Molecular Dynamics Workflow Decomposition for Hybrid Classic/Quantum Systems

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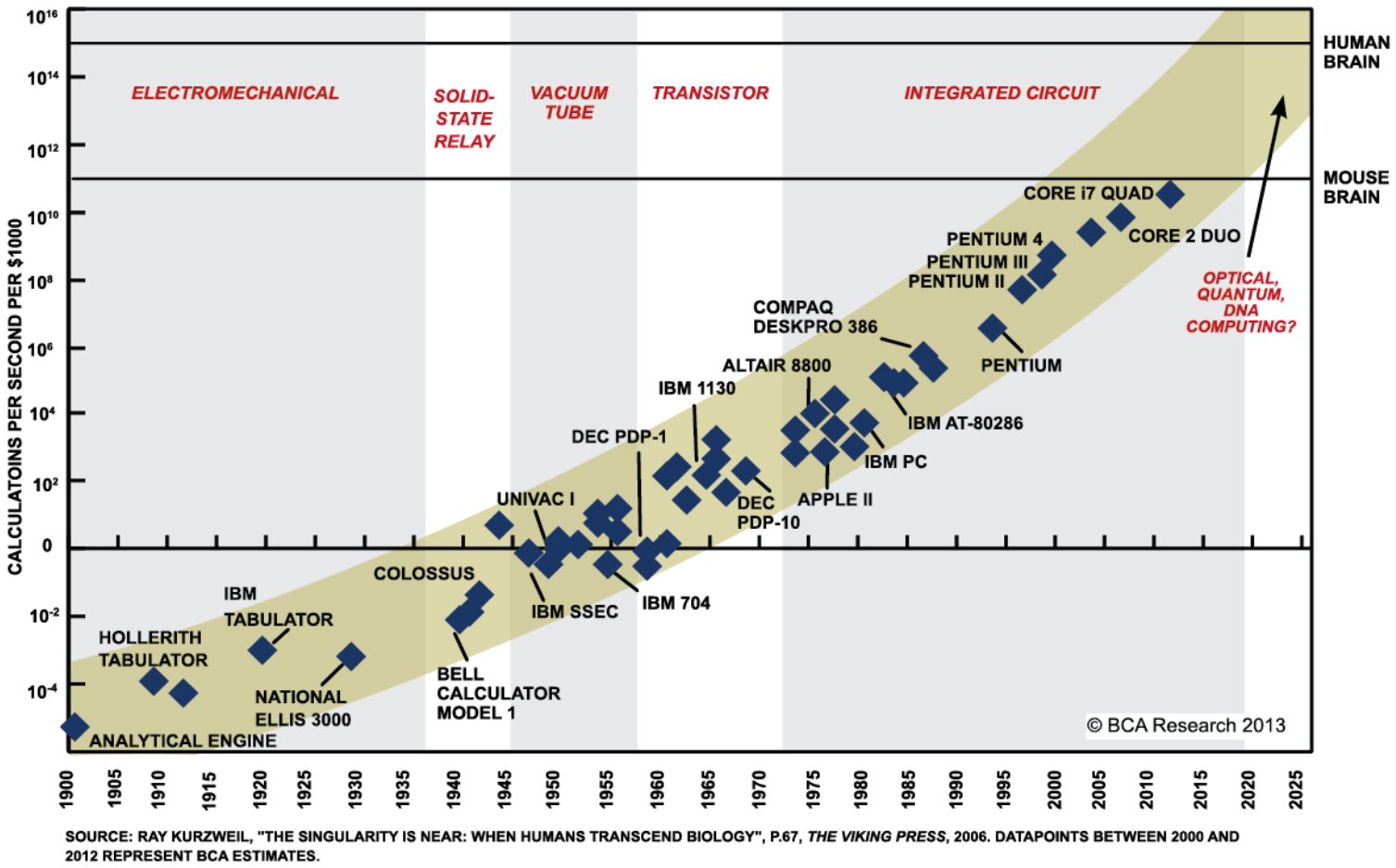
Post-Moore Computing



SOURCE: RAY KURZWEIL, "THE SINGULARITY IS NEAR: WHEN HUMANS TRANSCEND BIOLOGY", P.67, *THE VIKING PRESS*, 2006. DATAPOINTS BETWEEN 2000 AND 2012 REPRESENT BCA ESTIMATES.

- To improve performance of current architectures, we need to reduce component size…
- Component size: hitting the atom limit!
- Time to consider alternative (post-Moore's Law) forms of computing

Known Quantum Speedup

- Grover's algorithm: $O(\sqrt{n})$ vs $O(n)$
- Shor's algorithm: Polynomial vs Exponential
- Quantum ML

"Quantum random access memory", V. Giovannetti et al., Phys. Rev. Letters, vol. 100 p. 160501

"BQP and the polynomial hierarchy", Scott Aaronson

"Machine Learning: Quantum vs Classical", Tariq M. Khan et al., IEEE Access, November 2020

Scientific Quantum Computing

- Native 3D modelling of scientific problems
  - N-body
  - Particle physics
  - …
- Many calculations can benefit from quantum speedup
  - Approximate optimization,
  - Eigenvalues
  - …

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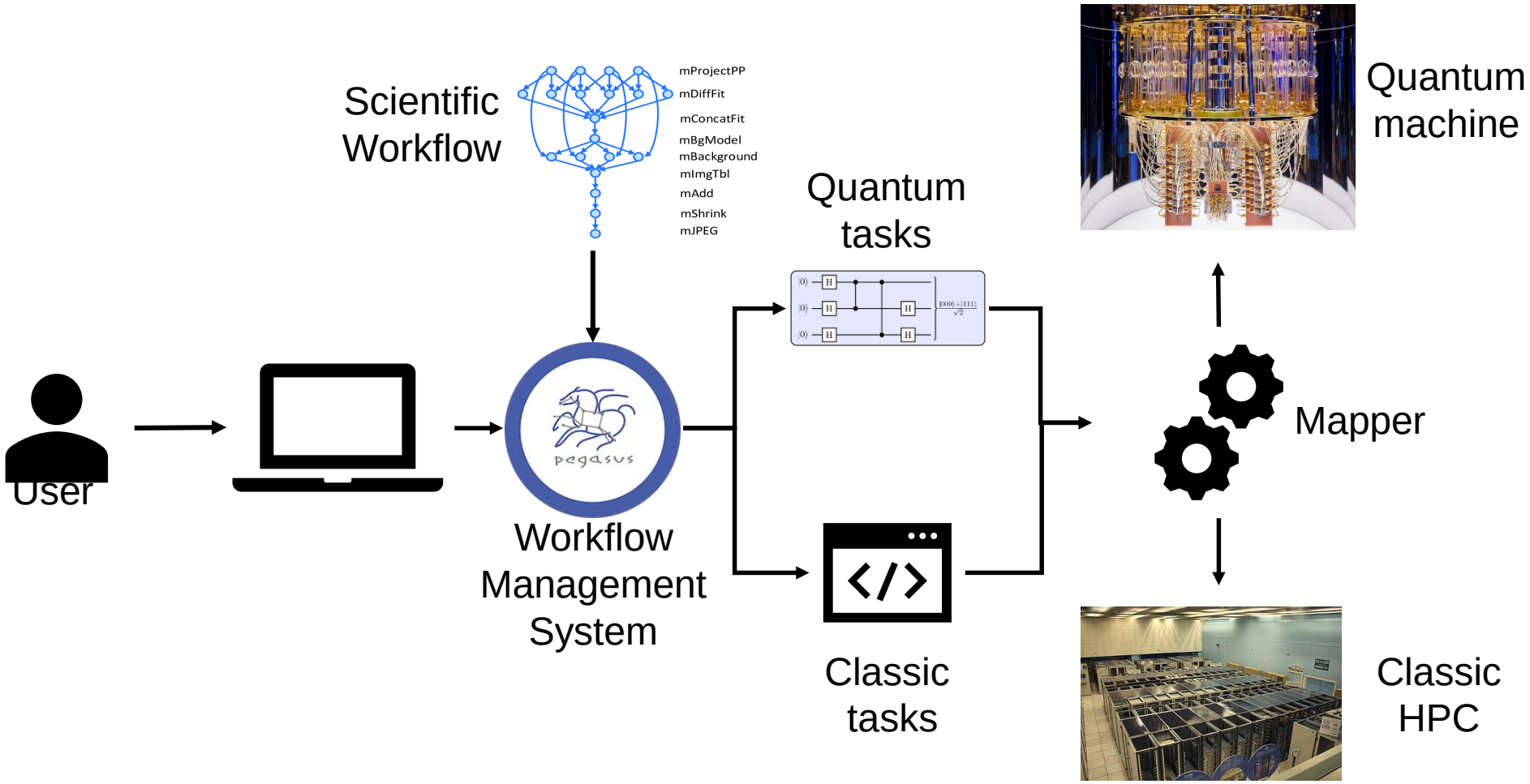
IDEA: integrate quantum as accelerator

Hybrid Classic/Quantum Systems

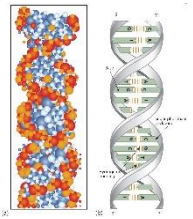


Molecular Dynamics

- Analyzing trajectories of backbone $C\alpha$ atoms of amino-acids segments
- Identifying collective variables capturing molecular motions in a region of interest

User input

Read trajectory file



Atom segments

$$D = \begin{bmatrix} 0 & \cdots & D_{IJ} \\ \vdots & \ddots & \vdots \\ D_{IJ}^T & \cdots & 0 \end{bmatrix}$$

Distance matrix

$$Dv = \lambda v$$

Find maximum eigenvalue

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Molecular Dynamics

- Analyzing trajectories of backbone $C\alpha$ atoms of amino-acids segments
- Identifying collective variables capturing

Question: are there application parts that could benefit from quantum execution?

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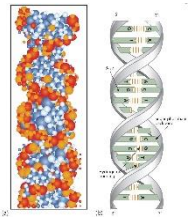
Quantum Decomposition

User input

Read trajectory file

End Device



Atom segments

Classic HPC

$$\begin{bmatrix} 0 & \cdots & D_{IJ} \\ \vdots & \ddots & \vdots \\ D_{IJ}^{T} & \cdots & 0 \end{bmatrix}$$

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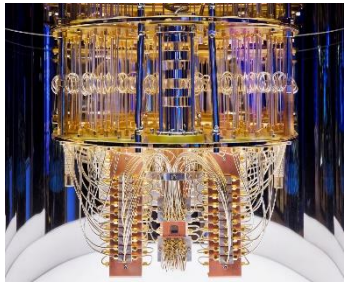

Quantum machine

Quantum Decomposition

User input

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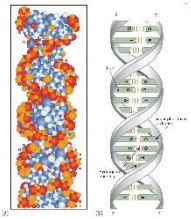
End Device



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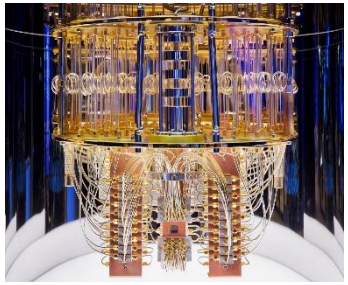

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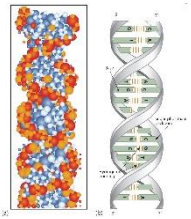

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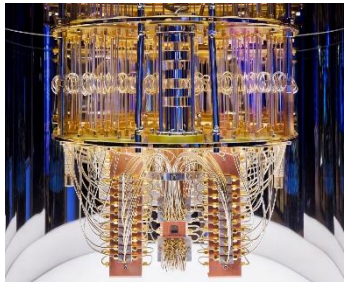
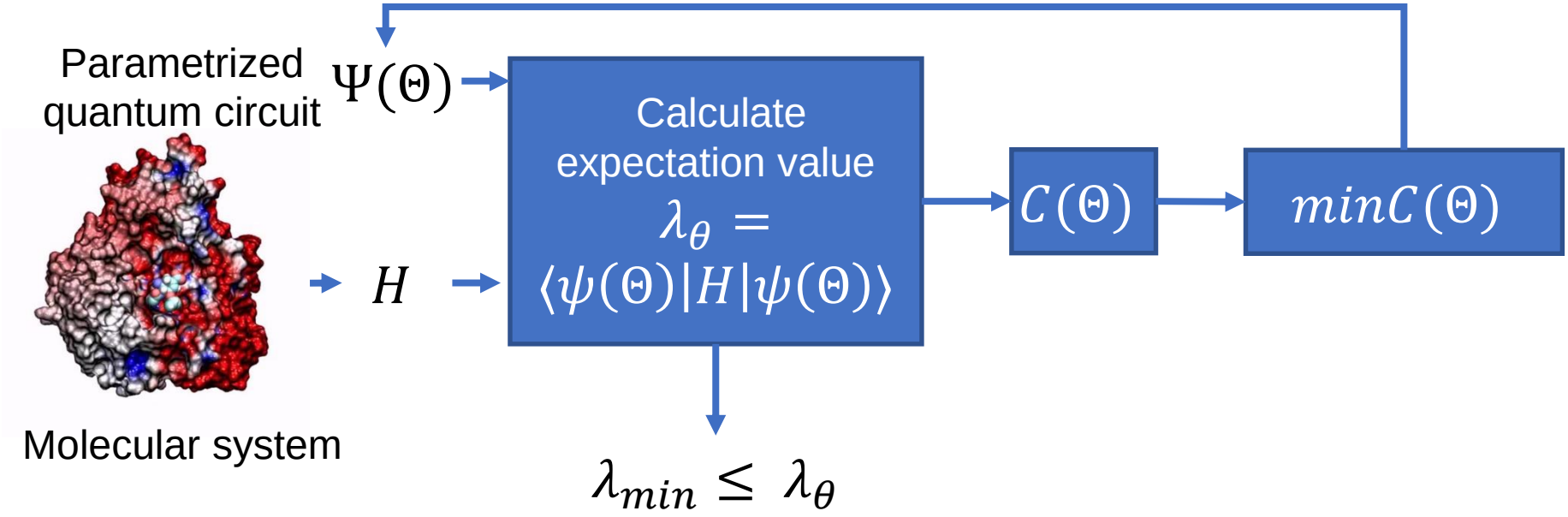


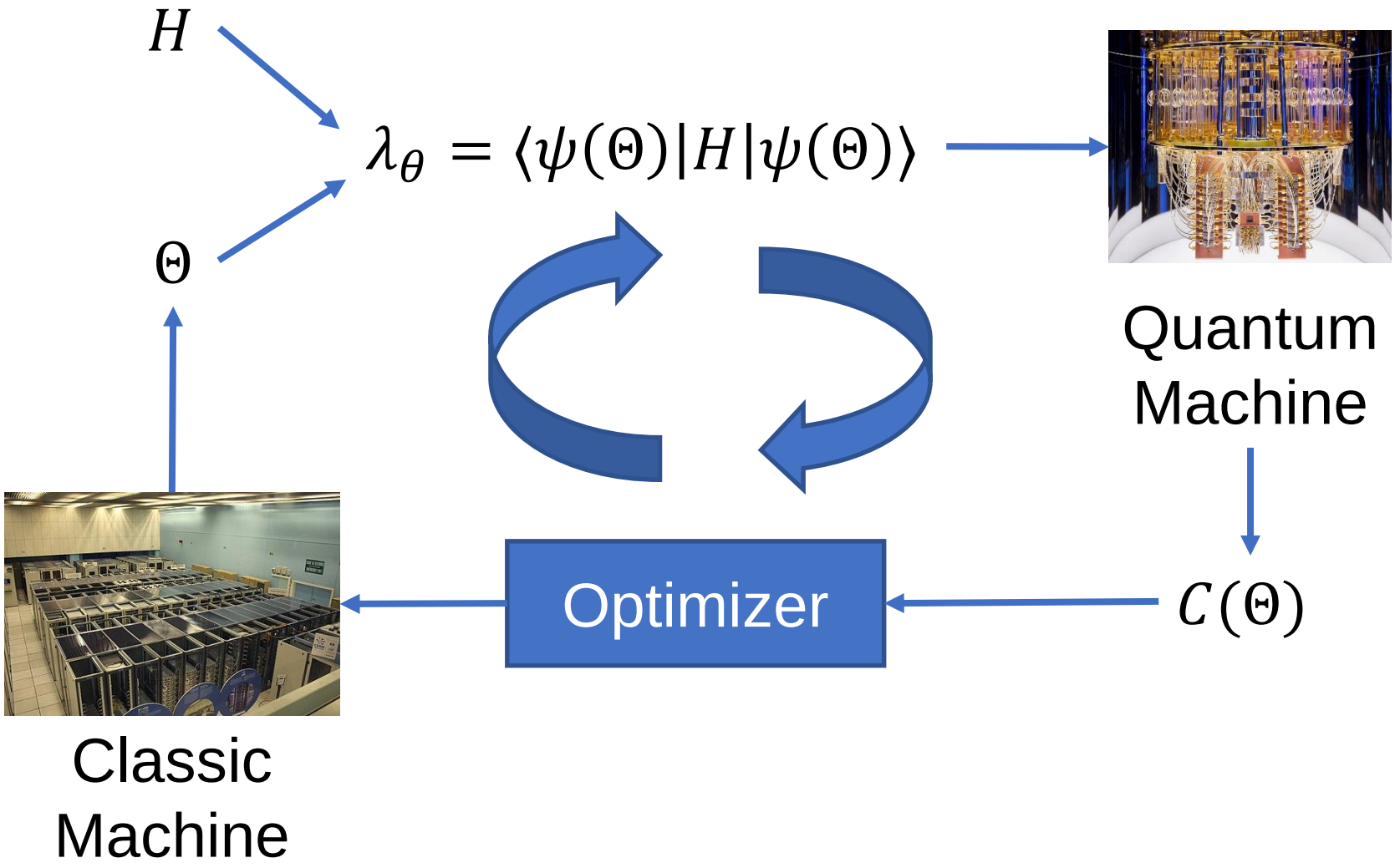
Quantum machine

Variational Quantum Eigensolver (VQE)

- In quantum mechanics, a system of particles can be described as a Hamiltonian representing the energy of the system.
- Finding eigenvalue ≡ Finding Hamiltonian ground state

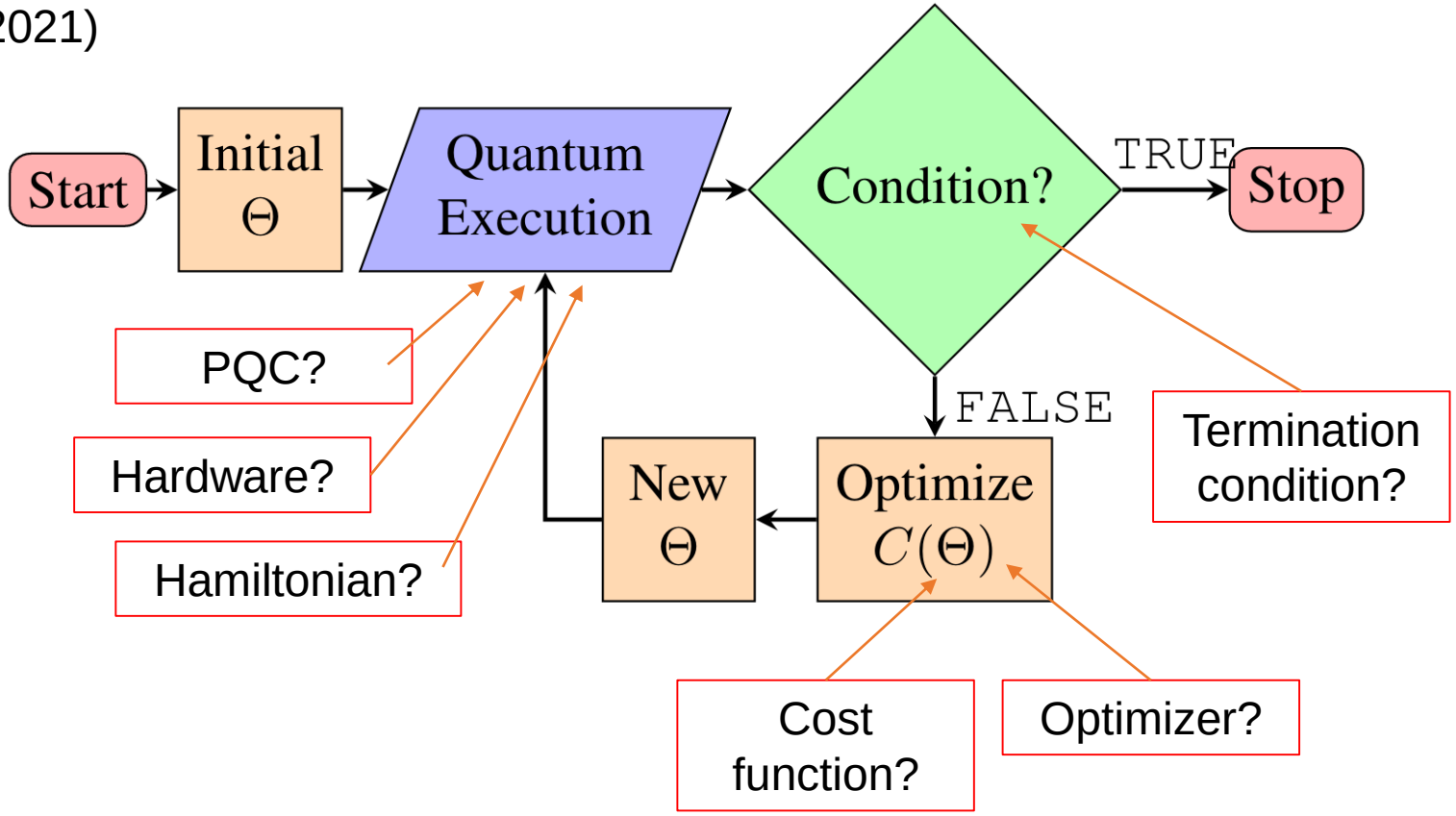


VQE mapping


H
Θ
$\lambda_\theta = \langle\psi(\Theta)|H|\psi(\Theta)\rangle$
Quantum Machine
$C(\Theta)$
Optimizer
Classic Machine

Variational quantum algorithms

- Defined by a set of **hyperparameters**
- Main candidates to achieve Quantum Supremacy (Cerezo et al., 2021)



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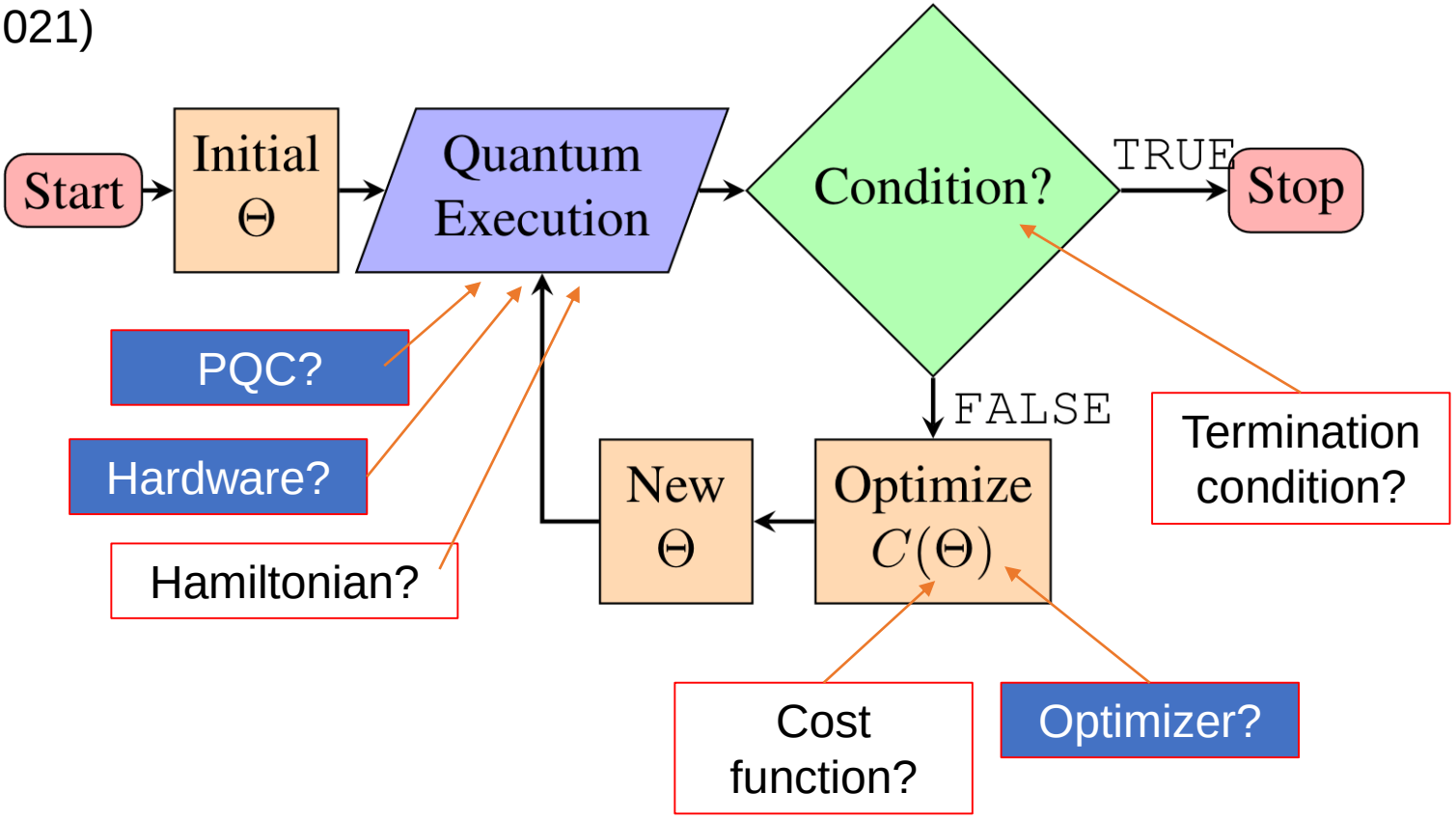
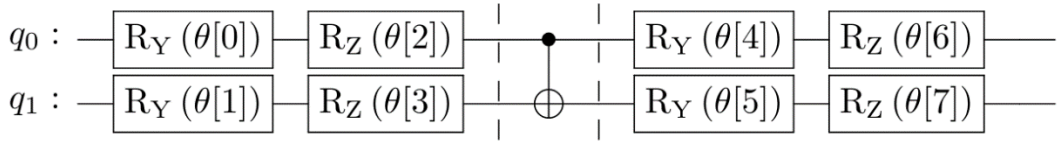
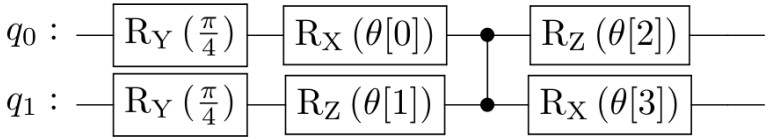


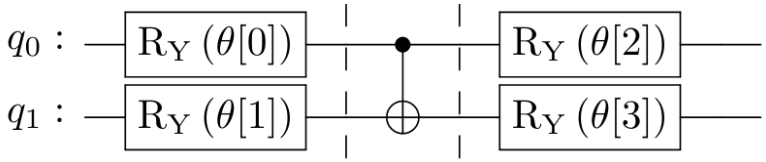
Parametrized Quantum Circuits



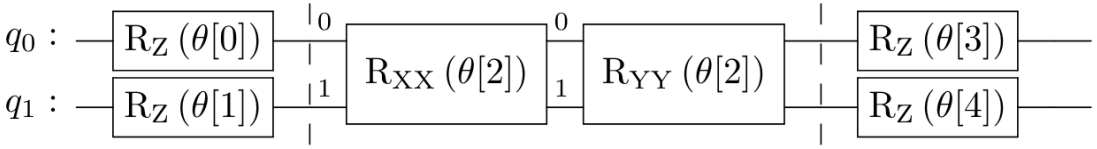
SU2



Pauli Two Design



Real Amplitudes



Excitation Preserving

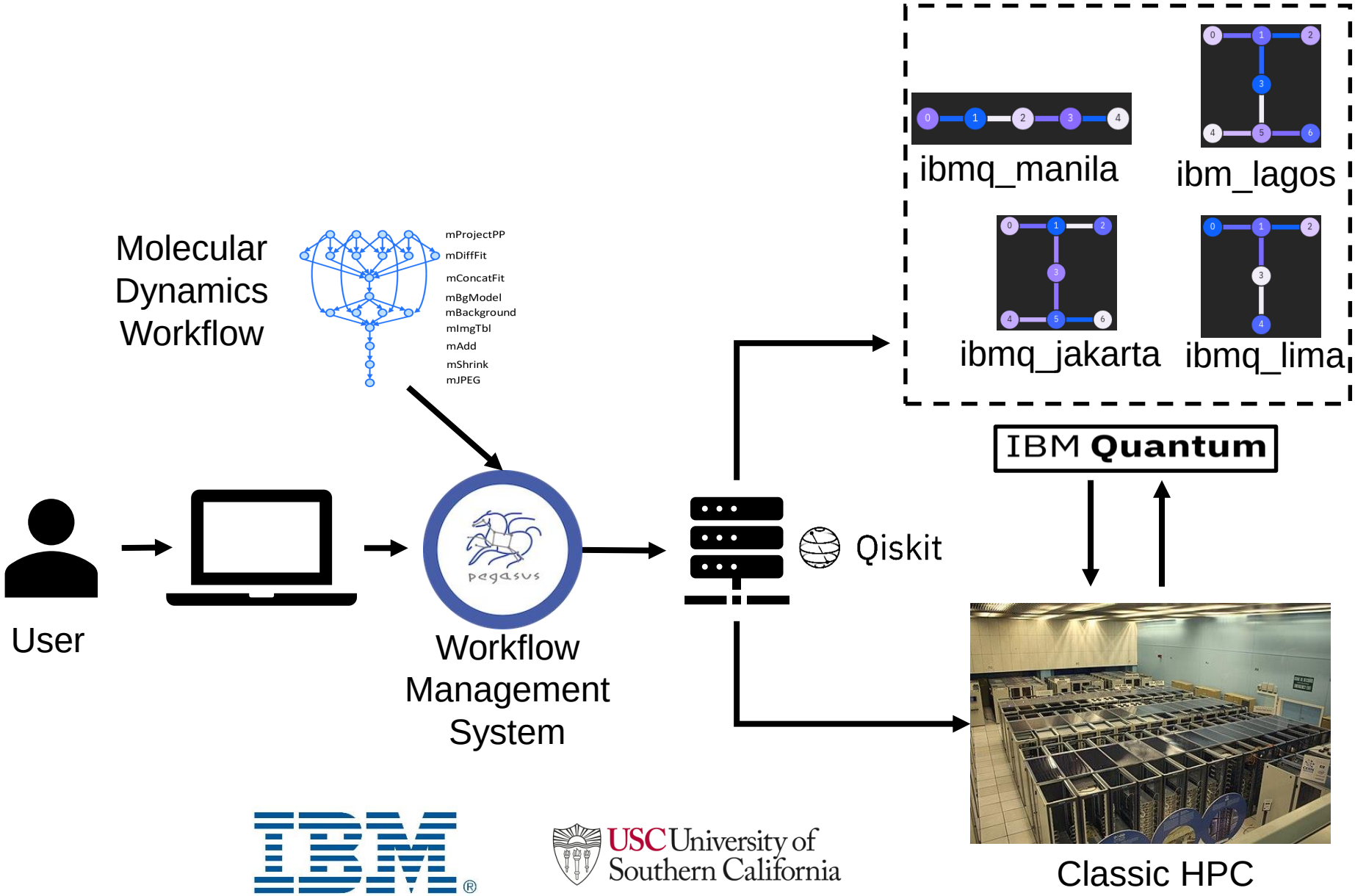
- Standard “well-known” circuits
- Entanglement
- Repetitions

Optimizers

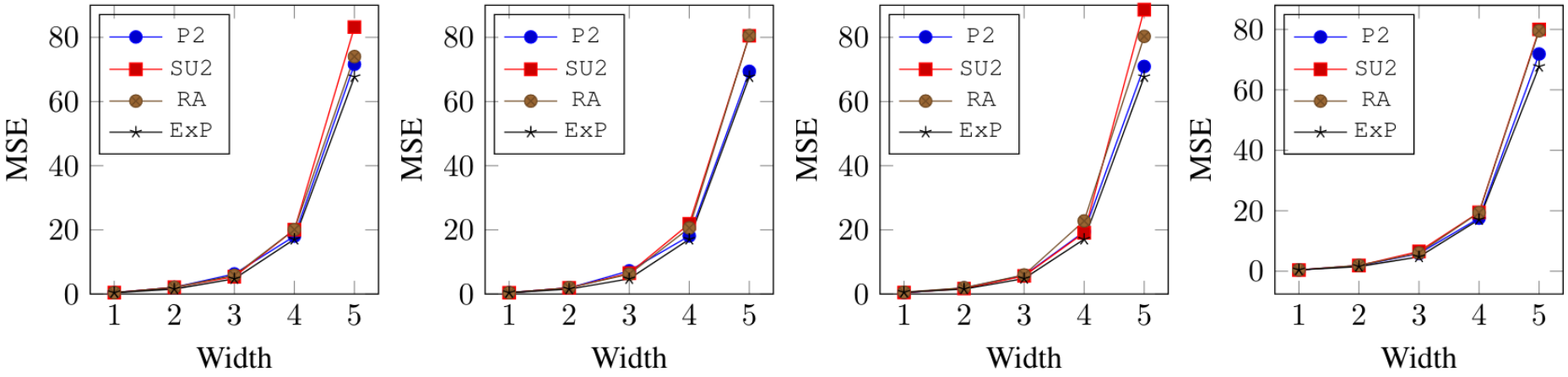
- Optimizers affect convergence rate and error

- We select three optimizers for our evaluation
  - COBYLA
  - SPSA
  - GRADIENT DESCENT

Experimental testbed



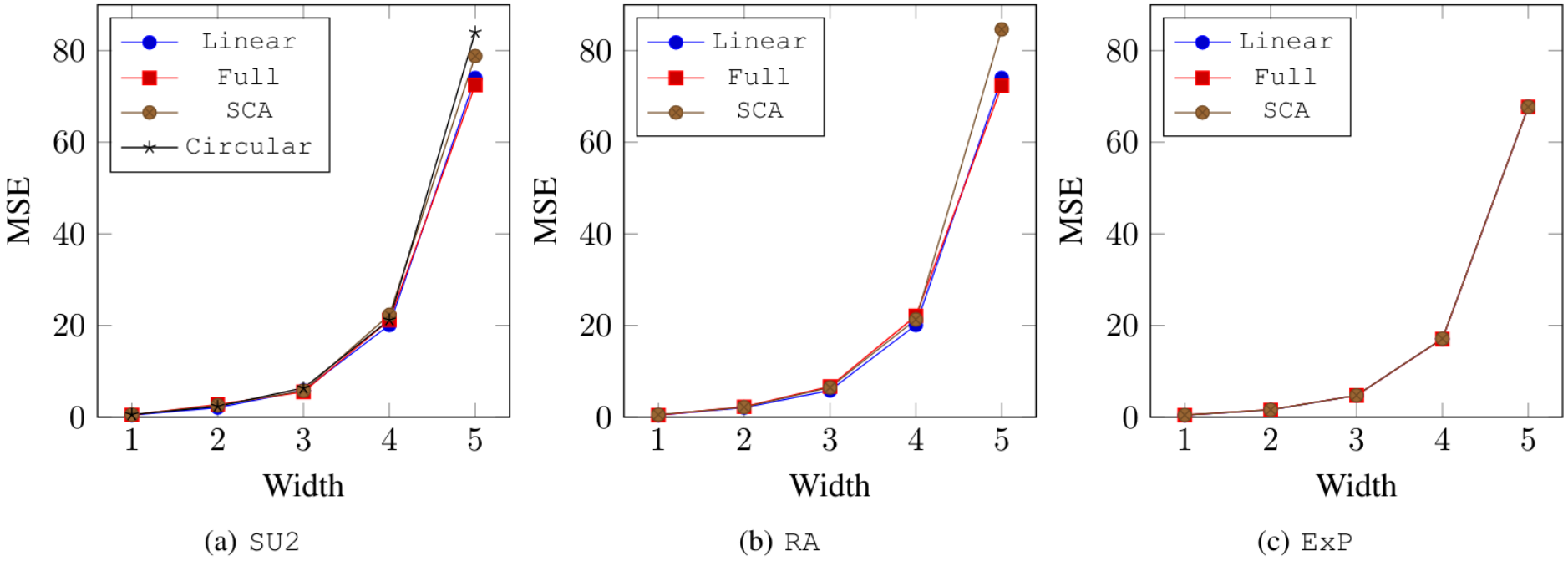
PQC vs Hardware



(a) ibm_jakarta (b) ibm_lagos (c) ibmq_manila (d) ibmq_santiago

- Width: amount of qubits required to represent input matrix ($n \cdot n = \log n$)
- Error due to decoherence and quantum noise

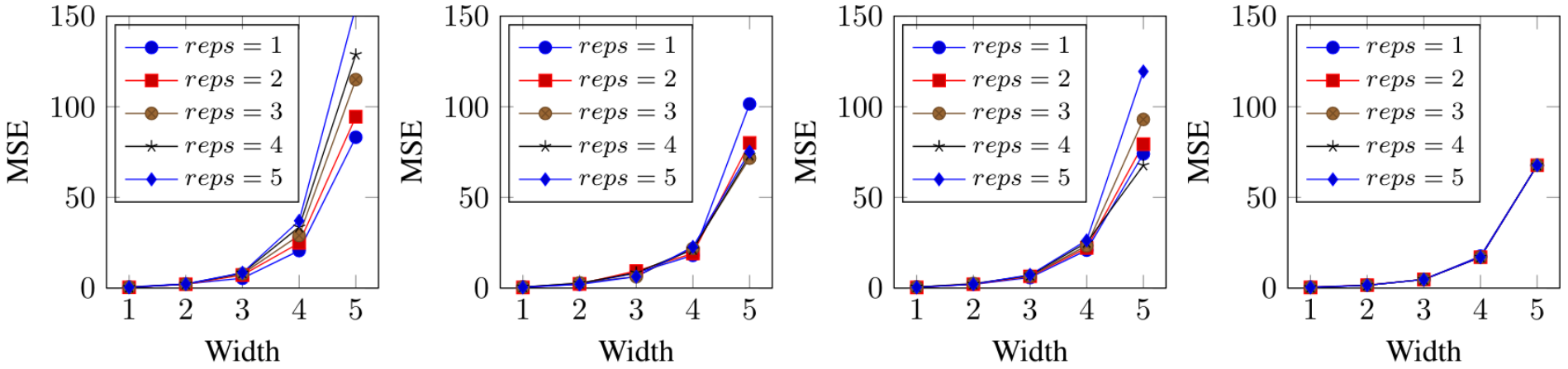
PQC vs entanglement



(a) SU2 (b) RA (c) ExP

- Entanglement:
  - LINEAR: $q_0 \rightarrow q_1 \rightarrow \ldots \rightarrow q_n$
  - FULL: $q_0 \rightarrow \{q_1, q_2, \ldots, q_n\}, q_1 \rightarrow \{q_0, q_2, \ldots, q_n\}, \ldots, q_n \rightarrow \{q_0, q_1, \ldots, q_{n-1}\}$
  - SCA: $q_0 \rightarrow \{q_2, q_4 \ldots, q_n\}$
  - CIRCULAR: $q_0 \rightarrow q_1 \rightarrow \ldots \rightarrow q_n \rightarrow q_0$

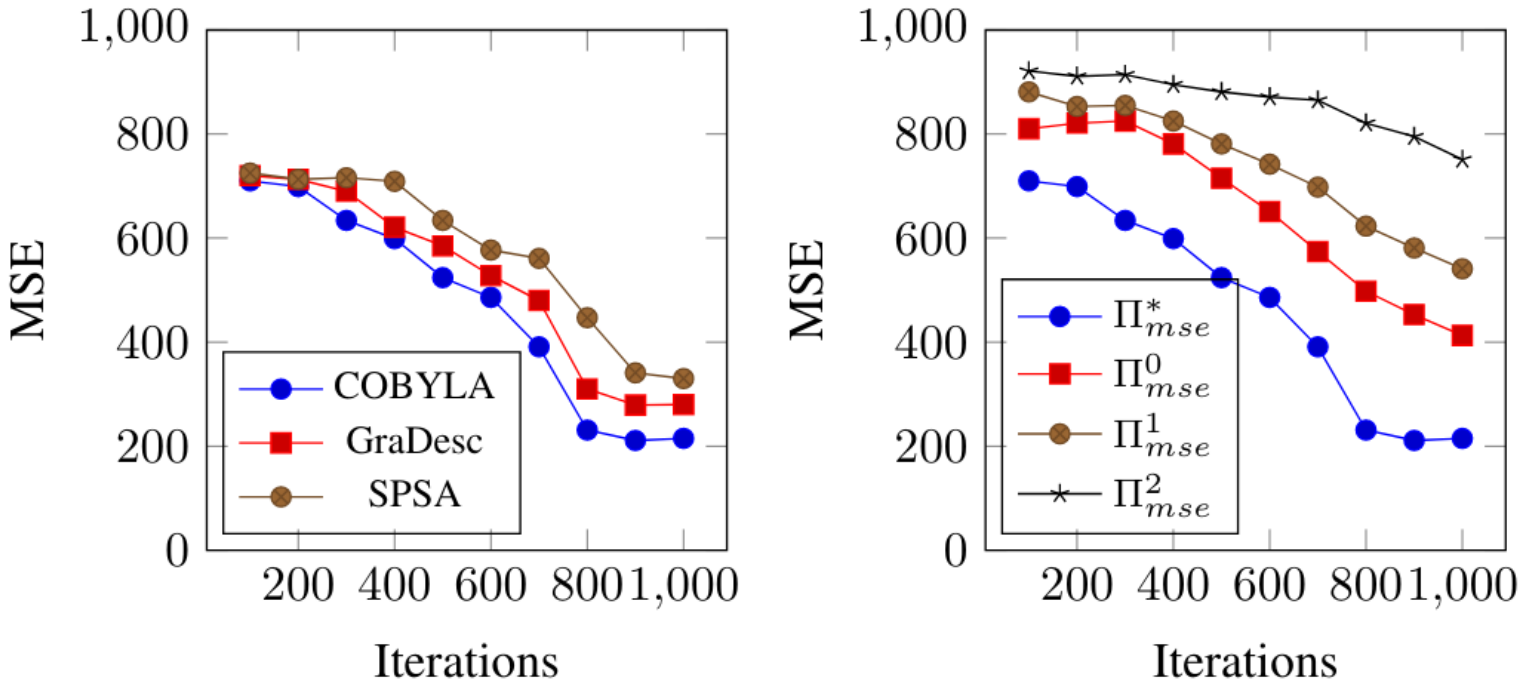
PQC vs repetitions



(a) SU2 (b) P2 (c) RA (d) ExP

- Error due to decoherence and quantum noise increases with respect to repetitions
- Error correction?

Results



- VQE calculation using different hyperparameters
- Benchmarking data collected on different machines
- Hyperparameters' optimization is used to identify best hyperparameters set for a target metric m, Π^*_m

Conclusion

- We provided a first step in the design of scientific applications for hybrid classic/quantum systems
  - Identified quantum-suitable parts
  - Provided an example implementation

- Future work
  - Consider different use cases
  - Investigating impact of different quantum hardware
    - (semiconductors, ion-traps, d-wave…)
  - Error correction methods

Der Wissenschaftsfonds.

RUCON

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Faculty of Informatics

Questions?

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IBM

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MARIE CURIE ACTIONS

WWTF

cost EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

European Commission