QEst Hackaton: Hybrid use-case compilation

Alvaro Caride
Customers solution engineer

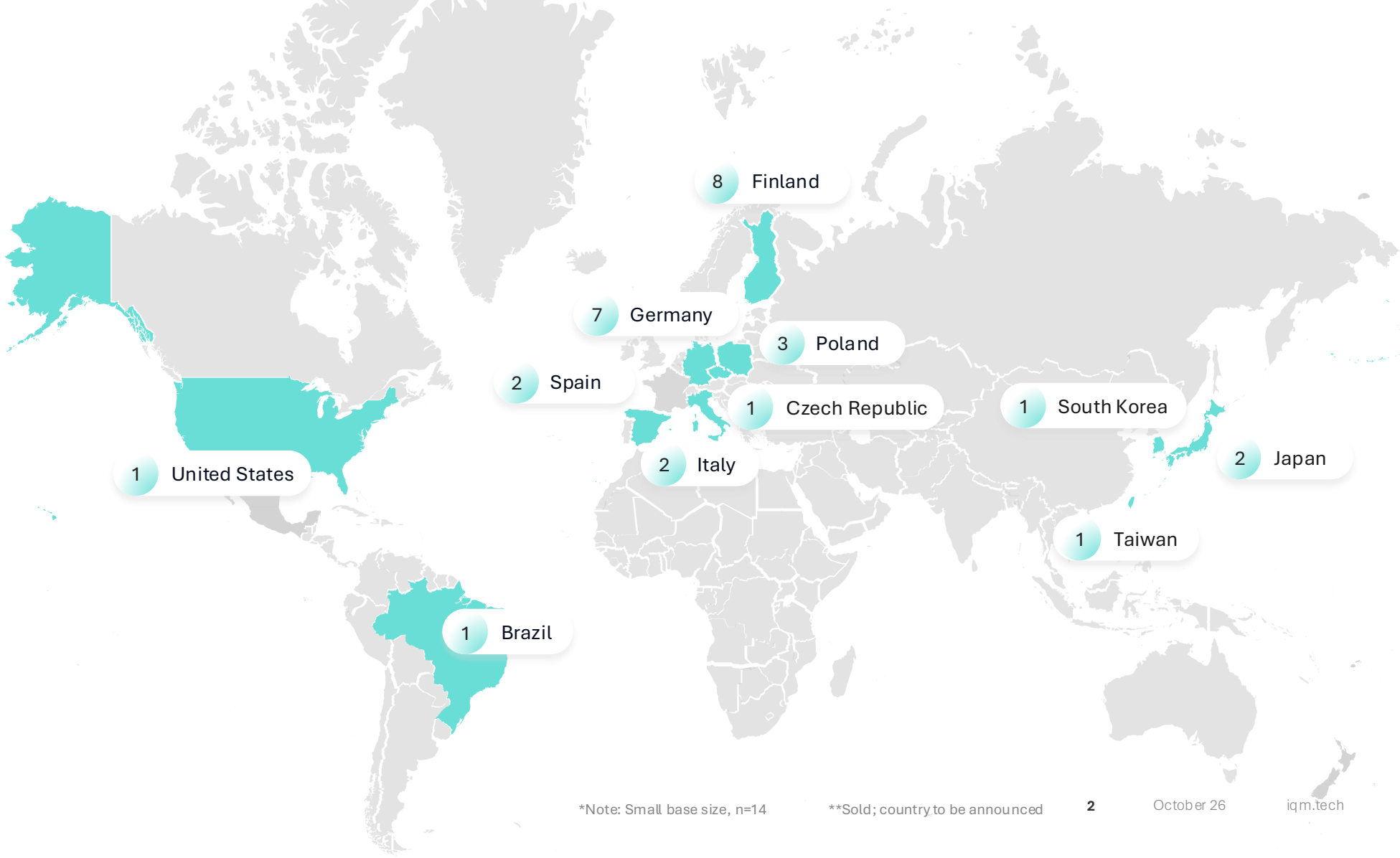
29 systems sold. 11 countries. 17 Delivered.

30+
Full systems built

29
Full systems sold

17,000+
Cloud users

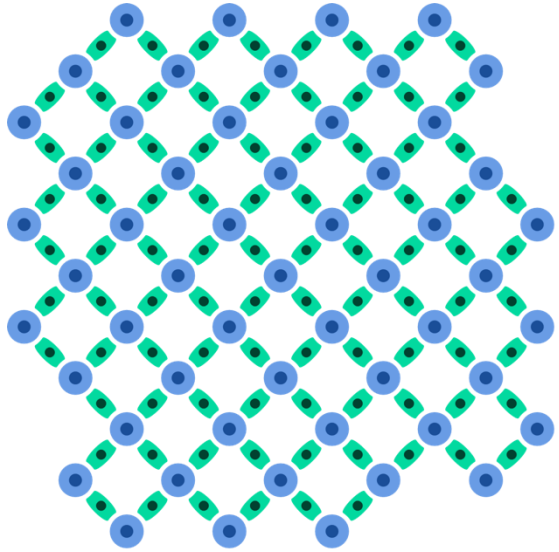
10
HPC integrations



*Note: Small base size, n=14

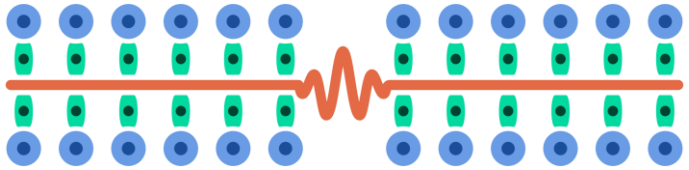
**Sold; country to be announced

IQM Develops Two QPU Topologies



Crystal

- Qubits and tunable couplers
- **Fast parallel gates**
- Nearest-neighbor connectivity
- Suitable for surface code



Star (cloud only)

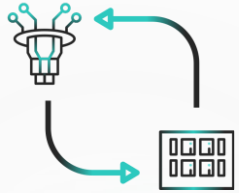
- Qubits, tunable couplers, and computational resonator (central element)
- **All-to-all connectivity**
- Disallowed parallel gates
- Promising for qLDPC codes

Why combine quantum and supercomputing?

Quantum

Strong at **high complexity**, **low data** problems (i.e. traveling salesperson)

Unique superpowers of **superposition** and **entanglement**



QC + HPC

New capabilities for **optimization**, **chemistry**
+
materials simulation
+
quantum machine learning (QML)

Supercomputing

Strong at **parallelized problems**, **big data**

General purpose computing

Product Portfolio Optimization

Partner: **DATEV**

Problem

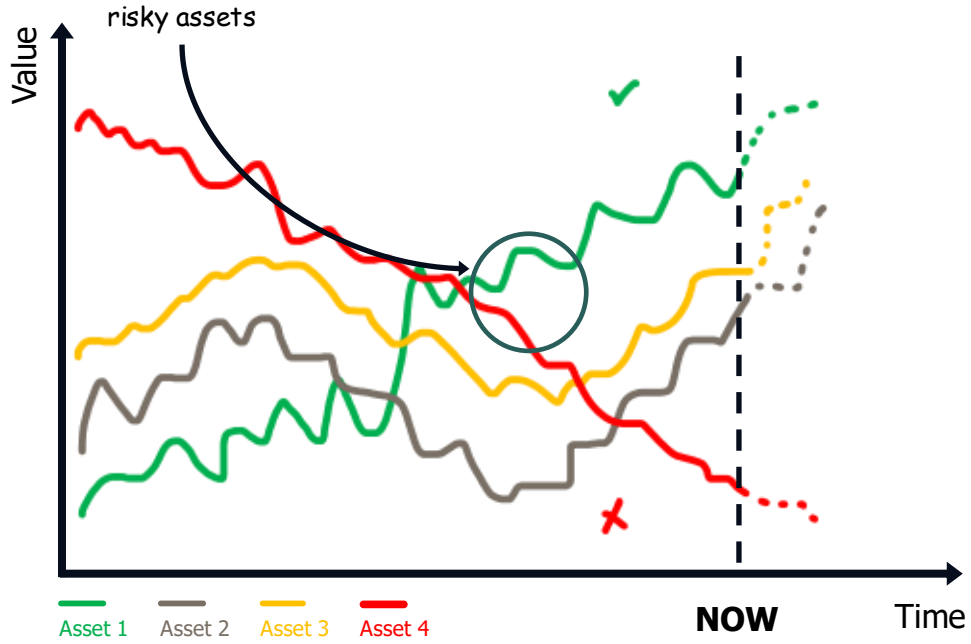
From a set of assets (such as stocks, bonds, or commodities) with a known historical value record, select a portfolio within a given budget to maximize returns while minimizing risks in the near term

Solution

Define the problem as Quadratic Unconstraint Binary Optimization (QUBO) amenable to be solved with QAOA. We implement an optimized QAOA algorithm tailored to our HW.

Why Quantum

QAOA can efficiently explore and optimize large solution spaces by leveraging quantum superposition, entanglement, and interference. Unlike classical algorithms, which evaluate solutions sequentially, QAOA simultaneously encodes and processes multiple candidate solutions, potentially offering faster convergence to optimal or near-optimal results for complex problems like combinatorial optimization.



Product Portfolio Optimization

Partner: **DATEV**

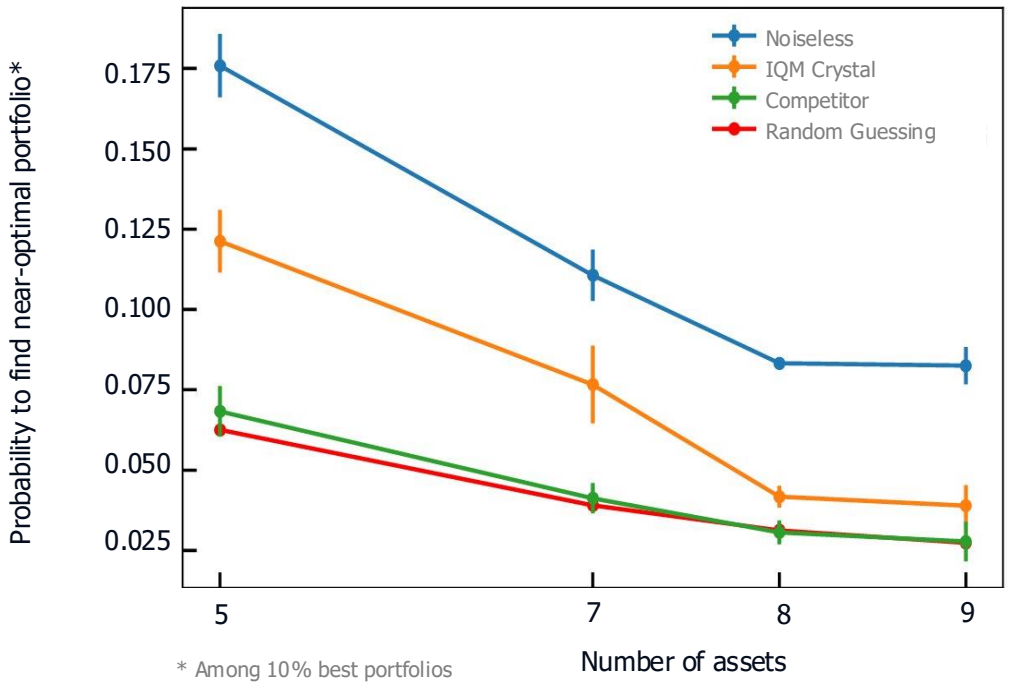
Executed on IQM Radiance Crystal 20

Probability to find near-optimal portfolio, solved with our optimized QAOA and routing

- → Different number of assets (5,7,8,9) are considered. For each case, the budget is set to half the number of assets
- → Data set provided by DATEV
- → NP-hard problem

First results show

- → When run in IQM machines, our optimized QAOA solution is closer to the noiseless simulation than standard Qiskit QAOA run on competitor systems.
- → Standard Qiskit QAOA on competitor systems offers a solution very close to uniformly random guessing



Clearly better results on IQM quantum due to

- → grid topology of the IQM quantum processing unit (QPU)
- → devising a specialized circuit for realizing the algorithm on IQM QPU

Power Plant Scheduling

The goal is to schedule the maintenance of a set of power plants for several years in the future.

01 The maintenance of every power plant has to be done regularly (e.g., once every 60 weeks)

02 The maintenance takes time (e.g., a week) during which the power plant is shut down

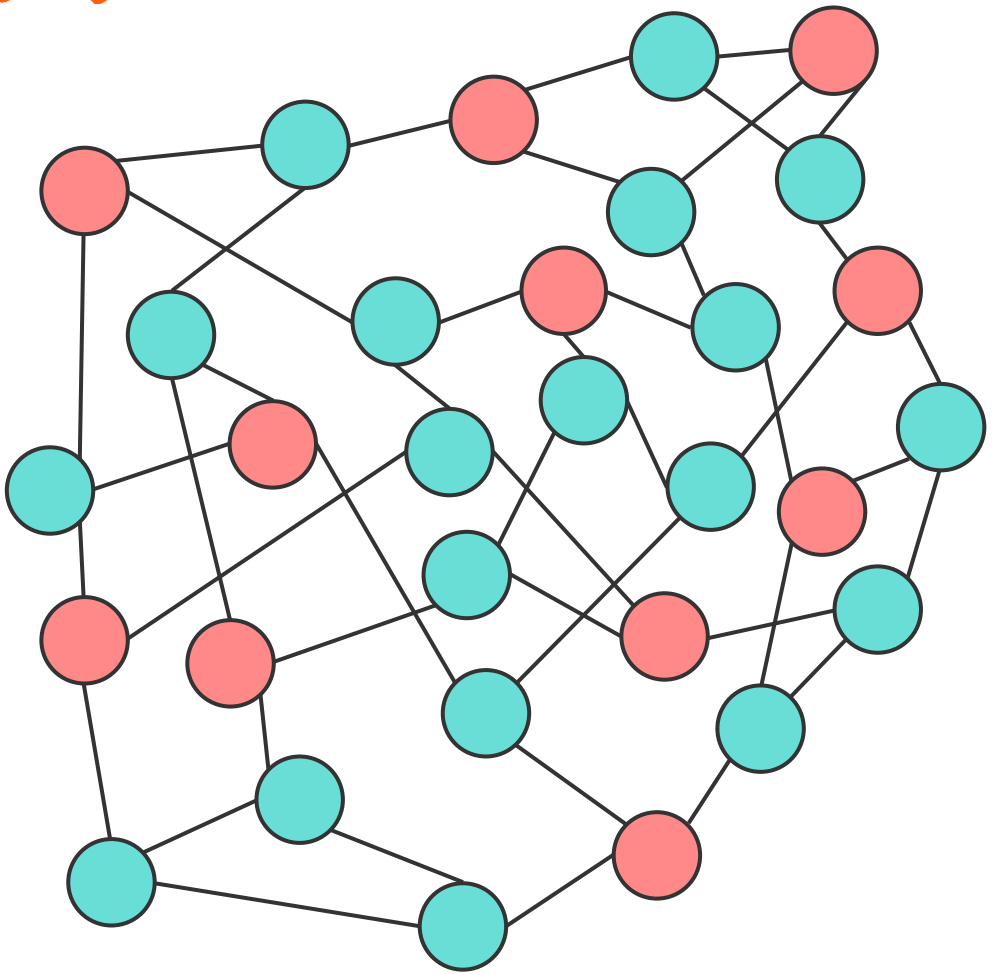
03 The maintenance can’t be performed at two power plants at the same time

04 Doing maintenance during low-demand season is preferred



QAOA Approach

1. Represent the problem as graph (nodes = individual schedules, edges = incompatibility)
2. Use QAOA to find maximum independent set (MIS)
3. MIS = valid schedule



Power Plant Maintenance Scheduling

Partner: **Électricité de France SA (EDF)**

Executed on IQM Radiance Crystal 20

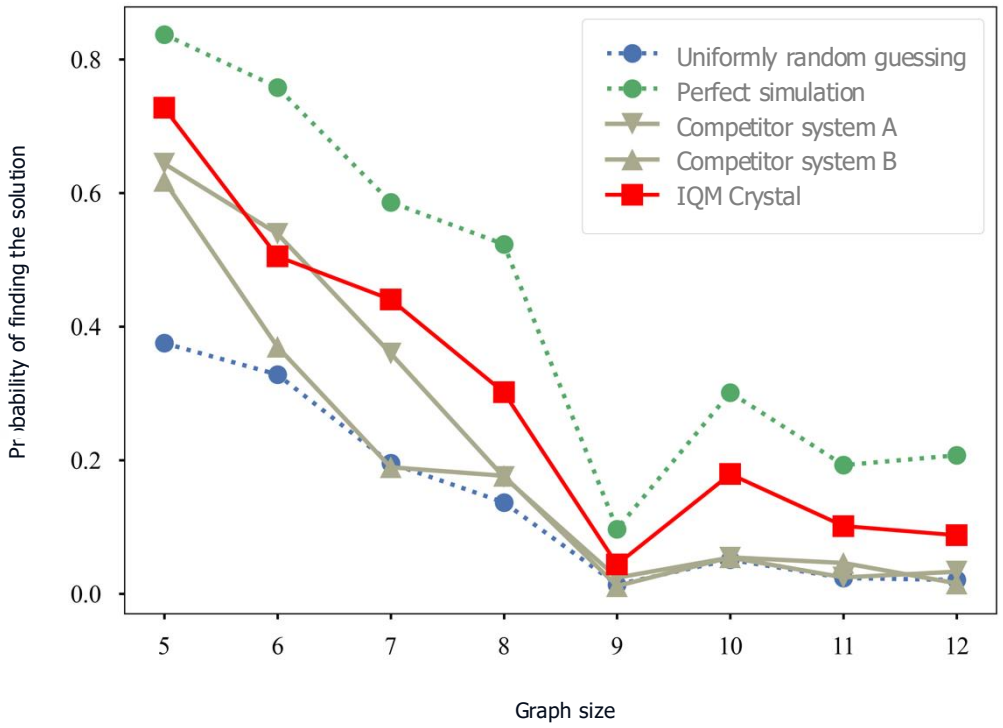
Maximum independent set (MIS) of graph, solved with QAOA

- → MIS = largest subset of vertices without any edges between
- → Data provided by EDF
- → NP-hard problem

First results show

- → When run in IQM machines, our QAOA solution is closer to the noiseless simulation than standard Qiskit QAOA run on competitor systems.
- → Standard Qiskit QAOA on competitor systems offers a solution very close to uniformly random guessing

X-axis: Graph size = number of schedules in the problem
Y-axis = probability of obtaining a correct solution after running the quantum circuit



Clearly better results on IQM quantum due to

- → grid topology of the IQM quantum processing unit (QPU)
- → devising a specialized circuit for realizing the algorithm on IQM QPU

Rolling Stock Rotation Planning

We are given a timetable. We need to plan the train routes to service all trips in the timetable.

01 All trips in the timetable have to be serviced.

02 A train needs to undergo regular maintenance.

03 The trains have to travel in cycles, so that the solution can be periodically extended.

04 The total distance travelled without passengers should be minimized.



Data



The timetable contains 190 trips



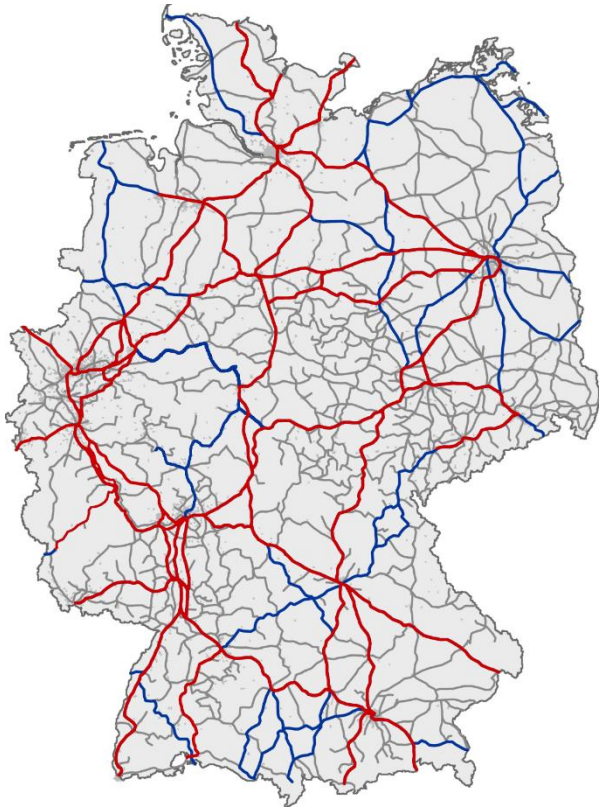
The trips cover 5 cities

Munich, Berlin, Hamburg, Frankfurt, Cologne



Maintenance location and frequency

Hamburg, every 4000 km



Hybrid QAOA-Based Algorithm

- ⇢ Enumerate all possible cycles that a train can take
- ⇢ Formulate the problem as a maximum-weight independent set (MWIS)
  - Nodes = train cycles
  - Edges = incompatible cycles
- ⇢ QUBO cost function

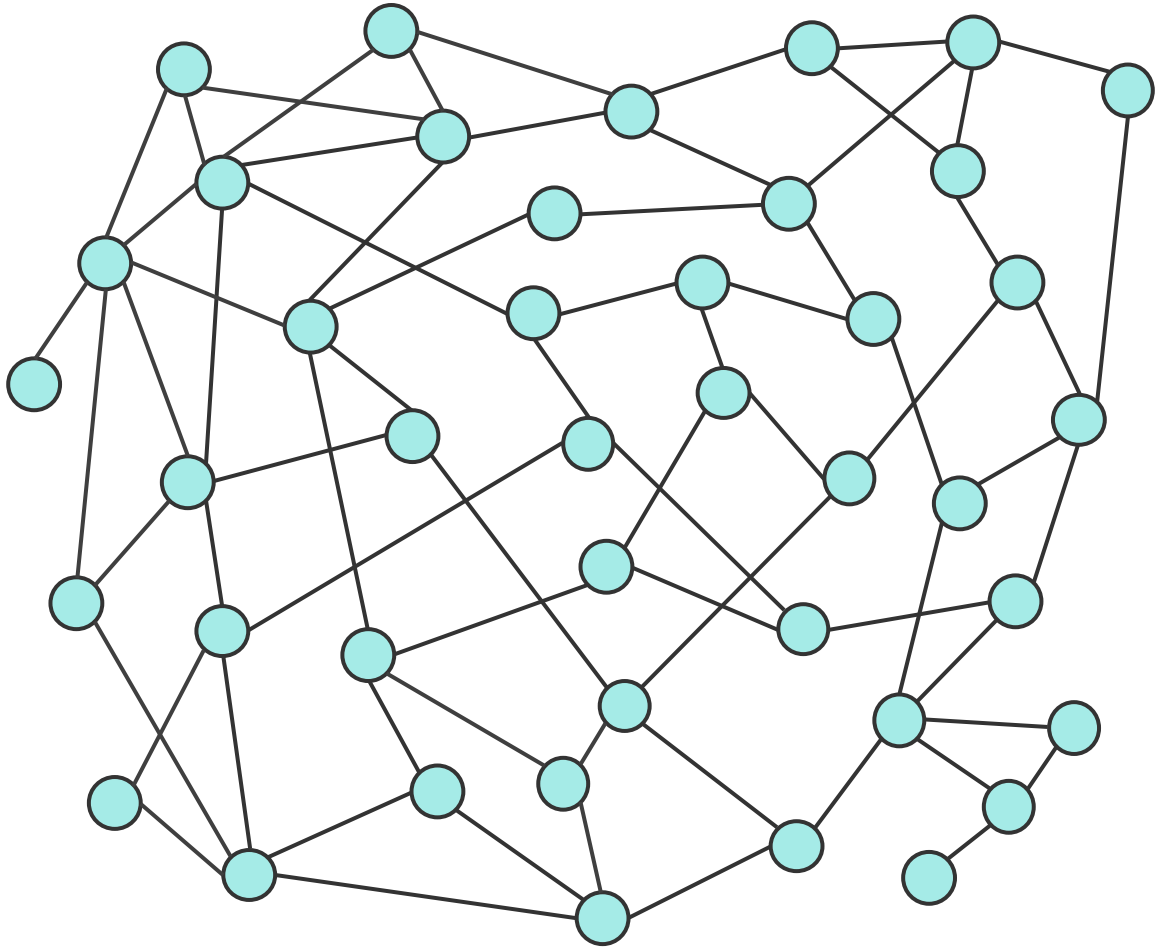
Weights of individual train cycles

$$C = -\sum_{i \in V} w_i x_i + \lambda \sum_{(i,j) \in E} x_i x_j$$

Penalty for selecting two incompatible cycles

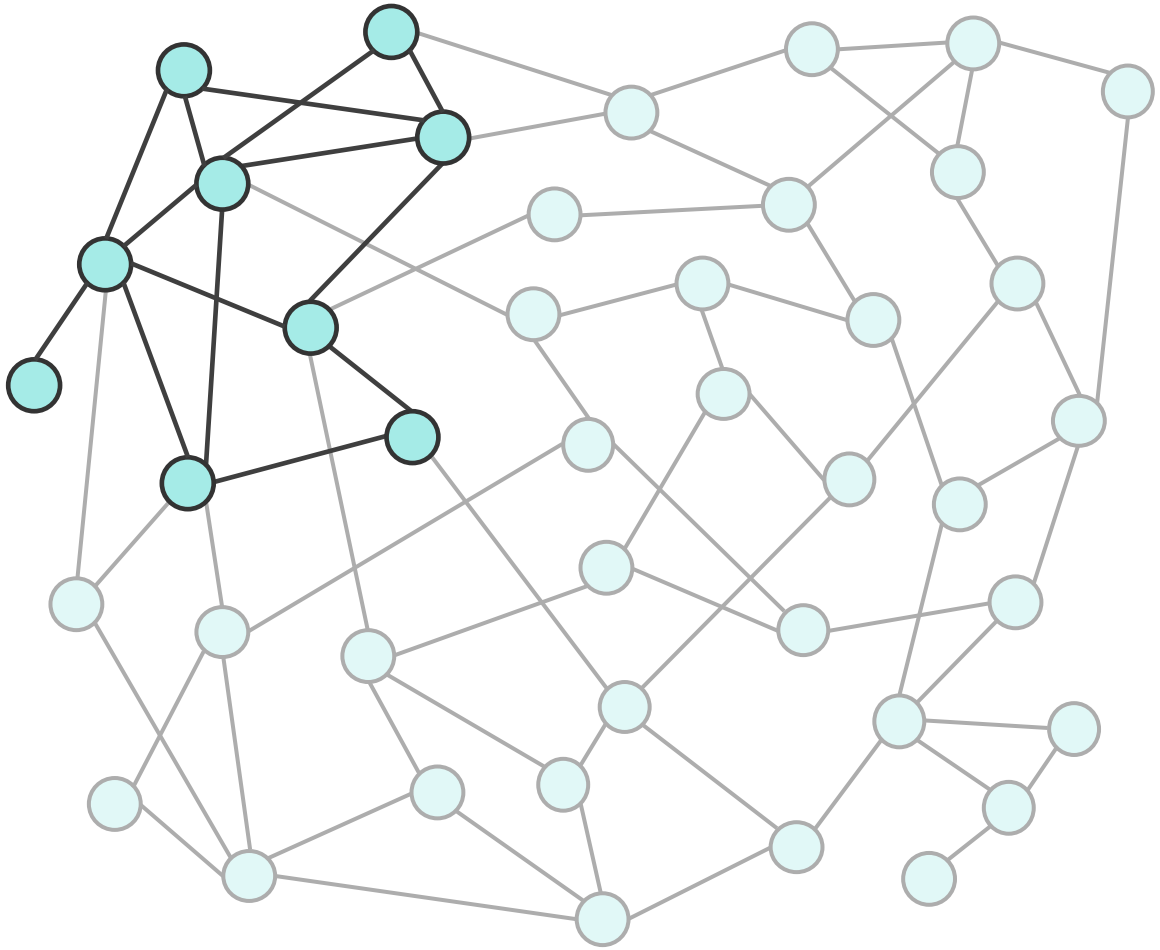
Hybrid QAOA-Based Algorithm

- ⇢ The resulting graph is too large for near-term quantum devices
- ⇢ We solve problem iteratively through a divide-and-conquer technique
  - Classical algorithm selects a subgraph
  - Quantum computer finds a solution on the subgraph using QAOA
  - The selected nodes and their neighbors are removed from the graph



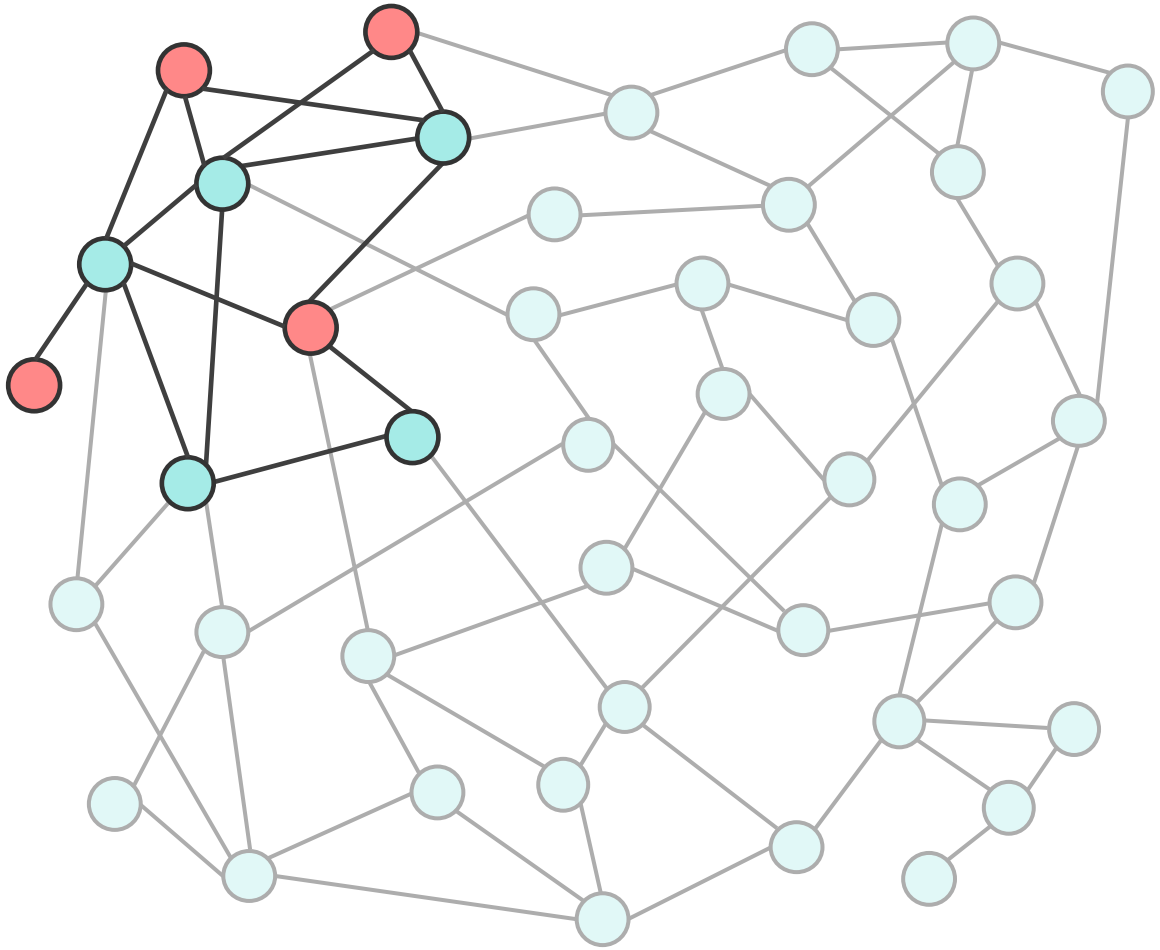
Hybrid QAOA-Based Algorithm

- ⇢ The resulting graph is too large for near-term quantum devices
- ⇢ We solve problem iteratively through a divide-and-conquer technique
  - **Classical algorithm selects a subgraph**
  - Quantum computer finds a solution on the subgraph using QAOA
  - The selected nodes and their neighbors are removed from the graph



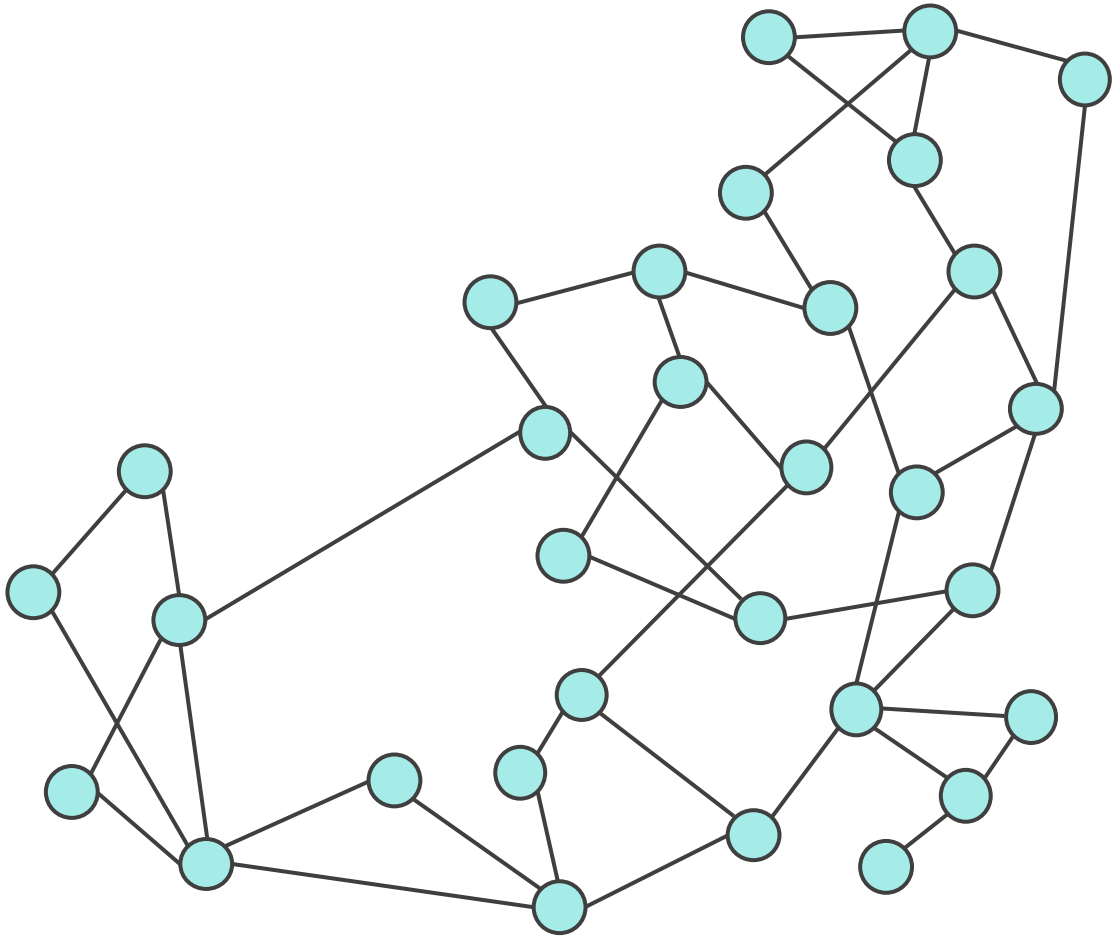
Hybrid QAOA-Based Algorithm

- ⇢ The resulting graph is too large for near-term quantum devices
- ⇢ We solve problem iteratively through a divide-and-conquer technique
  - Classical algorithm selects a subgraph
  - **Quantum computer finds a solution on the subgraph using QAOA**
  - The selected nodes and their neighbors are removed from the graph



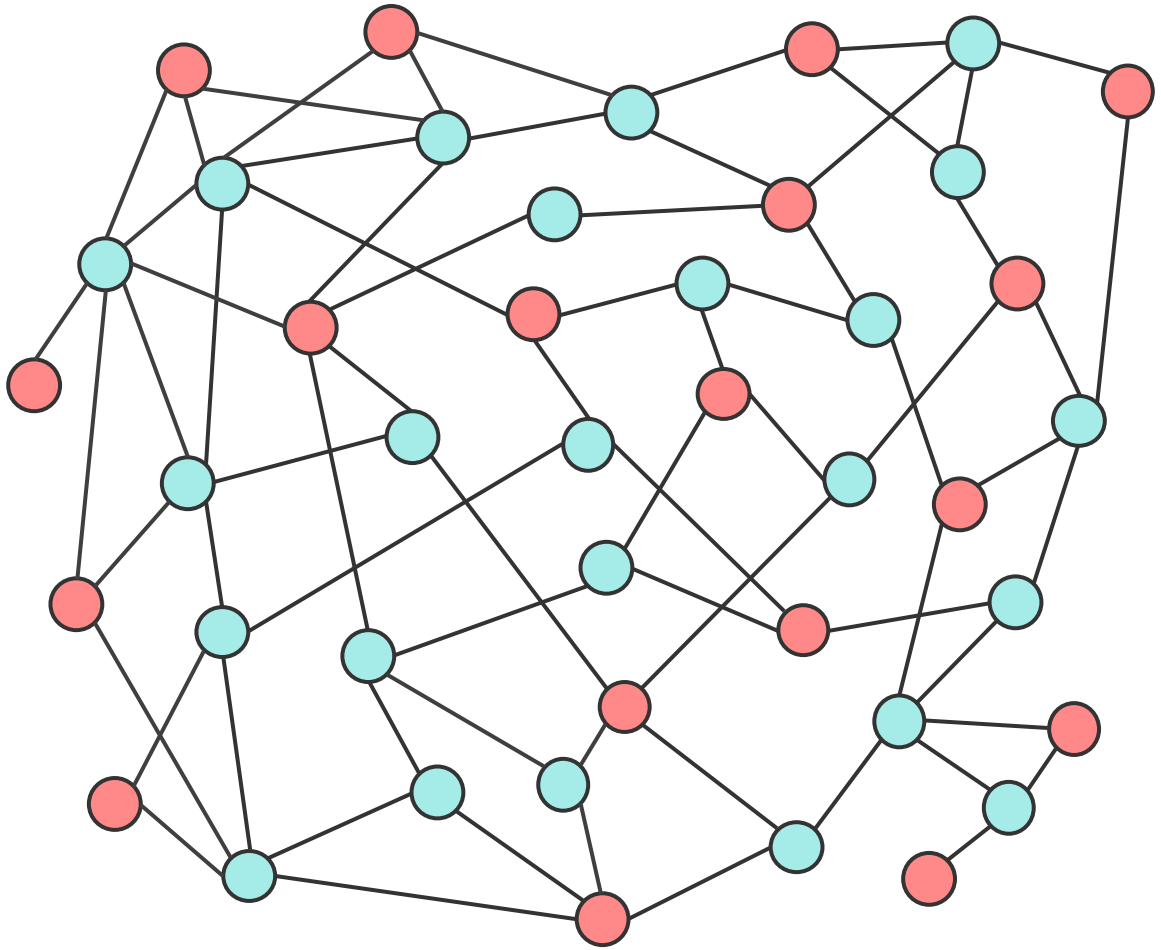
Hybrid QAOA-Based Algorithm

- ⇢ The resulting graph is too large for near-term quantum devices
- ⇢ We solve problem iteratively through a divide-and-conquer technique
  - Classical algorithm selects a subgraph
  - Quantum computer finds a solution on the subgraph using QAOA
  - **The selected nodes and their neighbors are removed from the graph**



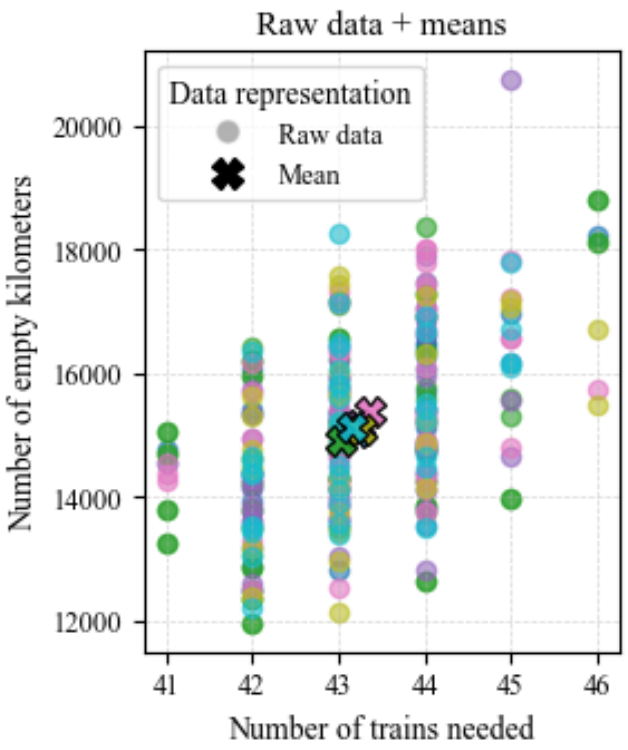
Hybrid QAOA-Based Algorithm

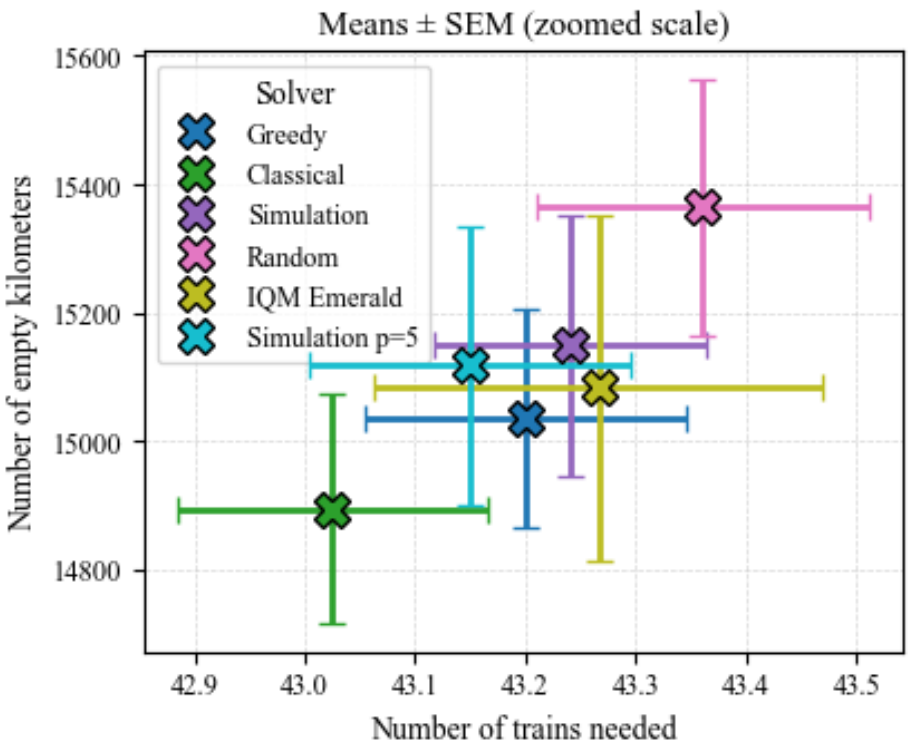
- ⇢ The resulting graph is too large for near-term quantum devices
- ⇢ We solve problem iteratively through a divide-and-conquer technique
  - Classical algorithm selects a subgraph
  - Quantum computer finds a solution on the subgraph using QAOA
  - The selected nodes and their neighbors are removed from the graph
- ⇢ The algorithm is iterated until the entire graph is solved
- ⇢ The partial solutions are combined to form the global solution



Results

- ⇢ The result quality has large variance
- ⇢ Improving subgraph solver (e.g., more QAOA layers) improves the overall solution
- ⇢ Increasing subgraph size improves the overall solution





Lithium-air batteries have 5.0x theoretical energy density of Li-ion batteries

Towards simulation of next generation batteries



Battery materials are strongly-correlated

Approximations cannot capture the behavior of strongly-correlated systems, such as battery materials

Need to understand the reaction pathways



Computational cost too high for practical use

QC-AFQMC is a hybrid method that is a quantization of a promising classical method. While efficient, it is still too slow for any practical chemical system



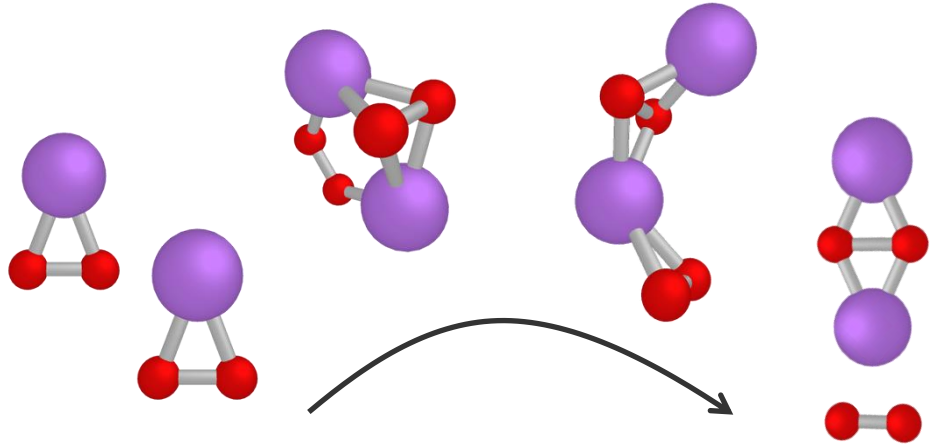
Improved SOTA runtime estimates by 248x using LUMI supercomputer

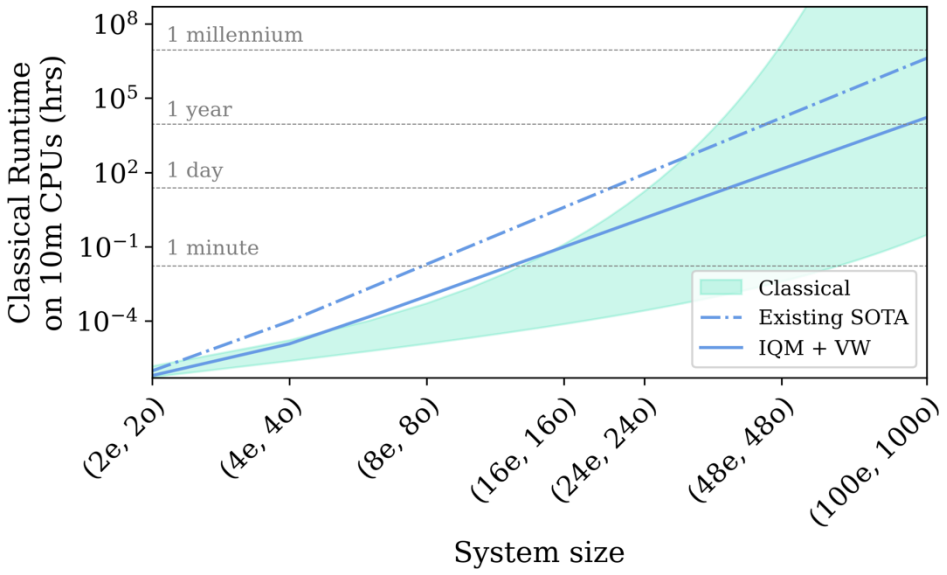
Combining algorithmic and implementation improvements, we bring the projected runtime for a 100-orbital system down to a couple years from half a millennium



Largest demonstration of this hybrid method

Contextualize the work with a reaction pathway for lithium-air batteries that fitted to 40 qubits





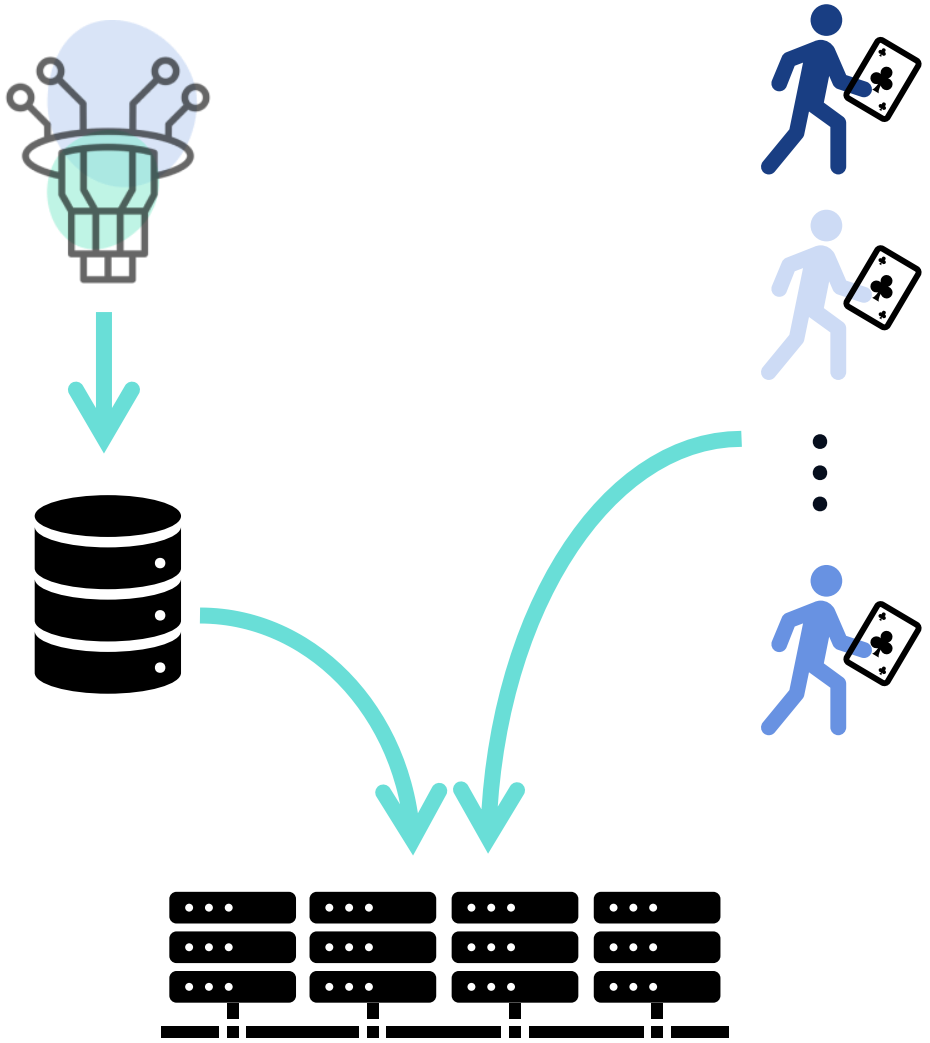
Why QC-AFQMC and HPC?

Most of the **load** of QC-AFQMC is expected to be on the **classical portion**

The workflow of QC-AFQMC lends itself to **parallelization**. The post-processing of the quantum data can be split across multiple cores for each walker at each time step

System size	Est. Quantum Runtime*	Est. Classical Runtime**
50 orbitals	5.5 days	1.1 weeks
70 orbitals	11.4 days	9.6 weeks
100 orbitals	19.8 days	1.8 years

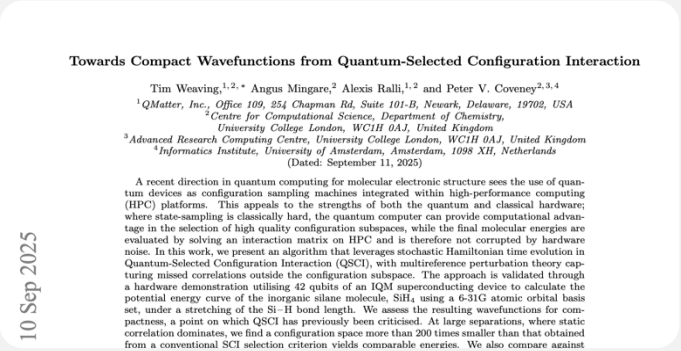
~43% → ~3% of total runtime



arXiv:2606.19239

*Using one fault-tolerant quantum device **Using ten million cores

Promising early results have been shown



Towards Compact Wavefunctions from Quantum-Selected Configuration Interaction

Tim Weaving,[1,2,*] Angus Mingare,[2] Alexis Ralli,[1,2] and Peter V. Coveney[2,3,4]

[1] QMatter, Inc., Office 109, 254 Chapman Rd, Suite 101-B, Newark, Delaware, 19702, USA
[2] Centre for Computational Science, Department of Chemistry, University College London, WC1H 0AJ, United Kingdom
[3] Advanced Research Computing Centre, University College London, WC1H 0AJ, United Kingdom
[4] Informatics Institute, University of Amsterdam, Amsterdam, 1098 XH, Netherlands

(Dated: September 11, 2025)

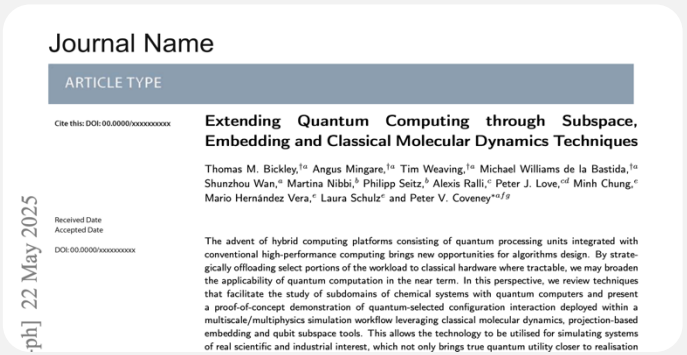
A recent direction in quantum computing for molecular electronic structure sees the use of quantum devices as configuration sampling machines integrated within high-performance computing (HPC) platforms. This appeals to the strengths of both the quantum and classical hardware; where state-sampling is classically hard, the quantum computer can provide computational advantage in the selection of high quality configuration subspaces, while the final molecular energies are evaluated by solving an interaction matrix on HPC and is therefore not corrupted by hardware noise. In this work, we present an algorithm that leverages stochastic Hamiltonian time evolution in Quantum-Selected Configuration Interaction (QSCI), with multireference perturbation theory capturing missed correlations outside the configuration subspace. The approach is validated through a hardware demonstration utilising 42 qubits of an IQM superconducting device to calculate the potential energy curve of the inorganic silane molecule, SiH_4 using a 6-31G atomic orbital basis set, under a stretching of the Si–H bond length. We assess the resulting wavefunctions for compactness, a point on which QSCI has previously been criticised. At large separations, where static correlation dominates, we find a configuration space more than 200 times smaller than that obtained from a conventional SCI selection criterion yields comparable energies. We also compare against

10 Sep 2025

Industrial Chemistry

200x increase in speed modeling of a complex molecule, Silane, using 42 QB





Journal Name

ARTICLE TYPE

Cite this: DOI: 00.0000/xxxxxxxxxx

Extending Quantum Computing through Subspace, Embedding and Classical Molecular Dynamics Techniques

Thomas M. Bickley,[†a] Angus Mingare,[†a] Tim Weaving,[†a] Michael Williams de la Bastida,[†a] Shunzhou Wan,[a] Martina Nibbi,[b] Philipp Seitz,[b] Alexis Ralli,[c] Peter J. Love,[cd] Minh Chung,[e] Mario Hernández Vera,[e] Laura Schulz[e] and Peter V. Coveney*[afg]

Received Date
Accepted Date

DOI: 00.0000/xxxxxxxxxx

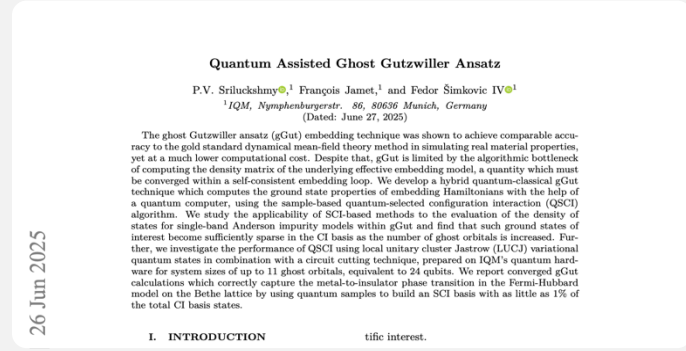
The advent of hybrid computing platforms consisting of quantum processing units integrated with conventional high-performance computing brings new opportunities for algorithms design. By strategically offloading select portions of the workload to classical hardware where tractable, we may broaden the applicability of quantum computation in the near term. In this perspective, we review techniques that facilitate the study of subdomains of chemical systems with quantum computers and present a proof-of-concept demonstration of quantum-selected configuration interaction deployed within a multiscale/multiphysics simulation workflow leveraging classical molecular dynamics, projection-based embedding and qubit subspace tools. This allows the technology to be utilised for simulating systems of real scientific and industrial interest, which not only brings true quantum utility closer to realisation

[ph] 22 May 2025

Solution Chemistry

Sophisticated modeling of proton transfer using intensive HPC and quantum resources





Quantum Assisted Ghost Gutzwiller Ansatz

P.V. Sriluckshmy,[1] François Jamet,[1] and Fedor Šimkovic IV[1]

[1] IQM, Nymphenburgerstr. 86, 80636 Munich, Germany

(Dated: June 27, 2025)

The ghost Gutzwiller ansatz (gGut) embedding technique was shown to achieve comparable accuracy to the gold standard dynamical mean-field theory method in simulating real material properties, yet at a much lower computational cost. Despite that, gGut is limited by the algorithmic bottleneck of computing the density matrix of the underlying effective embedding model, a quantity which must be converged within a self-consistent embedding loop. We develop a hybrid quantum-classical gGut technique which computes the ground state properties of embedding Hamiltonians with the help of a quantum computer, using the sample-based quantum-selected configuration interaction (QSCI) algorithm. We study the applicability of SCI-based methods to the evaluation of the density of states for single-band Anderson impurity models within gGut and find that such ground states of interest become sufficiently sparse in the CI basis as the number of ghost orbitals is increased. Further, we investigate the performance of QSCI using local unitary cluster Jastrow (LUCJ) variational quantum states in combination with a circuit cutting technique, prepared on IQM's quantum hardware for system sizes of up to 11 ghost orbitals, equivalent to 24 qubits. We report converged gGut calculations which correctly capture the metal-to-insulator phase transition in the Fermi-Hubbard model on the Bethe lattice by using quantum samples to build an SCI basis with as little as 1% of the total CI basis states.

I. INTRODUCTION

tific interest.

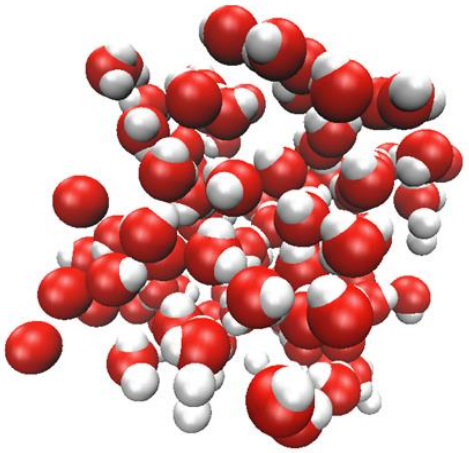
26 Jun 2025

Material Science

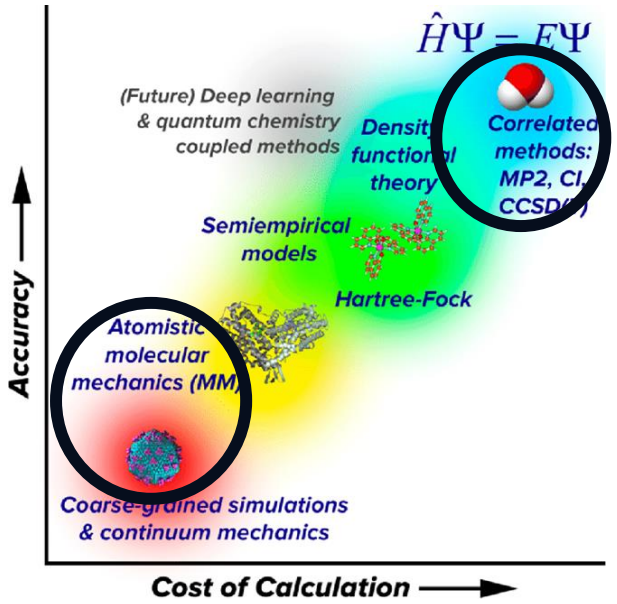
Simulating the behavior of metal-to-insulators transitions

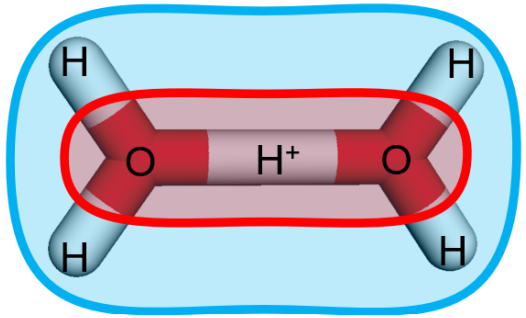


Combining the unique benefits of classical and quantum



Classical Computation using LAMMPS for coarse simulation of the background solvent





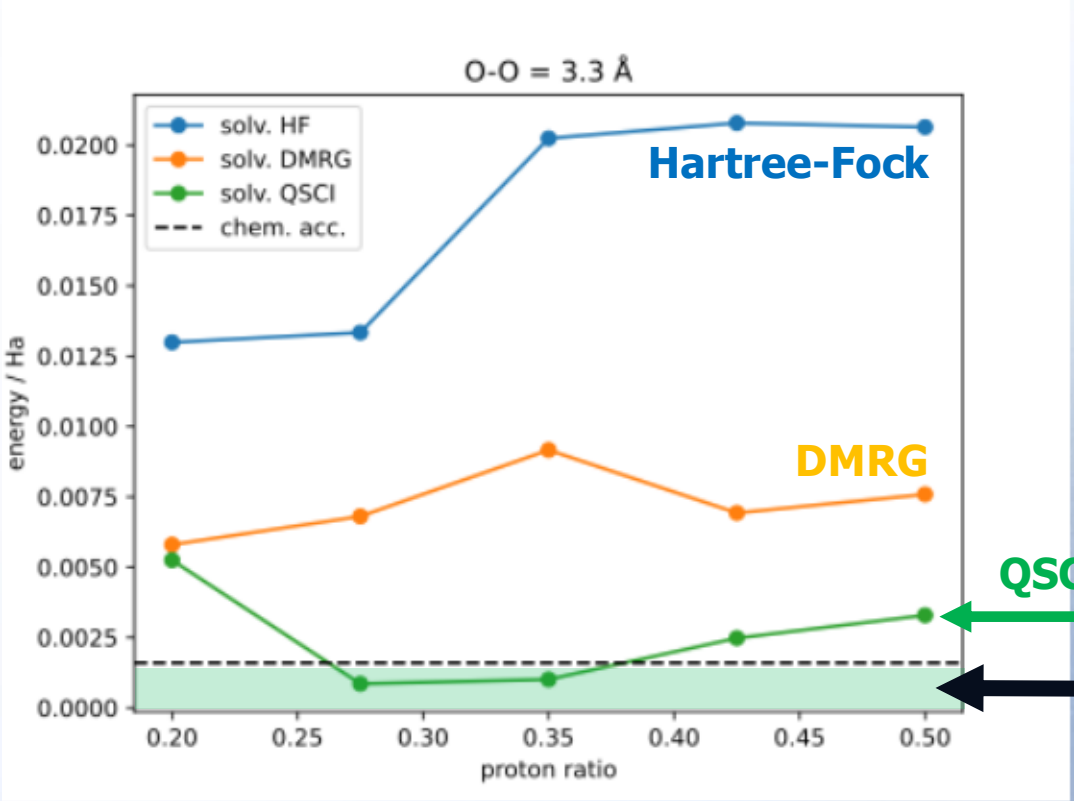
Active region:
16 qubit Hamiltonian

Environment region:
Density functional theory

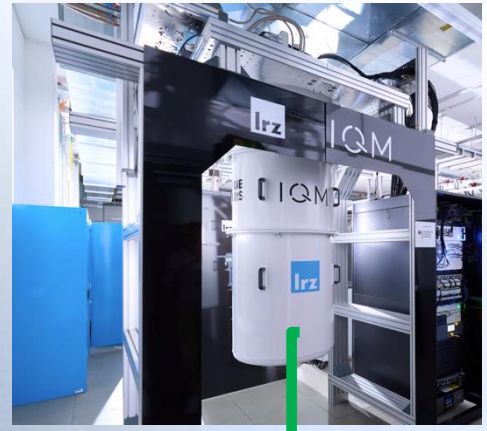
Difficult to simulate classically, quantum methods excel here with each qubit representing one valence state

T. Weaving; T. M. Bickley; A. Mingare; M. Williams de la Bastida; S. Wan; M. Nibbi; P. Seitz; A. Ralli; P. J. Love; M. Chung; M. Hernández Vera; L. Schulz; P. V. Coveney. "Extending quantum computing through subspace, embedding and classical molecular dynamics techniques", arXiv:2505.16796 (2025)

Results



IQM Q-Exa 20 device



With respect to the exact energy, the data from Q-Exa 20 device achieves **"chemical accuracy"** for some points along the proton transfer coordinate, and outperforms a DMRG solution at many step.

T. Weaving; T. M. Bickley; A. Mingare; M. Williams de la Bastida; S. Wan; M. Nibbi; P. Seitz; A. Ralli; P. J. Love; M. Chung; M. Hernández Vera; L. Schulz; P. V. Coveney. "Extending quantum computing through subspace, embedding and classical molecular dynamics techniques", arXiv:2505.16796 (2025)

Try it out for free!

- → **30 free credits per month** to use on as many jobs as you need
- → Access to IQM's **unique** quantum computer **topologies** and learning resources
- → Limited-time access to our **flagship Crystal 54** device for all Starter users

Sign up now

IQM Quantum Computers, Built for Real Impact

A major upgrade to IQM Resonance

Access to our 54-qubit Crystal system, pulse-level access, advanced error handling, upgrades to IQM Academy, a new QAOA library, and more.

Free sign up → Experience Resonance →

