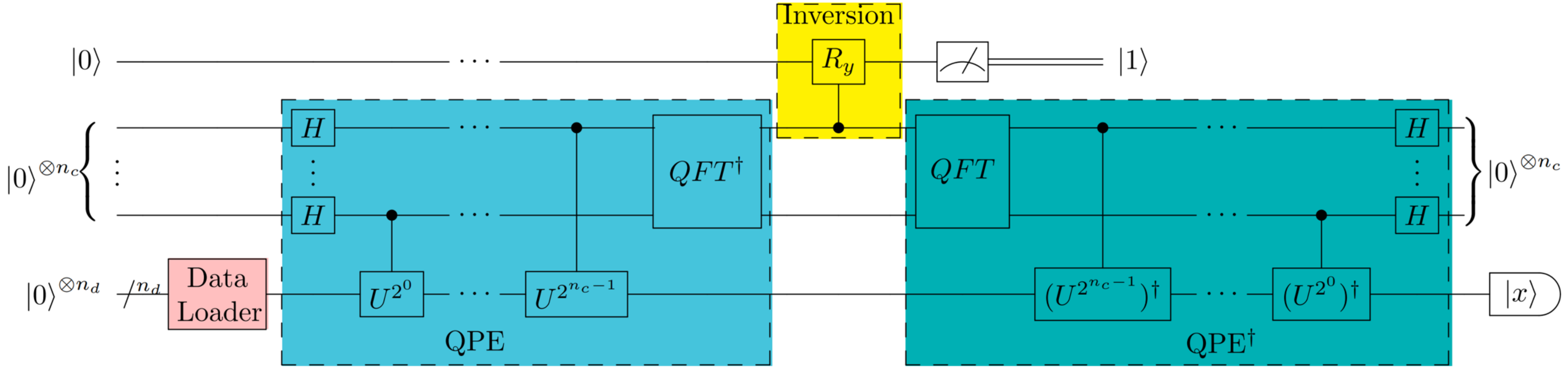
Harrow-Hassidim-Lloyd (HHL) Algorithm

- Quantum linear system problem: $A|x\rangle = |b\rangle$,
    - A is a Hermitian matrix, $|b\rangle = \frac{\vec{b}}{\left\|\vec{b}\right\|_2}, |x\rangle = \frac{A^{-1}|b\rangle}{||A^{-1}|b\rangle||_2}$



Load $|b\rangle$ into quantum computer

Eigen-decomposition

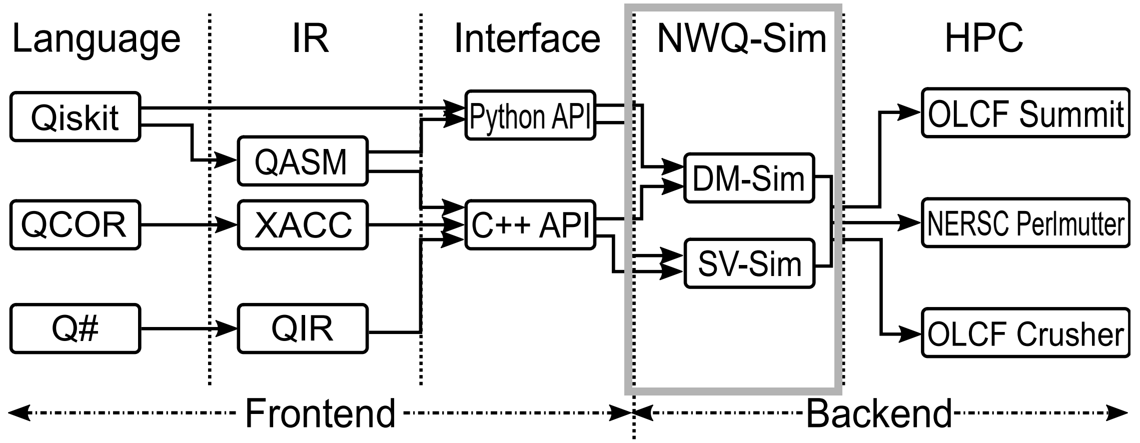
Post-selection and undo QPE to obtain $|x\rangle$

The phases estimated in QPE are stored as a n_c-bit binary string
- n_c is the number of clock qubits for QPE

Larger $n_c \Longrightarrow$ Higher precision in eigenvalue estimation $\Longrightarrow$ Lower HHL solution error

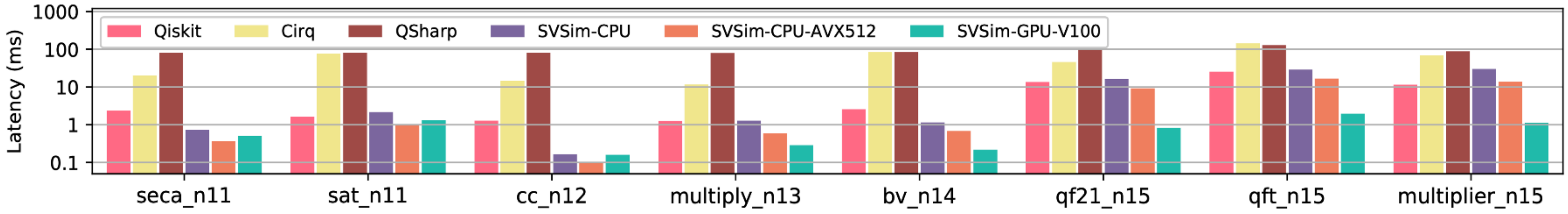
However, each additional clock qubit roughly doubles the total number of gates in the HHL circuit.

HPC Quantum Simulator: NWQSim (1/2)



Routine	Description	Qubits	Gates	CX
seca	Shor's error correction code for teleportation	11	216	84
sat	Boolean satisfiability problem	11	679	252
cc	Counterfeit-coin finding algorithm	12	22	11
multiply	Performing 3×5 in a quantum circuit	13	98	40
bv	Bernstein-Vazirani algorithm	14	41	13
qf21	Quantum phase estimation to factor 21	15	311	115
qft	Quantum Fourier transform	15	540	210
multiplier	Quantum multiplier	15	574	246

Quantum routines evaluated for SV-Sim



The simulation latency of SV-Sim to the default simulators of Qiskit (IBM), Cirq (Google), and Q# (Microsoft) on the V100-DGX-2 platform using a single CPU core or a single GPU

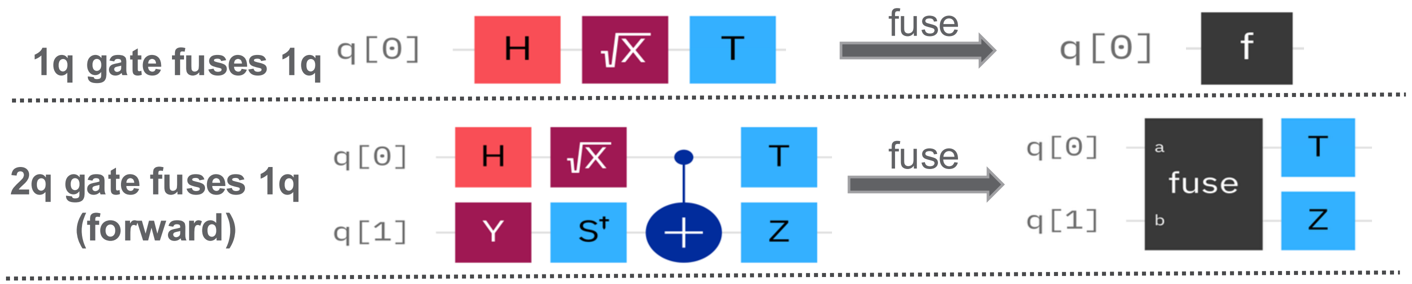
[1] Li, Ang, et al. "Density Matrix Quantum Circuit Simulation via the BSP Machine on Modern GPU Clusters." SC-2020. http://github.com/pnnl/DM-Sim
[2] Li, Ang, et al. "SV-Sim: Scalable PGAS-based State Vector Simulation of Quantum Circuits", SC-2021. http://github.com/pnnl/SV-Sim

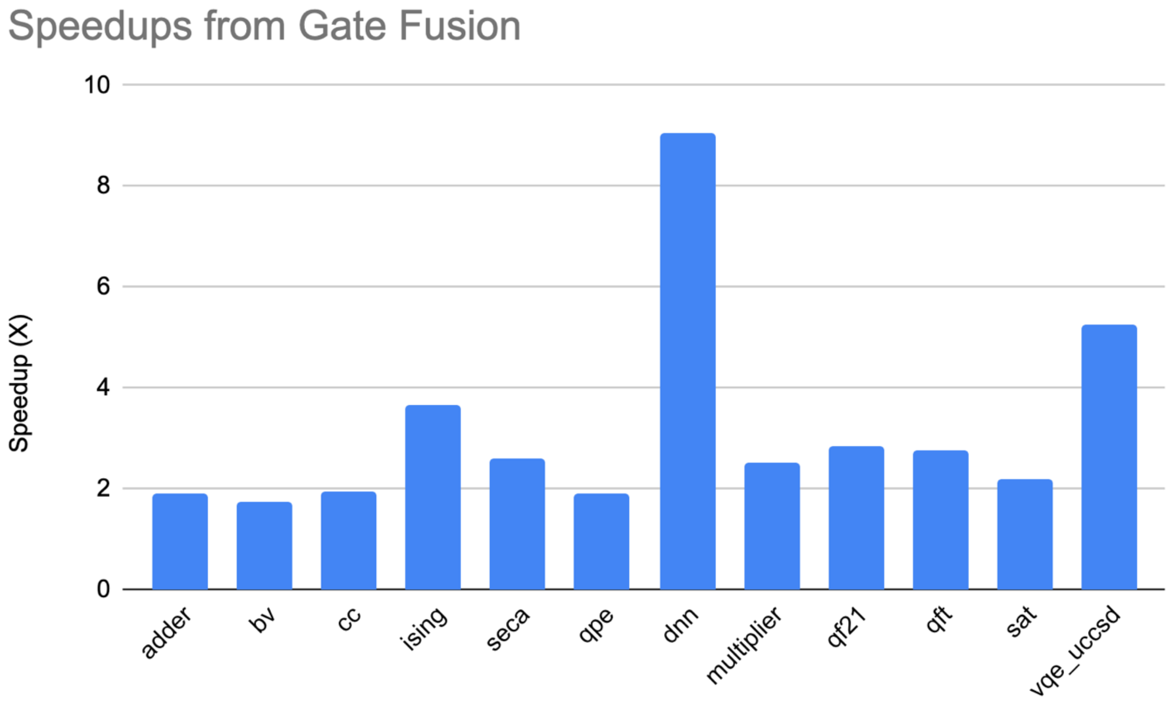
HPC Quantum Simulator: NWQSim (2/2)

Strategy: 1q fusion ➔ 2q-fuse-1q-forward ➔ 2q-fuse-1q-backward ➔ 2q fusion

- May switch qubits to enable more 2q fusion opportunities

- **Fusion can bring a 2x-12x reduction in total gate count**





[1] Li, Ang, et al. "Density matrix quantum circuit simulation via the BSP machine on modern GPU clusters." SC-2020. http://github.com/pnnl/DM-Sim
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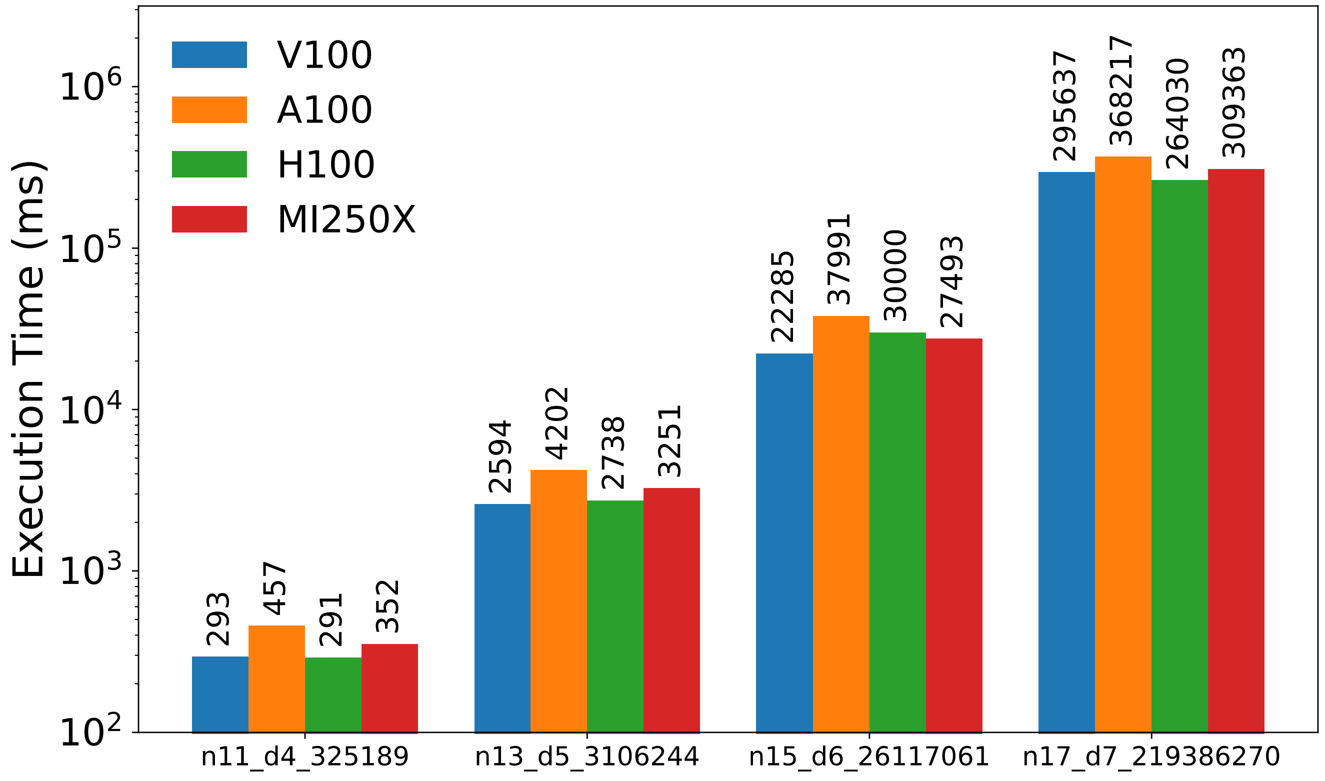
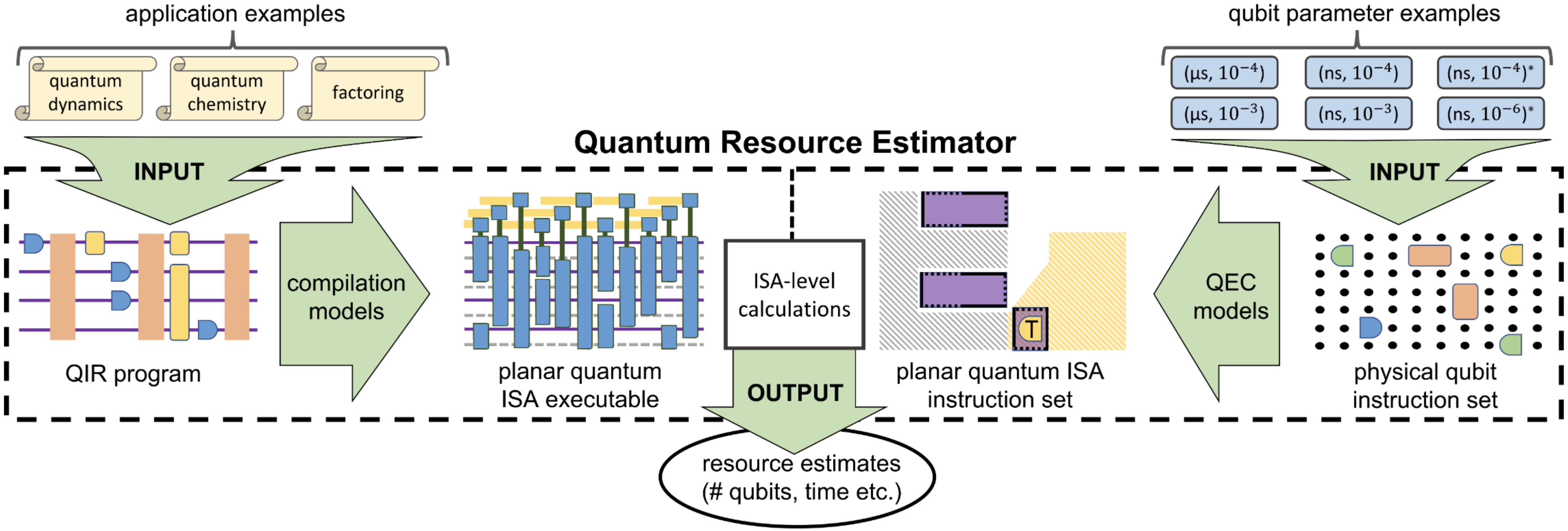
NWQSim Performance on Different GPUs



The tested HHL circuits use randomly generated sparse matrices and random RHS vectors. The three numbers in each circuit's name denote: (1) number of qubits in the circuit; (2) number of qubits used for data loading; and (3) total number of gates.

No. of Qubits n_d	n_c	CX gates	Depth	Total No. of Gates Before Fusion	After Fusion
4	6	116,535	248,084	325,189	70,804
5	7	1,111,178	2,373,842	3,106,244	665,921
6	8	9,335,345	19,969,964	26,117,061	5,557,777
7	9	78,420,632	167,816,254	219,386,270	46,631,320

Azure Quantum Resource Estimator



Error budget is the overall allowed errors for the algorithm. Its value is equally divided into

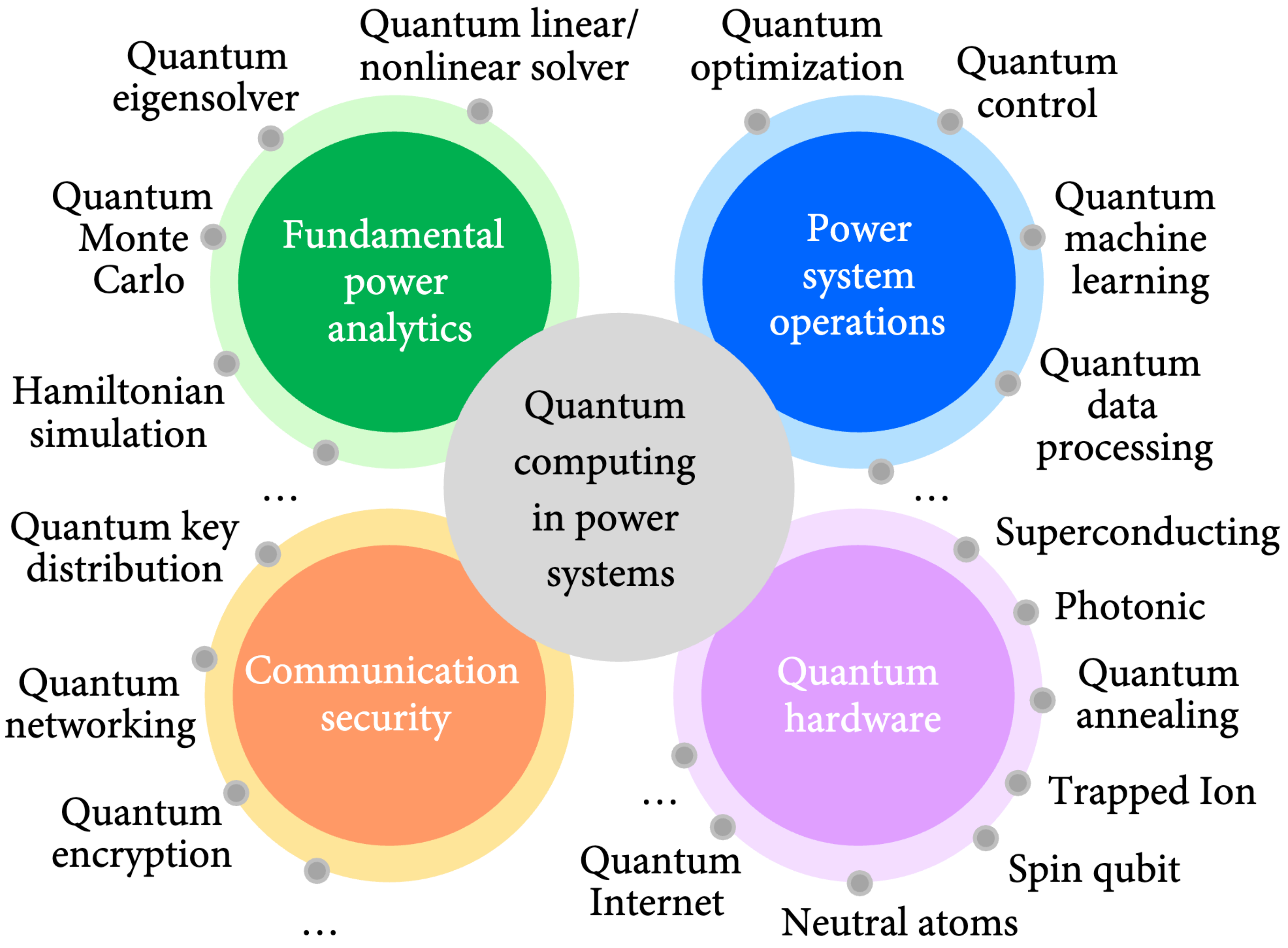
- logical error probability: the probability of at least one logical error
- T-distillation error probability: the probability of at least one faulty T-distillation
- rotation synthesis error probability: the probability of at least one failed rotation synthesis.

After or pre- layout: if enforce 2-D nearest-neighbor connectivity of the qubits or not

[1] Beverland, M.E., Murali, P., Troyer, M., Svore, K.M., Hoefler, T., Kliuchnikov, V., Low, G.H., Soeken, M., Sundaram, A. and Vaschillo, A., 2022. Assessing requirements to scale to practical quantum advantage. arXiv preprint arXiv:2211.07629.

QC Applications in Power Systems

- Power flow and state estimation problems
  - The goal is to analyze the steady-state behavior of power systems by describing the relationship between bus voltages (magnitude and phase angles), currents, and power injections in a power system



[1] Zhou, Y., Tang, Z., Nikmehr, N., Babahajiani, P., Feng, F., Wei, T.C., Zheng, H. and Zhang, P., 2022. Quantum computing in power systems. *IEnergy*, *1*(2), pp.170-187.

AC Power Flow Problem

- For a system with B buses and G generators → $2(B-1)-(G-1)$ unknowns
  - **voltage magnitudes**, $|Vk|$,
  - **phase angles**, θ_k , for load buses and voltage phase angles for generator buses
- Power flow equations

$$P_k = \sum_{j=1}^{n} \left(|V_k||V_j|\mathrm{Re}(Y_{kj}^*)\cos(\theta_{kj}) + |V_k||V_j|\mathrm{Im}(Y_{kj}^*)\sin(\theta_{kj}) \right)$$

$$Q_k = \sum_{j=1}^{n} \left(|V_k||V_j|\mathrm{Re}(Y_{kj}^*)\sin(\theta_{kj}) - |V_k||V_j|\mathrm{Im}(Y_{kj}^*)\cos(\theta_{kj}) \right)$$

- P_k: real power injection at bus k
- Q_k: reactive power injection at bus k
- $|V_k|$: voltage magnitude at bus k
- θ_{kj}: phase angle difference between bus k and bus j
- Y_{kj}: admittance between bus k and bus j

Newton-Raphson Method

- Solve $f(\vec{y}) = \vec{d}$ where f is a non-linear algebraic function

With 1st-order Taylor series expansion

$$\vec{d} = f\left(\vec{y}^{(0)}\right) + \left.\frac{df}{dy}\right|_{\vec{y}^{(0)}} \left(\vec{y} - \vec{y}^{(0)}\right)$$

$$\vec{y} = \vec{y}^{(0)} + J^{-1}\left(\vec{d} - f\left(\vec{y}^{(0)}\right)\right)$$

$$\vec{y}^{(\nu+1)} = \vec{y}^{(\nu)} + \boxed{J^{-1}\left(\vec{d} - f\left(\vec{y}^{(\nu)}\right)\right)}$$

In the N-R iteration $\nu + 1$

- Solve

$$\boxed{J\Delta\vec{y}^{(\nu+1)} = \Delta\vec{f}^{(\nu)}}$$

where $\Delta\vec{f}^{(\nu)} = \vec{d} - f\left(\vec{y}^{(\nu)}\right)$

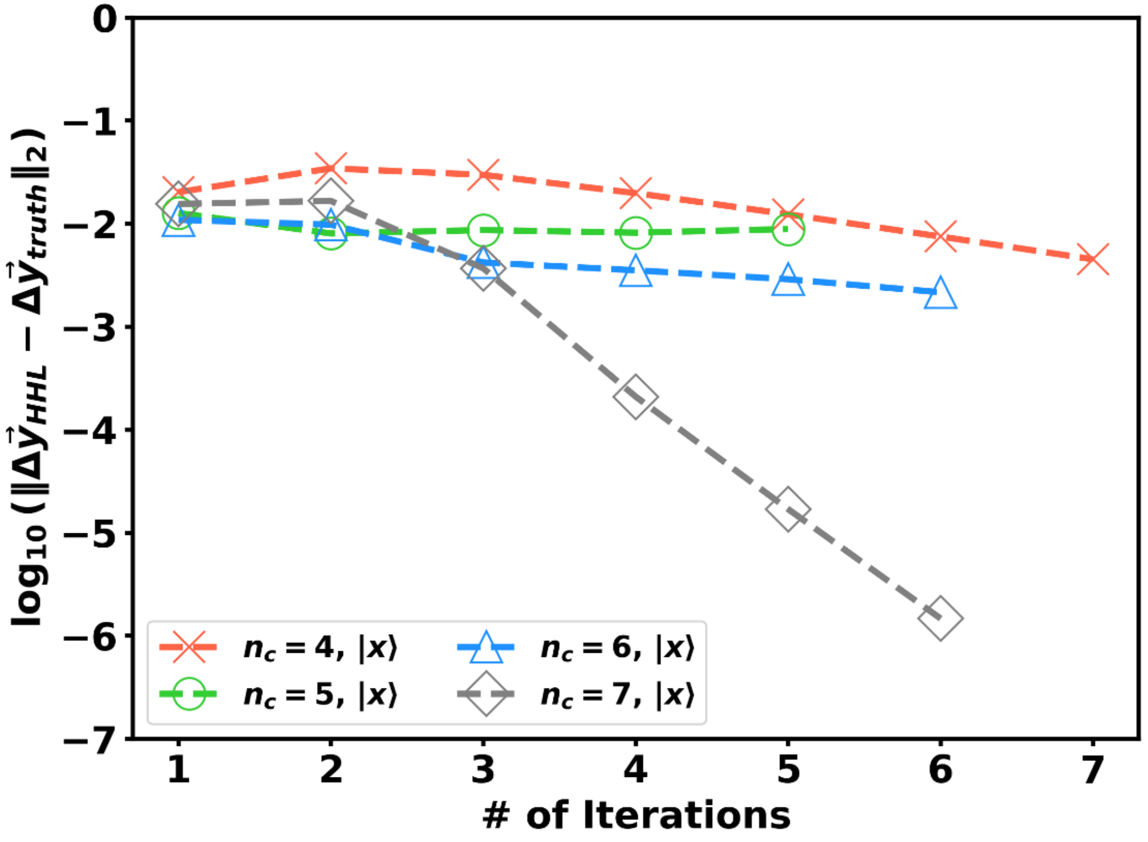
- Update
  - $\vec{y}^{(\nu+1)} = \vec{y}^{(\nu)} + \Delta\vec{y}^{(\nu+1)}$
  - $\Delta\vec{f}^{(\nu+1)} = \vec{d} - f\left(\vec{y}^{(\nu+1)}\right)$
- Set to converge when $\left\|\Delta\vec{f}^{(\nu)}\right\|$ is small

$$\begin{bmatrix} \frac{\partial \Delta\vec{P}}{\partial\vec{\theta}} & \frac{\partial \Delta\vec{P}}{\partial|\vec{V}|} \\ \frac{\partial \Delta\vec{Q}}{\partial\vec{\theta}} & \frac{\partial \Delta\vec{Q}}{\partial|\vec{V}|} \end{bmatrix} \begin{bmatrix} \Delta\vec{\theta} \\ \Delta|\vec{V}| \end{bmatrix} = -\begin{bmatrix} \Delta\vec{P} \\ \Delta\vec{Q} \end{bmatrix}$$

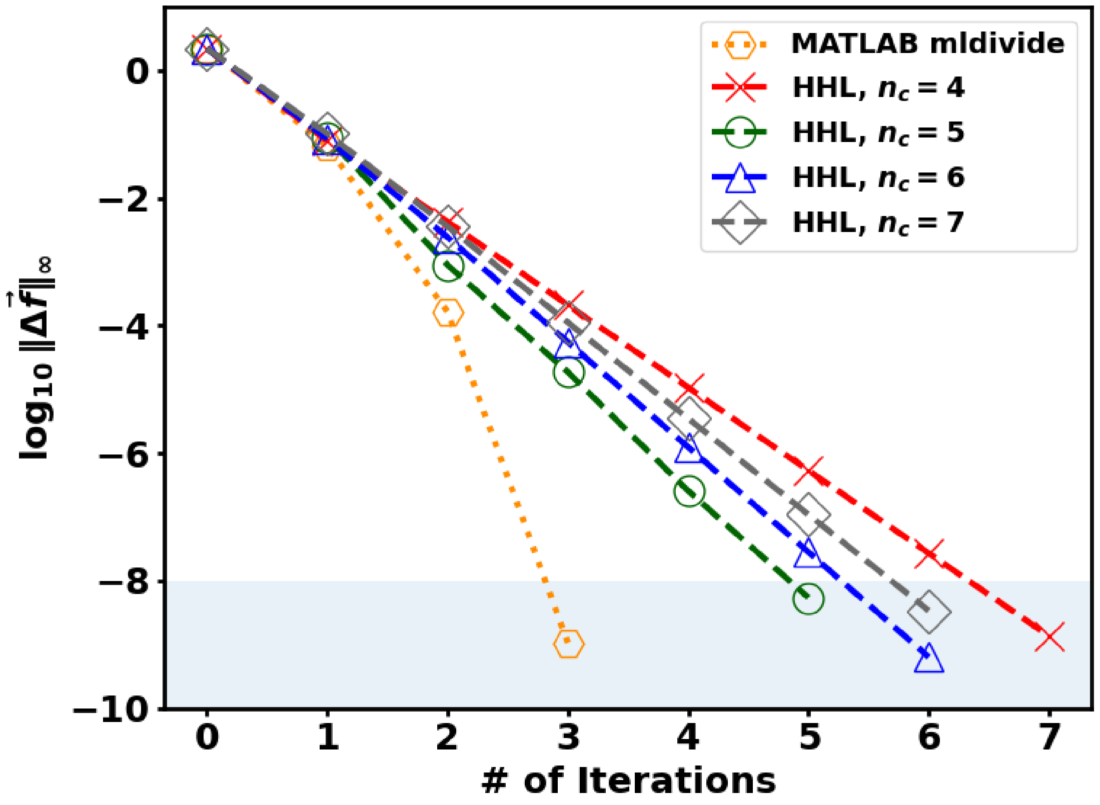
in AC power flow problem

HHL and Newton-Raphson Method

- Linear systems solved are in the size of 16×16
- All quantum and classical runs converge at the same $\vec{y}$



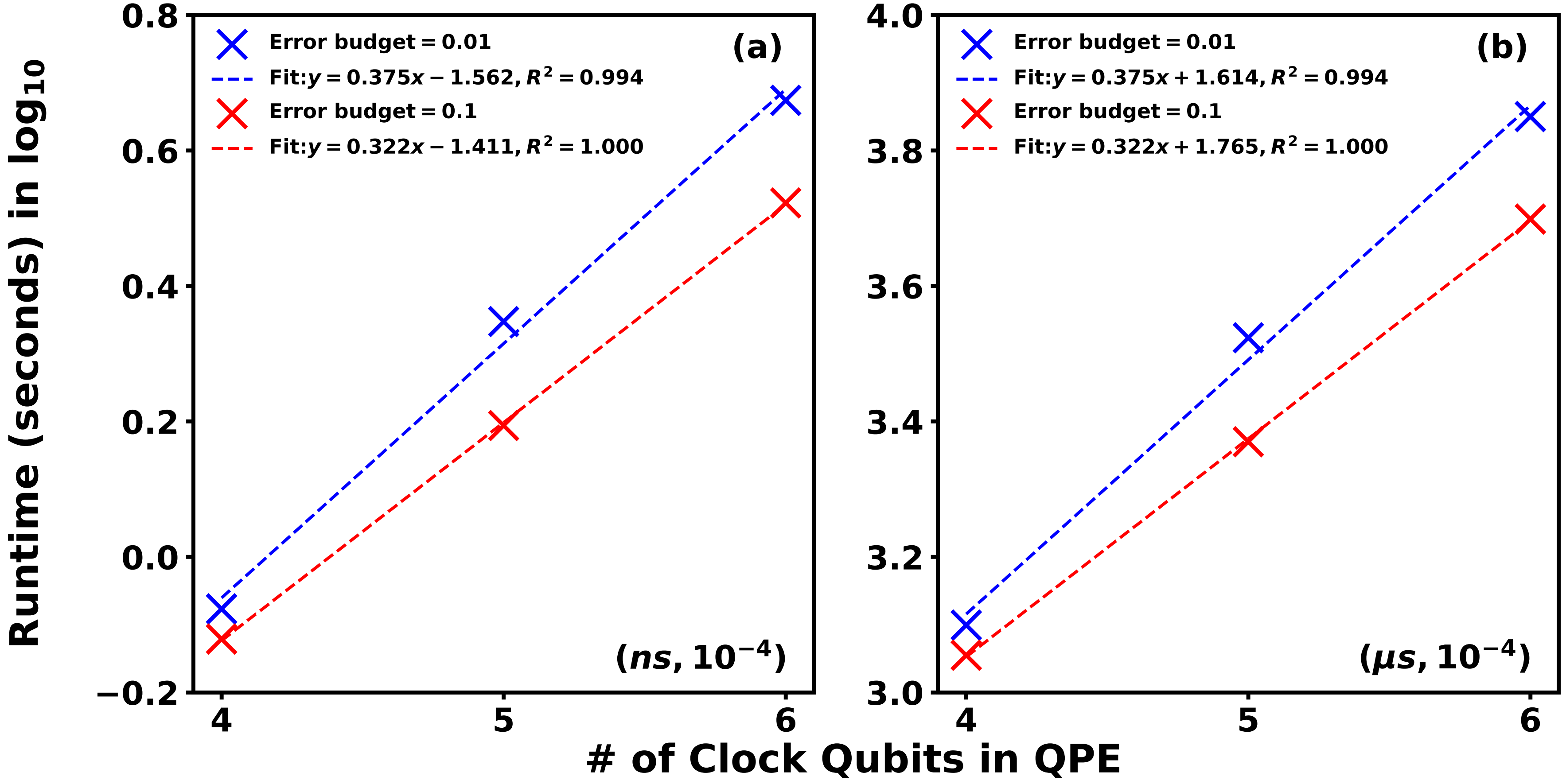
HHL Errors



Convergence Criteria $\left\|\Delta\vec{f}^{(\nu)}\right\|$

Runtime Estimation under a Surface Code

Estimate the runtime under a surface code that encodes 98 physical qubits into a logical qubit



Qubit parameters from [1]:

- $(\mu s, 10^{-4})$: 100 μs operation time, 10^{-4} error rate for Clifford gates and 10^{-6} for non-Clifford gates
- $(ns, 10^{-4})$: 100 ns operation time, 10^{-4} error rate for Clifford gates and 10^{-4} for non-Clifford gates

[1] Beverland, M.E., Murali, P., Troyer, M., Svore, K.M., Hoefler, T., Kliuchnikov, V., Low, G.H., Soeken, M., Sundaram, A. and Vaschillo, A., 2022. Assessing requirements to scale to practical quantum advantage. arXiv preprint arXiv:2211.07629.

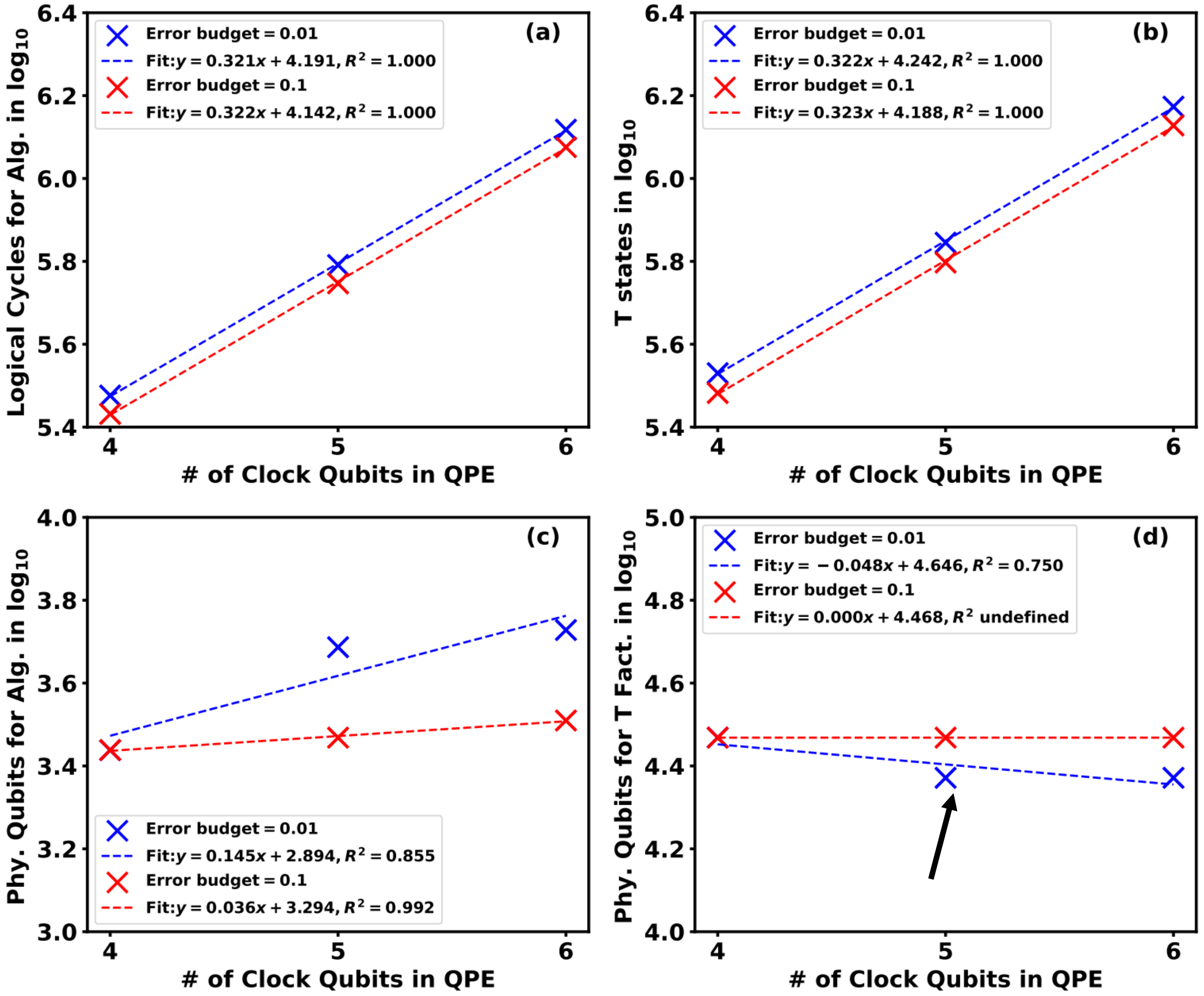
HHL Circuit and QEC Cost

Estimate the resource cost under a surface code that encodes 98 physical qubits into a logical qubit

- The logical qubit error rate is 10^{-9} to 10^{-10}

Error budget	n_c	Physical qubits after layout	Logical qubits pre- and after layout	Min. logical qubit error rate	Min. T state error rate
0.01	4	32,144	9 to 28	3.977×10^{-10}	9.831×10^{-9}
	5	28,380	10 to 30	1.797×10^{-10}	4.762×10^{-9}
	6	28,866	11 to 33	7.700×10^{-11}	2.236×10^{-9}
0.1	4	32,144	9 to 28	4.406×10^{-9}	1.098×10^{-7}
	5	32,340	10 to 30	1.990×10^{-9}	5.319×10^{-8}
	6	32,634	11 to 33	8.487×10^{-10}	2.483×10^{-8}

Faster runtime growth reduces the number of T-factories needed, thereby reducing the total number of physical qubits.



**Tool: Microsoft Azure Quantum Resources Estimator*

Quantum Linear Solver in Differential Equation (DE) Solving

- Example: 2-D heat-diffusion PDE discretized via finite differences.

$$\frac{\partial T}{\partial t} = D\nabla^2 T + F \;\Rightarrow\; AT = F$$

where

  - T is the temperature at a given 2-D point and time
  - D is the transfer coefficient
  - F is the forcing term that includes boundary / initial conditions

After discretization, the linear system becomes $AT = F$

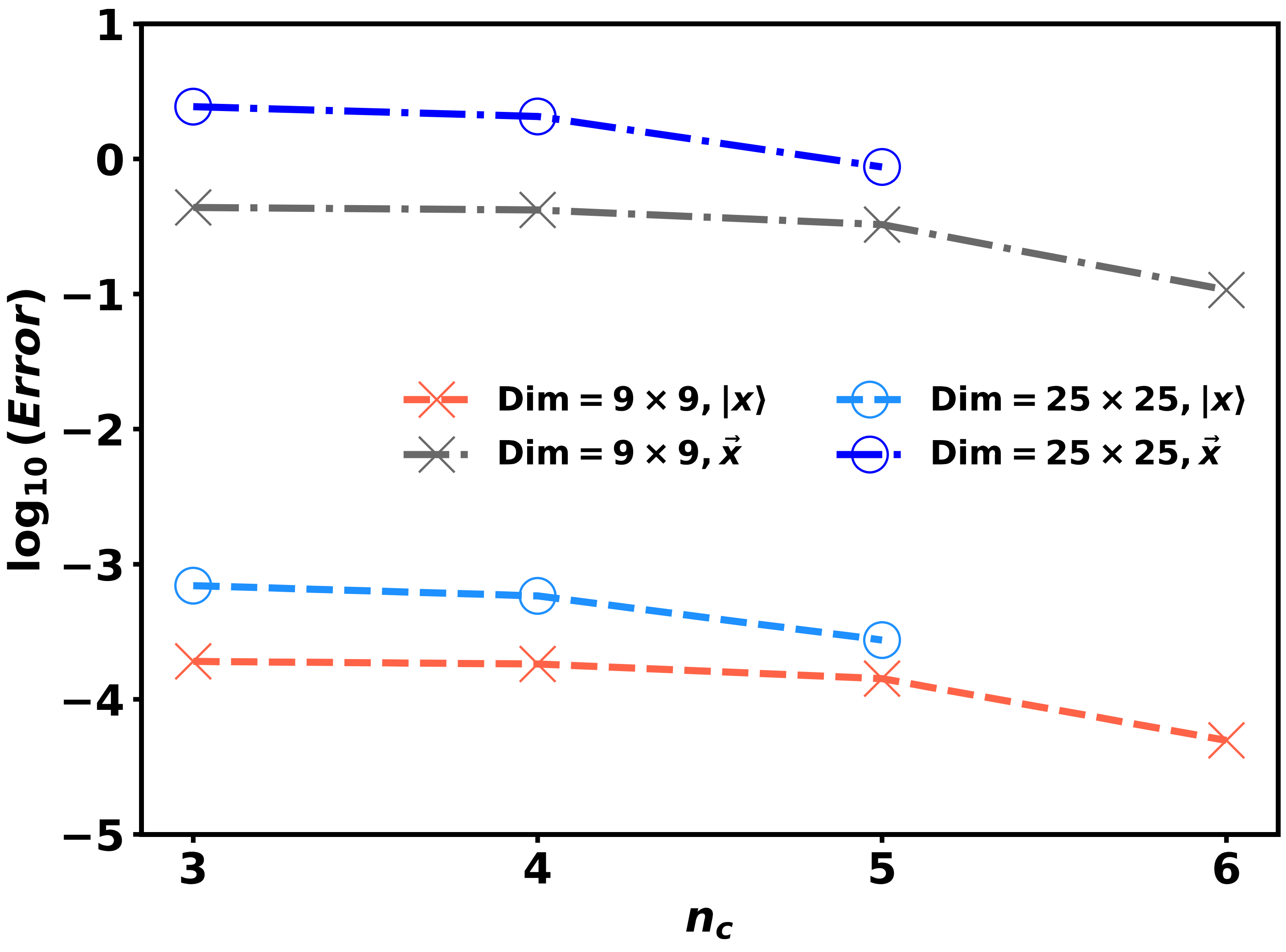
  - $A_{pq} = \begin{cases} 1 + 4r, p = q \\ -r, p = q \pm 1 \; or \; p = q \pm l \\ 0, otherwise \end{cases}$ for l number of grid points

We tested 3-point (9×9 matrix) and 5-point (25×25 matrix)

HHL Performance in DE Solving

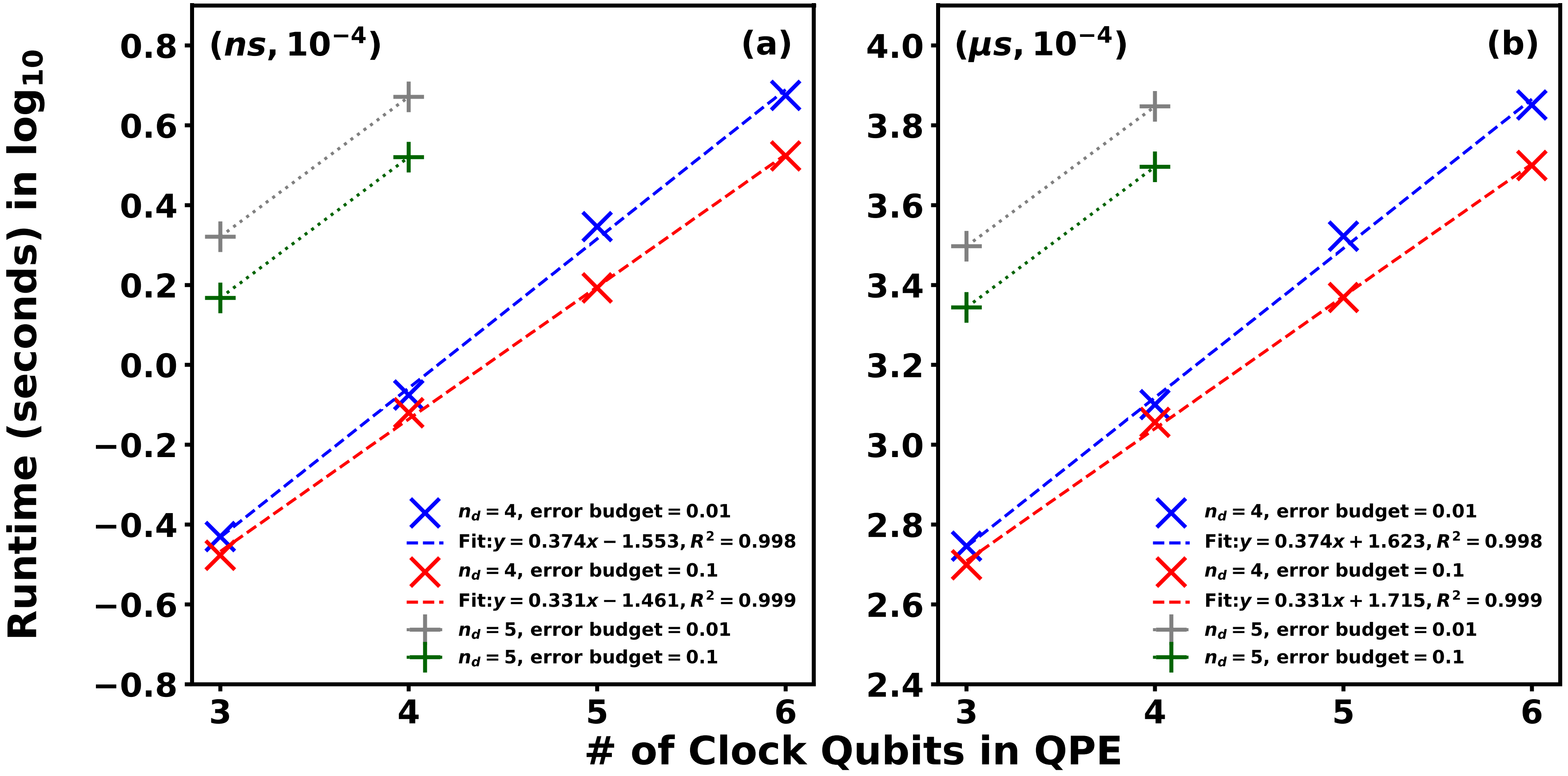
- Errors are defined as (1) $\| |x\rangle - |x\rangle_{HHL} \|_2$ and (2) $\| \vec{x} - \vec{x}_{HHL} \|_2$.
- The incremental of n_c shows limited reduction towards errors.

Dim.	n_d	n_c	Depth	# of gates	#of 2-qubit gates	# of gates after fusion
9 × 9	4	3	30742	40290	14315	8445
9 × 9	4	4	65824	86262	30651	18061
9 × 9	4	5	135986	178180	63315	37284
9 × 9	4	6	276308	361980	128631	75718
25 × 25	5	3	133966	175253	62546	37147
25 × 25	5	4	287134	375643	134046	79547
25 × 25	5	5	593948	777069	277230	164338



Runtime Estimation in QEC Settings

Estimate the runtime under a surface code that encodes 98 physical qubits into a logical qubit



Qubit parameters from [1]:

- $(\mu s, 10^{-4})$: 100 μs operation time, 10^{-4} error rate for Clifford gates and 10^{-6} for non-Clifford gates
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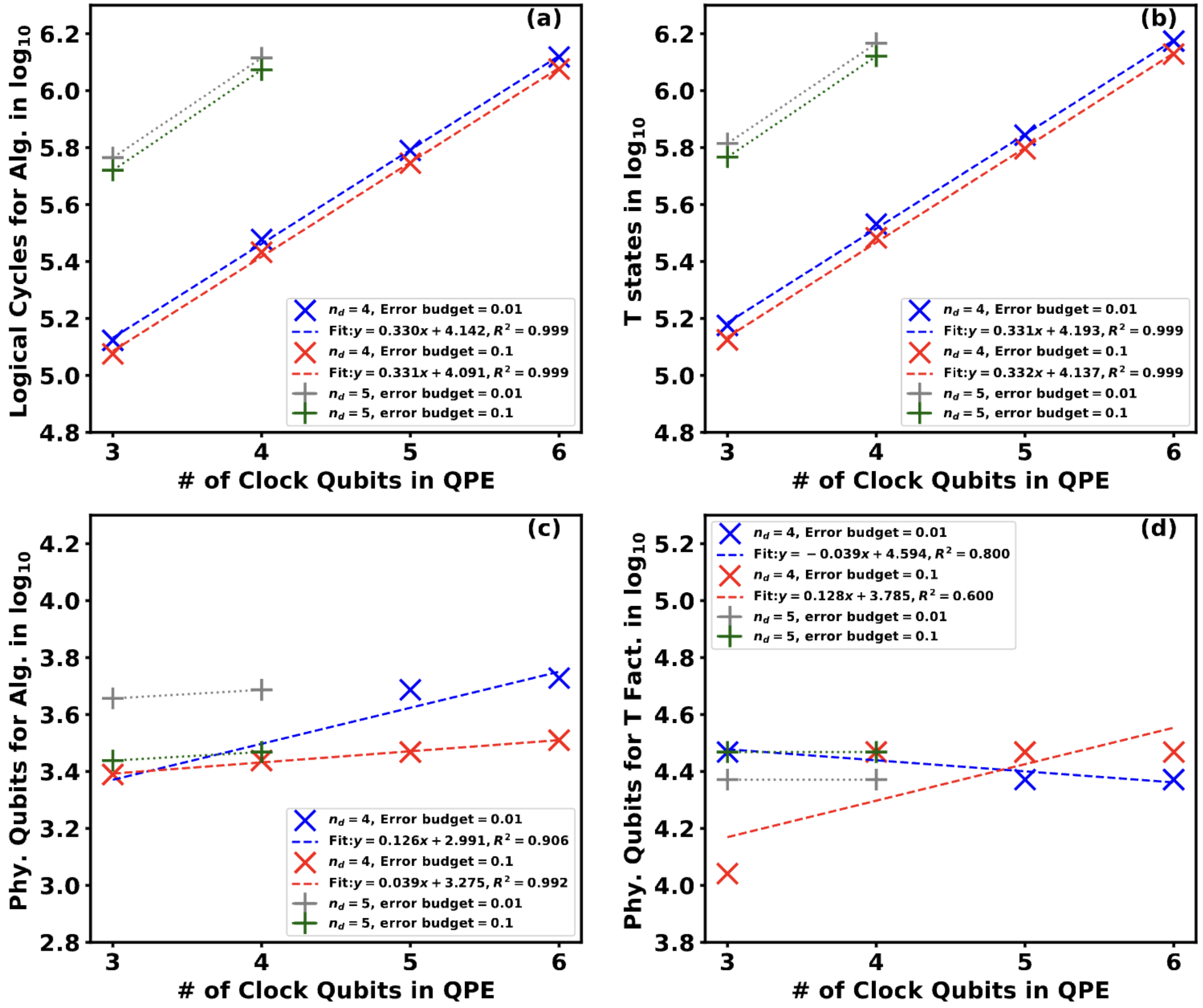
QEC Cost in DE Solving

Estimate the resource cost under a surface code that encodes 98 physical qubits into a logical qubit

- The logical qubit error rate is 10^{-9} to 10^{-10}

Error budget	(n_d, n_c)	Physical qubits after layout	Logical qubits pre- and after layout	Min. logical qubit error rate	Min. T state error rate
0.01	(4,3)	31850	8 to 25	1.01×10^{-9}	2.22×10^{-8}
	(4,4)	32144	9 to 28	3.97×10^{-10}	9.81×10^{-9}
	(4,5)	28380	10 to 30	1.80×10^{-10}	4.77×10^{-9}
	(4,6)	28866	11 to 33	7.69×10^{-11}	2.23×10^{-9}
	(5,3)	28056	9 to 28	2.05×10^{-10}	5.11×10^{-9}
	(5,4)	28380	10 to 30	8.53×10^{-11}	2.27×10^{-9}
0.1	(4,3)	13450	8 to 25	1.12×10^{-8}	2.50×10^{-7}
	(4,4)	32144	9 to 28	4.40×10^{-9}	1.10×10^{-7}
	(4,5)	32340	10 to 30	2.00×10^{-9}	5.33×10^{-8}
	(4,6)	32634	11 to 33	8.47×10^{-10}	2.48×10^{-8}
	(5,3)	32144	9 to 28	2.27×10^{-9}	5.70×10^{-8}
	(5,4)	32340	10 to 30	9.39×10^{-10}	2.52×10^{-8}



Conclusion

- Highlighted the benefits of the utilization of low-precision QPE in HHL for both iterative and non-iterative methods in practice:
  - low-precision QPE can exponentially reduce the gate counts and circuit depth in an HHL circuit, while keeping the same solution accuracy in iterative methods like Newton-Raphson method and maintain a similar level of accuracy in a non-iterative method like finite difference method.
- Demonstrated that runtime, number of logical cycles, and number of T states all grow exponentially with the number of clock qubits in QPE
- Showed how the faster growth in runtime can offset physical-qubit requirements for T factories preparation.