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Overview of Distributed Variational Optimization Algorithms on Large-scale Quantum-HPC Ecosystems

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Quantum-HPC Group, NCCS

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U.S. DEPARTMENT OF ENERGY

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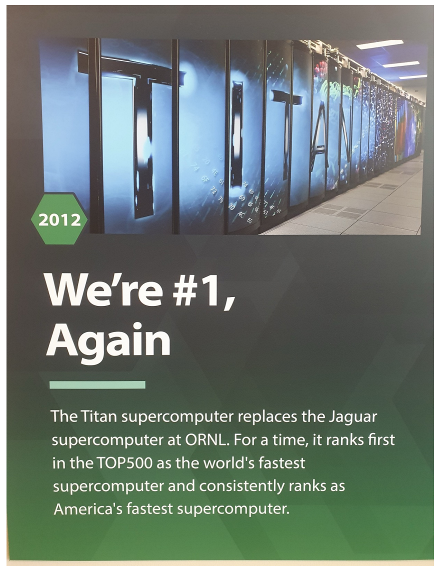
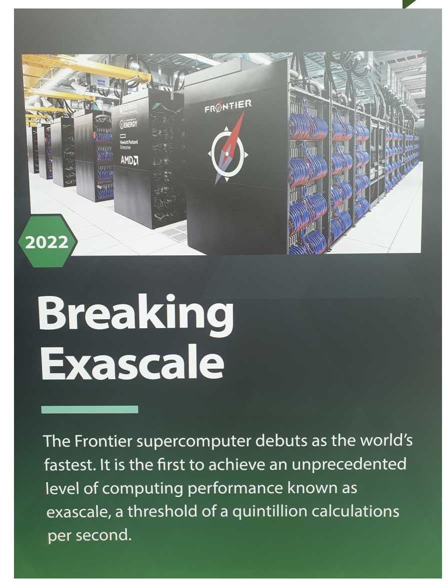
Advanced Computing





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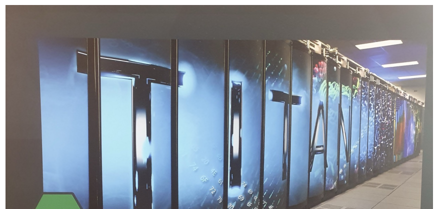
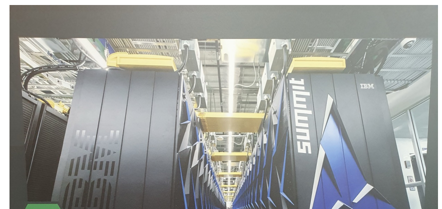
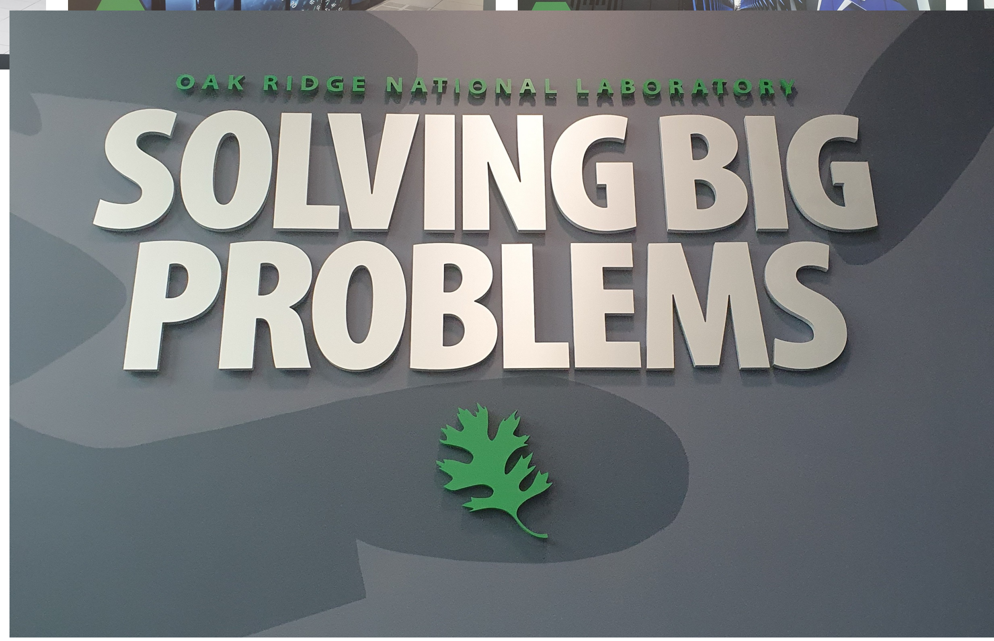
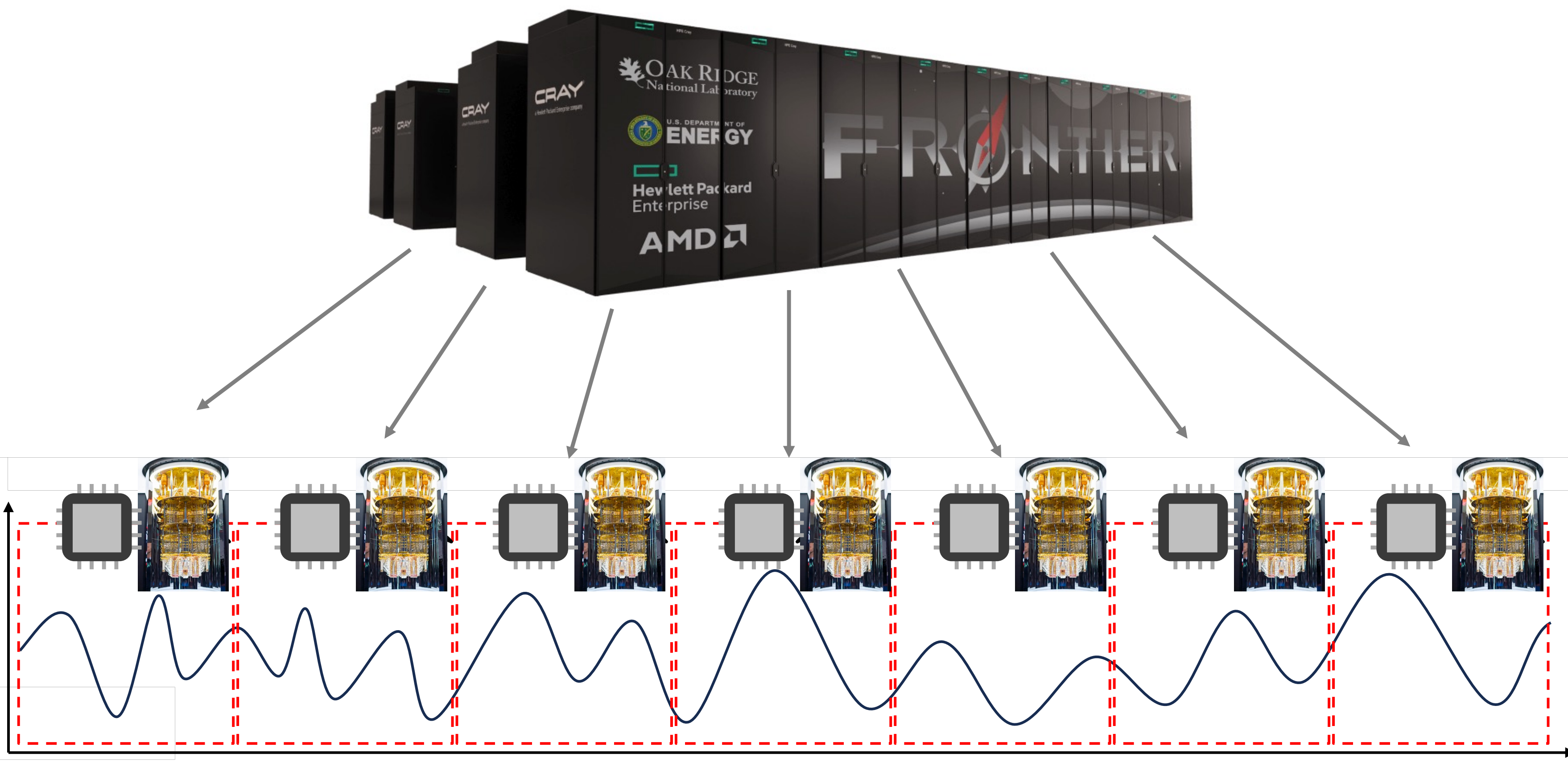
Advanced Computing for Solving Big Problems



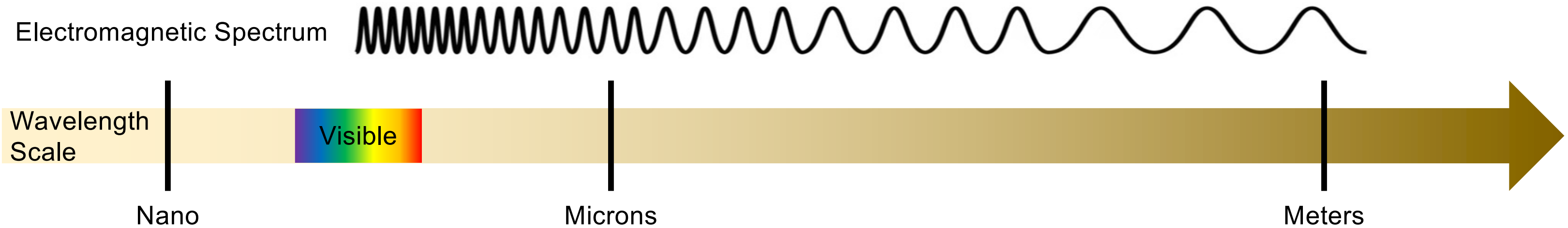


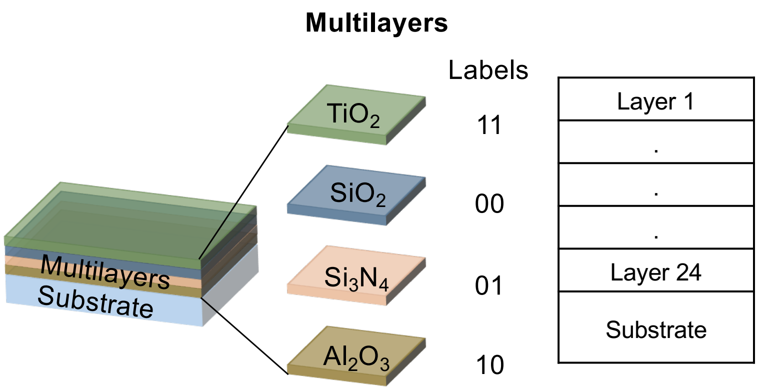


Advanced Computing for Optimization Challenges



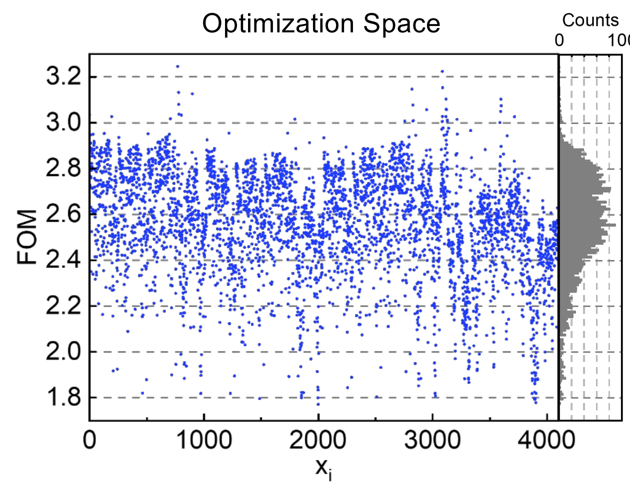
Materials Optimization Challenges





Multilayer structure (***x***): [11 00 01 10 … 10 11]

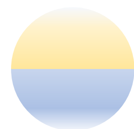
$4^{24} \approx 2.81\times10^{14}$



Quantum Computing in Material Science

0 state   1 state

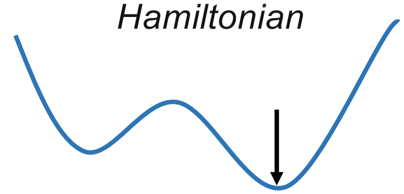
Classical computer - Bit



Superposition of 0 or 1 state

Quantum computing (QC) – Qubit

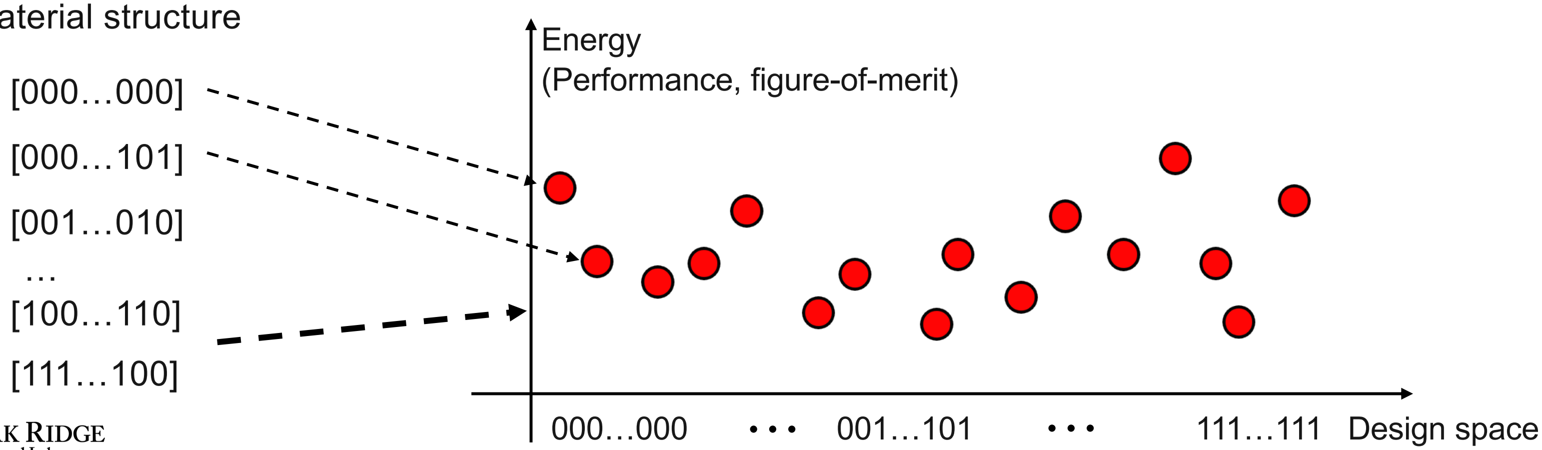
Optimization Landscape: Hamiltonian



Lowest energy state

→ Solution

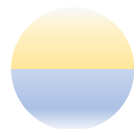
Material structure



Quantum Computing in Material Science

0 state or 1 state

Classical computer - Bit



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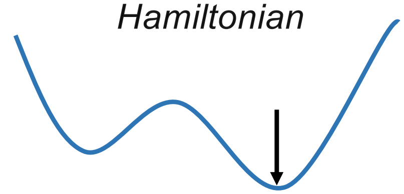
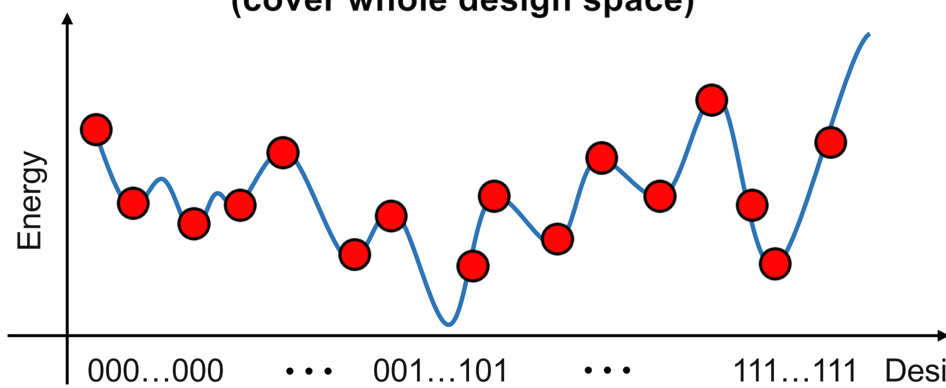


Lowest energy state

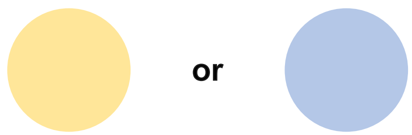
→ Solution

Datasets (sparse points)

Material structures (binary vectors) & Performance (FOMs) → ***Hamiltonian*** **(cover whole design space)**

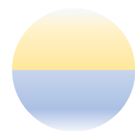


Quantum Computing in Material Science



0 state 1 state

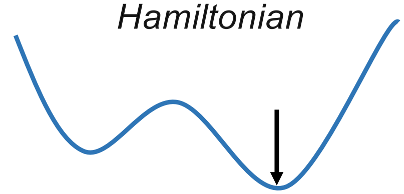
Classical computer - Bit



Superposition of 0 or 1 state

Quantum computing (QC) – Qubit

Optimization Landscape: Hamiltonian



Lowest energy state

→ Solution

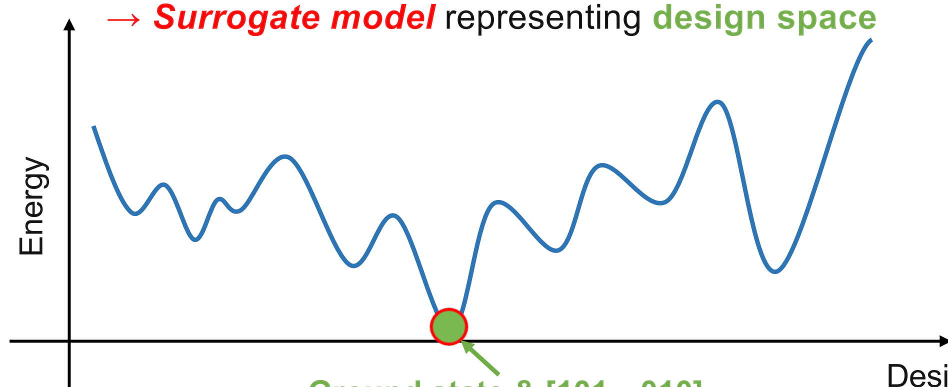
Datasets (sparse points)

Material structures (binary vectors) & Performance (FOMs) →

Hamiltonian

(cover whole design space)

→ ***Surrogate model*** representing **design space**



Machine Learning Model for Hamiltonian

Factorization machine (FM): Supervised learning model

Model equation

$$y \coloneqq w_0 + \sum_{i=1}^{n} w_i x_i + \sum_{f=1}^{n} \sum_{j=i+1}^{n} \langle \boldsymbol{v_i}, \boldsymbol{v_j} \rangle\, x_i, x_j \qquad \langle \boldsymbol{v_i}, \boldsymbol{v_j} \rangle \coloneqq \sum_{f=1}^{k} v_{i,f} \cdot v_{j,k}$$

Simple form for reducing computation

$$\boxed{y \coloneqq w_0 + \sum_{i=1}^{n} w_i x_i + \frac{1}{2} \sum_{f=1}^{k} \left[\left(\sum_{i=1}^{n} v_{i,f} x_i \right)^2 - \sum_{i=1}^{n} v_{i,f}^2 x_i^2 \right]}$$

Training with dataset {*x*, y} = {Metamaterials, FOMs}

Model parameters

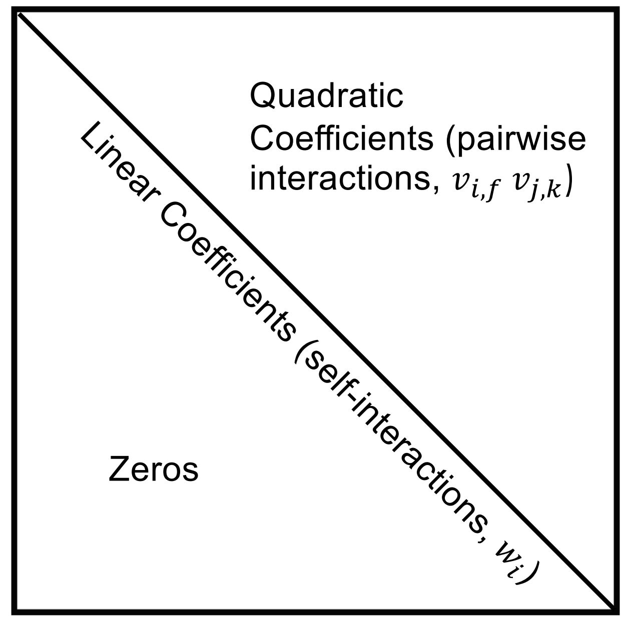
$w_0, w_i, v_{i,f}, v_{j,k}$

x_i: binary variable

w_0: global bias

w_i: models the strength of the i^{th} vaiable

$\langle \mathbf{v_i}, \mathbf{v_j} \rangle$: models the interaction between the i^{th} and j^{th} variabls



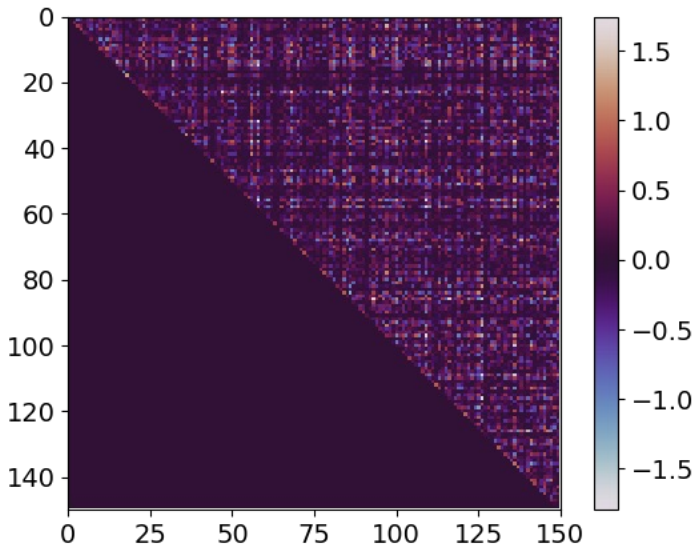
***Hamiltonian** (quadratic unconstrained binary optimization; **QUBO**)*

Surrogate model representing **design space**

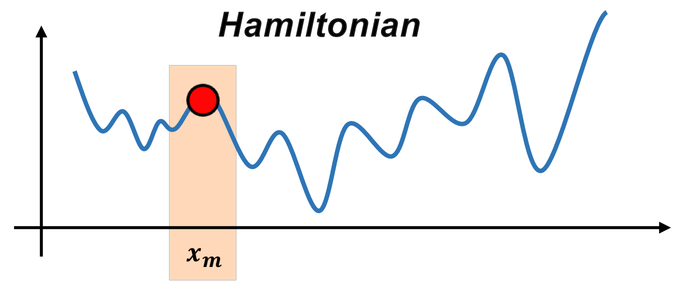
Steffen Rendle. 2010 IEEE International conference on data mining, 995 (2010)

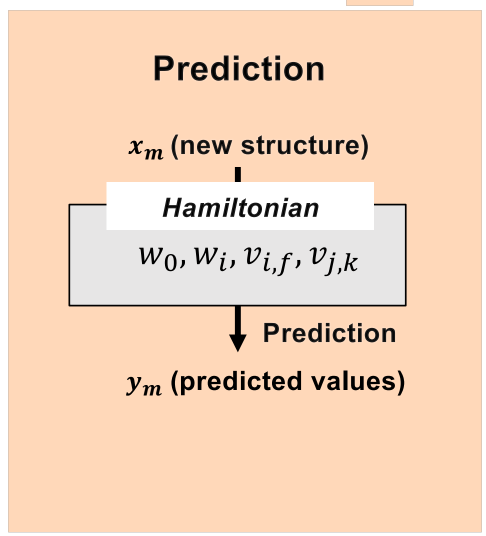
Machine Learning Surrogate Model for Hamiltonian

Factorization machine (FM): Supervised learning model



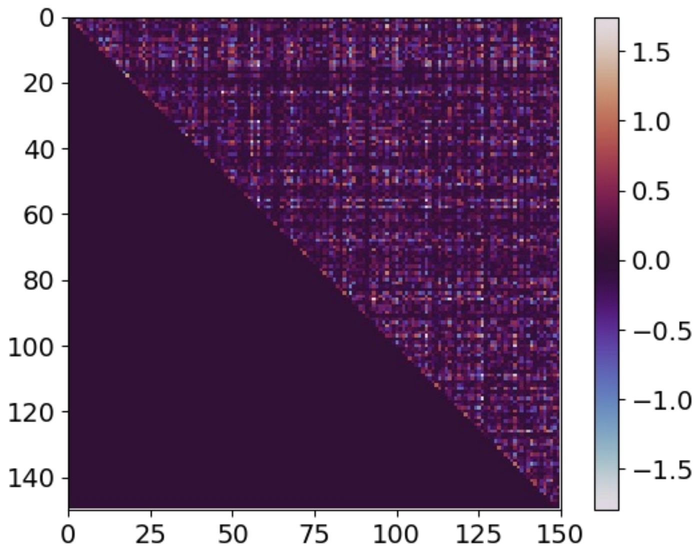
Hamiltonian *(quadratic unconstrained binary optimization;* ***QUBO****)*



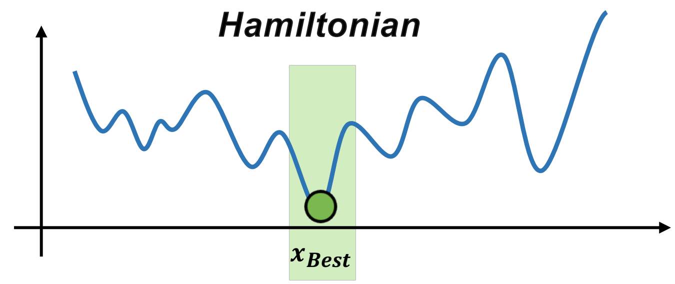


Machine Learning Surrogate Model for Hamiltonian

Factorization machine (FM): Supervised learning model



Hamiltonian *(quadratic unconstrained binary optimization;* ***QUBO****)*



Prediction

x_m **(new structure)**

Hamiltonian

$w_0, w_i, v_{i,f}, v_{j,k}$

Prediction

y_m **(predicted values)**

Inverse design

x_{Best} **(best structure)**

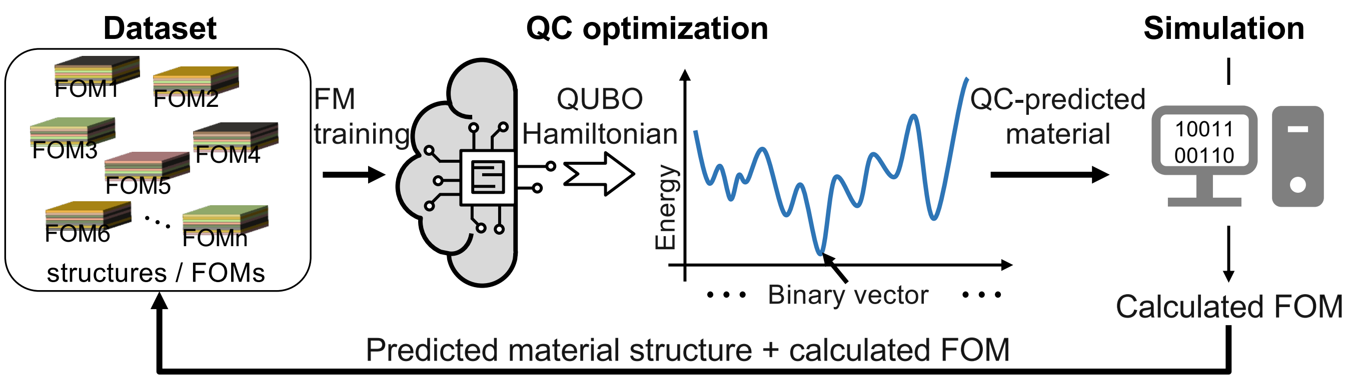
Hamiltonian

$w_0, w_i, v_{i,f}, v_{j,k}$

y_{Best} **(ground state)**

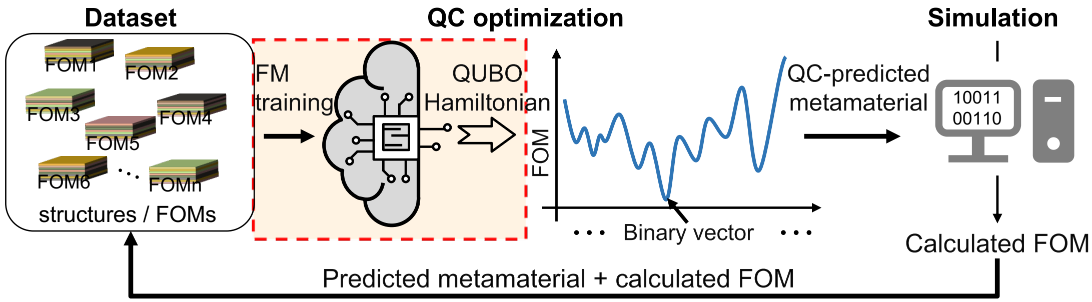
Pixels = 100 : $2^{100} \approx 1.26\times10^{30}$

Active Learning for Material Design (AI+HPC+QC integration)

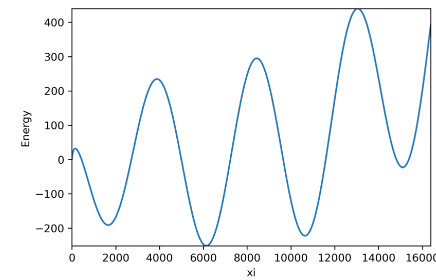


Active learning algorithm using machine Learning and quantum computing to find optimal material structures with low FOM

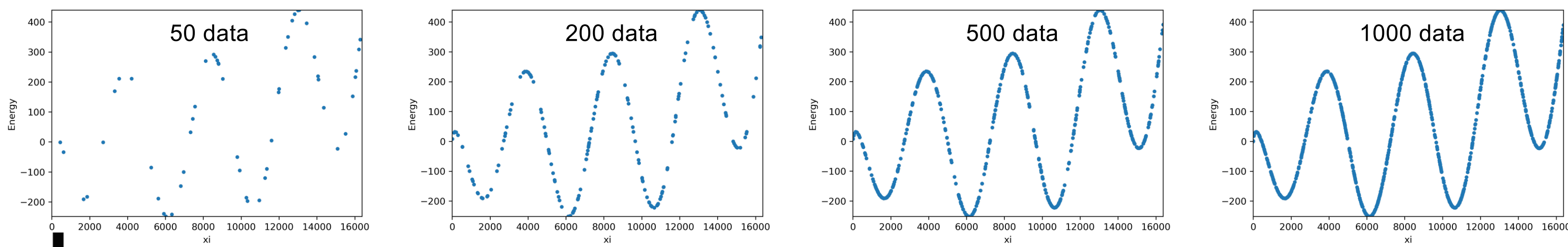
1. Initial data set is generated: {25 material structures, 25 FOMs} which are calculated by simulation
2. FM is trained with a dataset $\{x\text{:FOM}\}_n \rightarrow$ ***Hamiltonian***
3. QC predicts an optimal structure(x_{po}) with the lowest $\text{FOM}_{\text{QA:po}}$ based on the given QUBO surrogate
   - x_{po} may not be the true optimal state due to the limited extrapolative ability of the FM model trained on limited data.
4. Simulation takes the x_{po} and calculates FOM ($\text{FOM}_{\text{Simulation:po}}$)
5. The data set is updated by adding x_{po}:$\text{FOM}_{\text{simulation:po}}$ to $\{x\text{:FOM}\}_n \rightarrow \{x\text{:FOM}\}_{n+1}$
   - ✓ Iterate 1 – 5



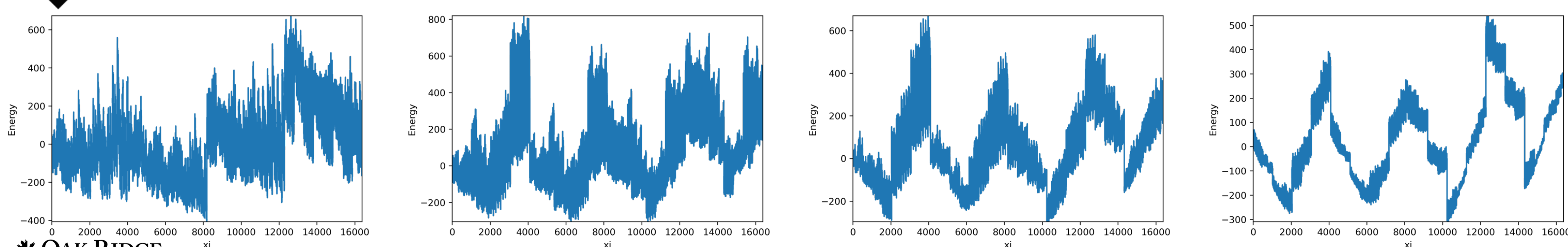
Design Space



Datasets

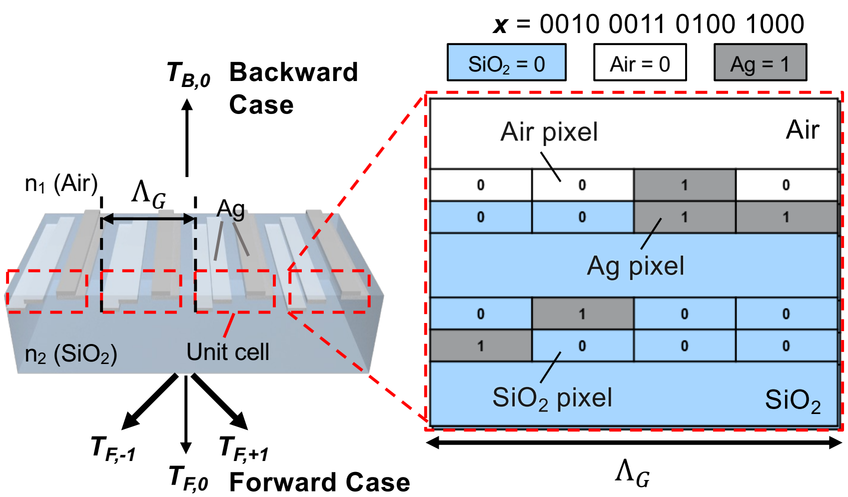


Energy Landscape of the **QUBO surrogate** (from FM)

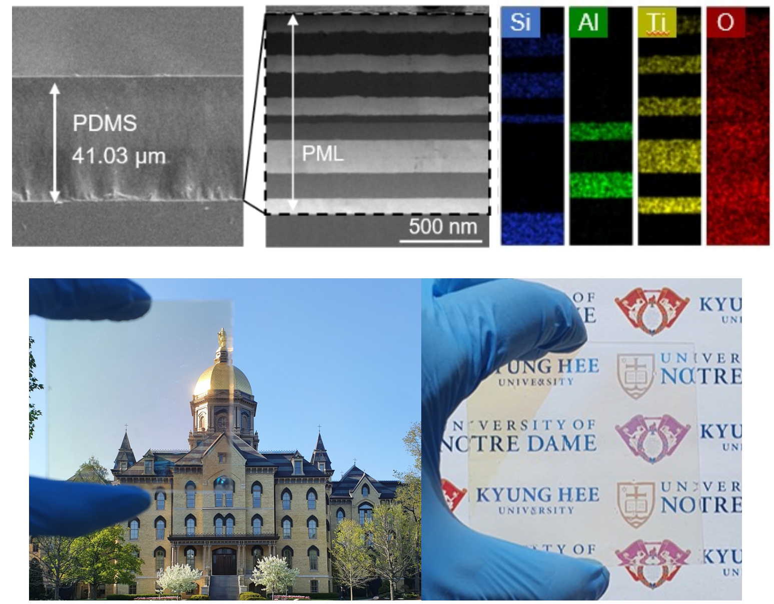


Designed Metamaterials

Metamaterial Optical Diode



Transparent Radiative Cooler



Kim et. al., ACS Energy Letters, 2022, 7, 4134–4141
Kim et. al., Nano Convergence, 2024, 11, 16

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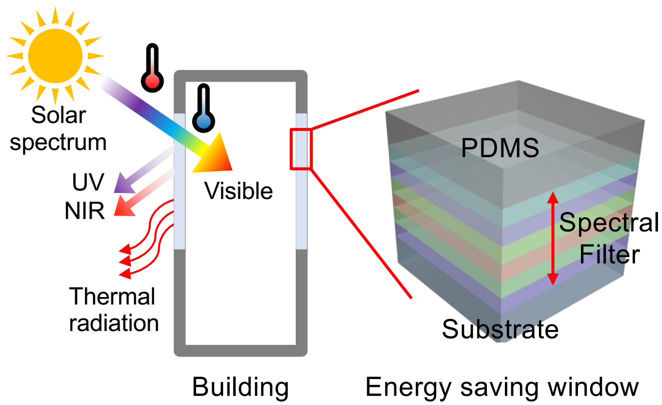
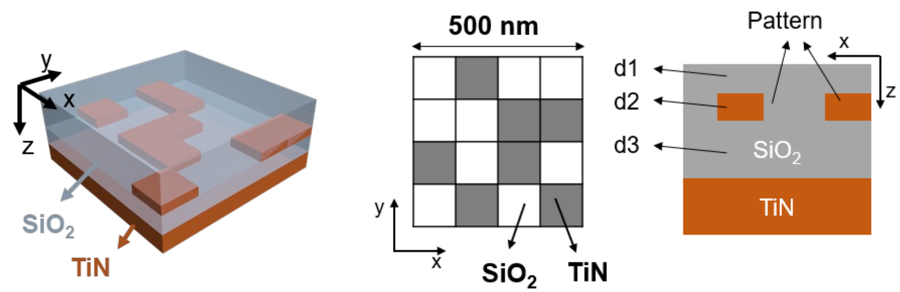
Designed Metamaterials

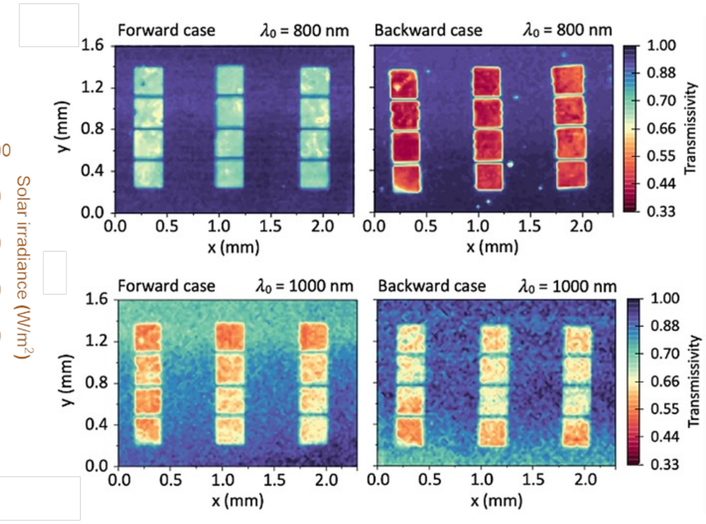
Wide-Angle Spectral Filter



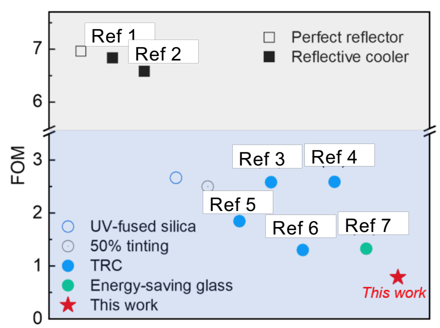
Metamaterial Solar Absorber

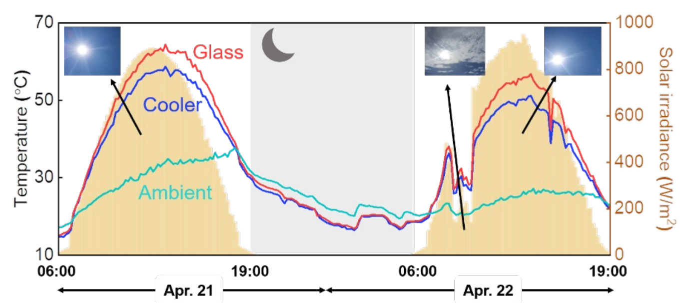


Kim et. al., ACS Applied Materials & Interfaces, 2023, 15, 40606-40613
Kim et. al., Cell Reports Physical Science, 2024, 5, 101847



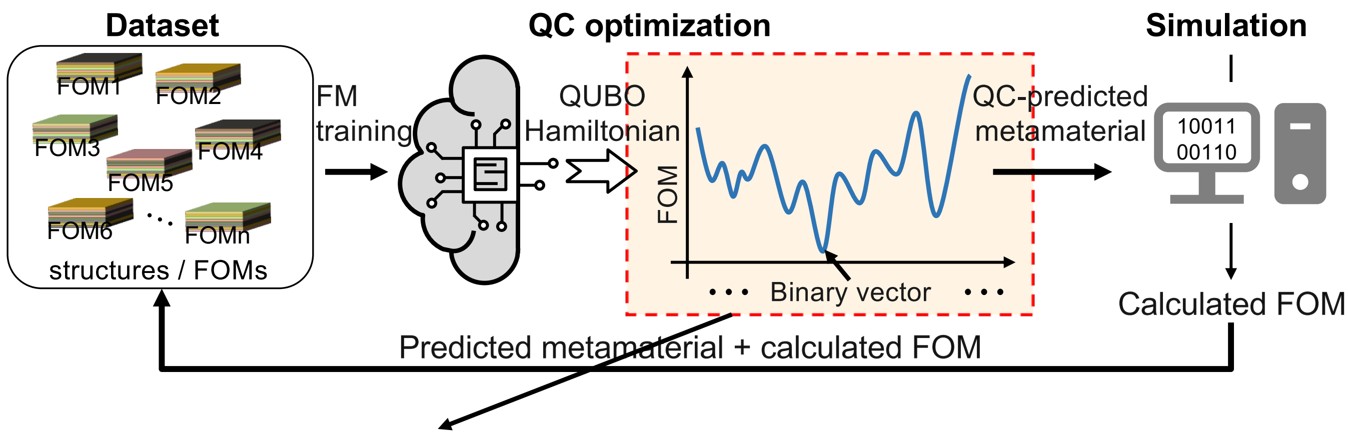
Performance Evaluation



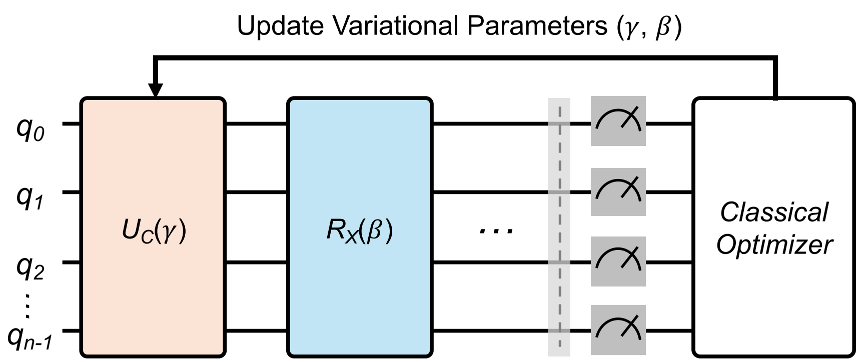


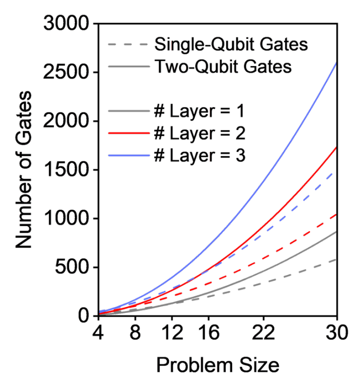
Refs: *Nat. Nanotechnol.* **2021**, *16* (12), 1342, *EcoMat.* **2022**, *4* (1), e12153, *Adv. Opt. Mater.* **2021**, *9* (13), 2002226, *Adv. Mater. Interfaces* **2021**, 2201050, *Adv. Funct. Mater.* **2022**, *32* (1), 2105882, *Nano Energy* **2021**, *89*, 106440, *Int. J. Appl. Glass Sci.* **2010**, *1* (1), 118

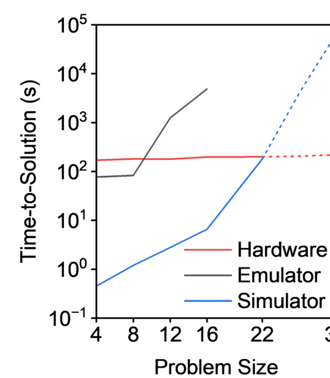
Gate-Based Quantum Computing to Solve QUBO Surrogates



Quantum Approximate Optimization Algorithm (QAOA)

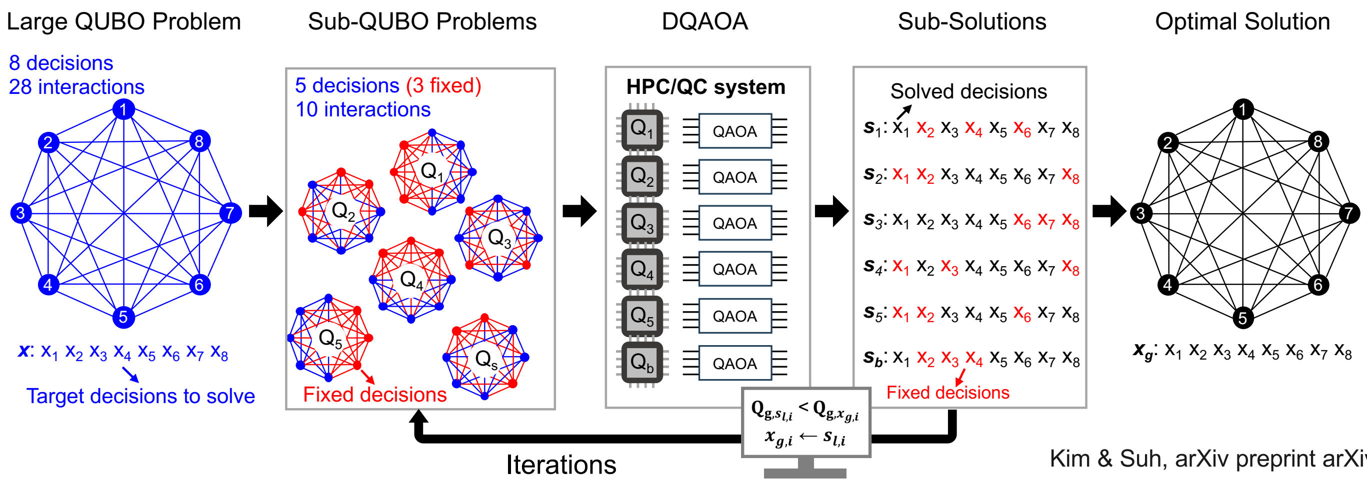






Kim & Suh, arXiv preprint arXiv:2407.20212, 2024

Distributed QAOA (DQAOA) on HPC-QC Integrated Systems



Kim & Suh, arXiv preprint arXiv:2407.20212, 2024

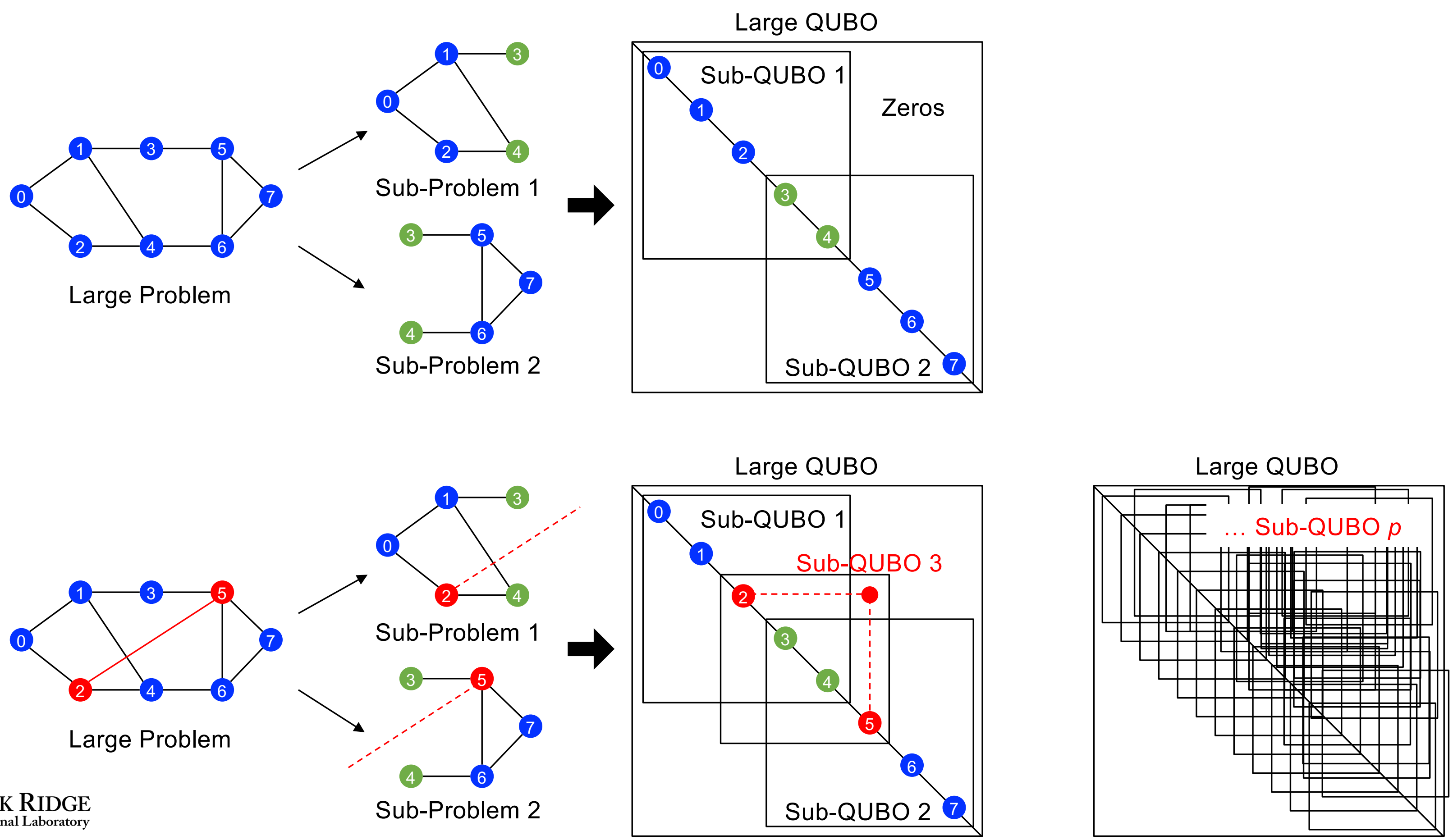
Why DQAOA?

- **Optimizing metamaterials for continuous variables** makes a **very large QUBO** (10,000 x 10,000)
  - ✓ Large QUBO (size: 10,000) **requires large sub-QUBOs** (size: ~100)
  - ⟶ **QAOA** (optimized algorithm with advanced simulators on HPC) **shows great potential** in solving QUBOs
- **Higher-order interactions** (not just pair-wise interactions) should be considered for metamaterial optimization (**HUBO**)
  - ✓ **QAOA is the best** for higher-order optimization problems
  - ⟶ QAOA shows a much better performance than other solvers

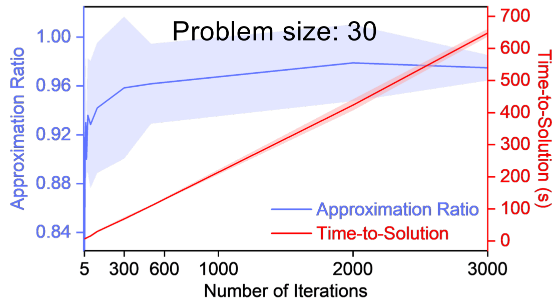
Shaydulin et. al., Science Advances, 2024, 10, 6761

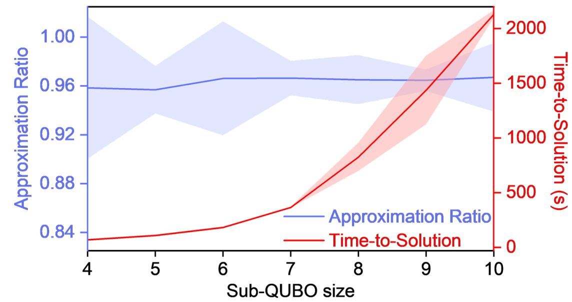
Bucher et. al., arXiv preprint arXiv:2405.07624, 2024

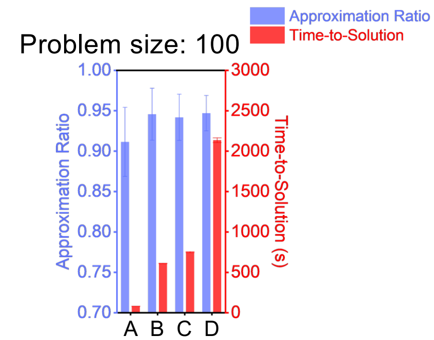
Decomposition Policy

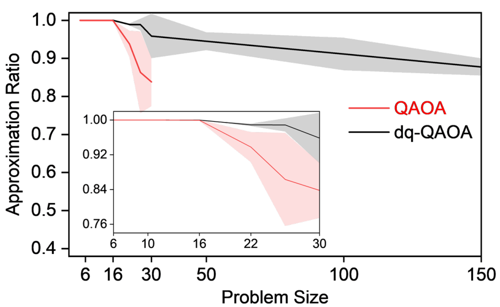


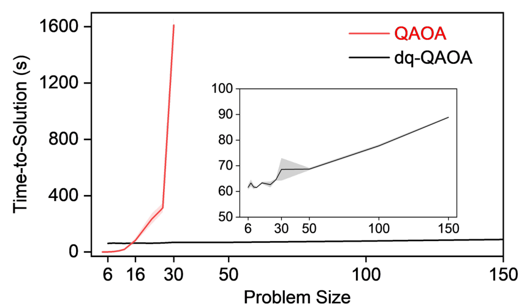
Performance Analysis of dq-QAOA (single core)

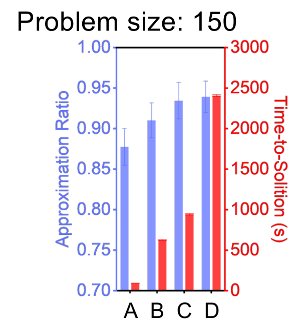








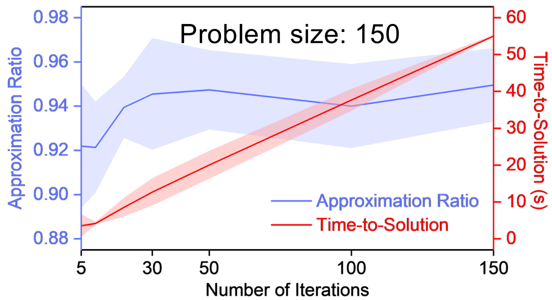


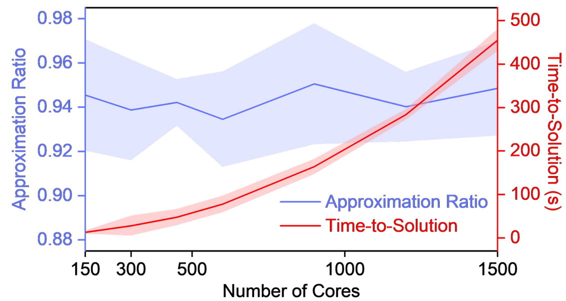


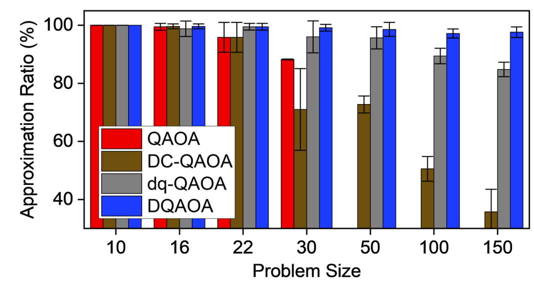
A: 300 iterations, 4 subQUBO size
B: 3000 iterations, 4 subQUBO size
C: 300 iterations, 8 subQUBO size
D: 1000 iterations, 8 subQUBO size

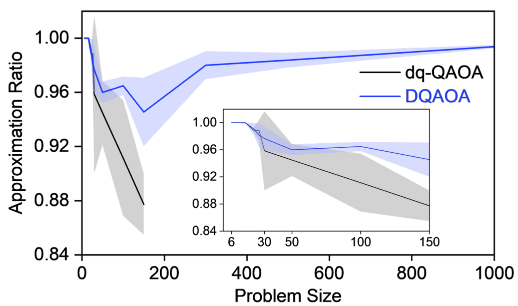
- QAOA on a single core (dq-QAOA) can efficiently solve QUBO problems (size: up to 150)
- Hyperparameter tuning (number of iterations, and sub-QUBO size) can improve the global solution quality, but increase time-to-solution a lot

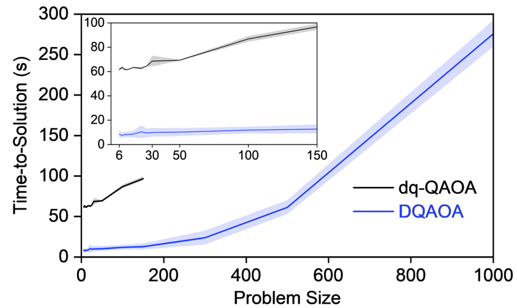
Performance Analysis of DQAOA (multi-cores/nodes)

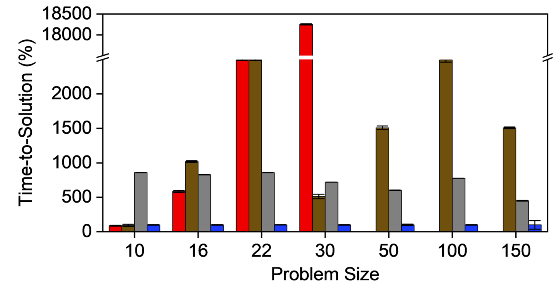






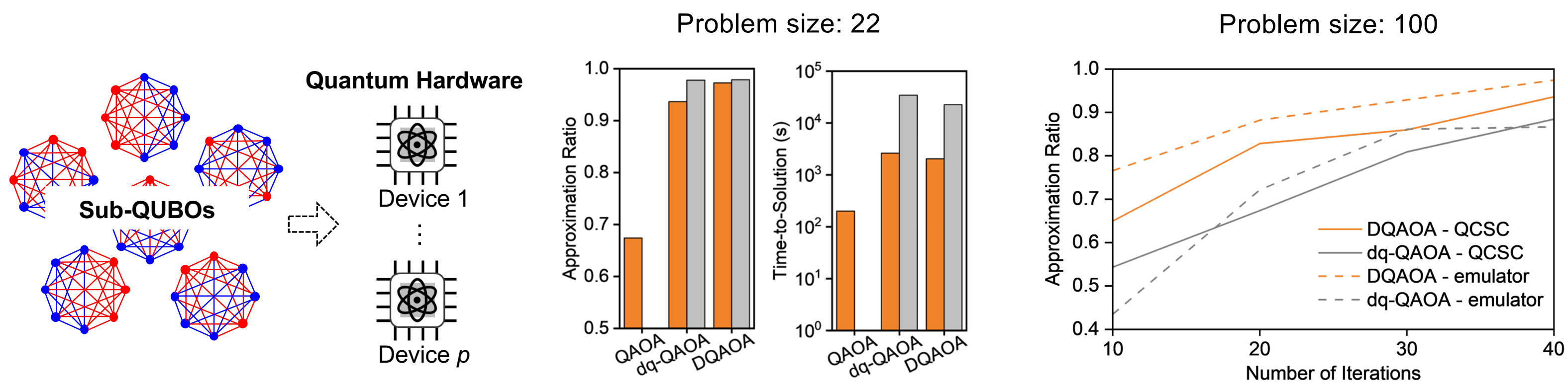






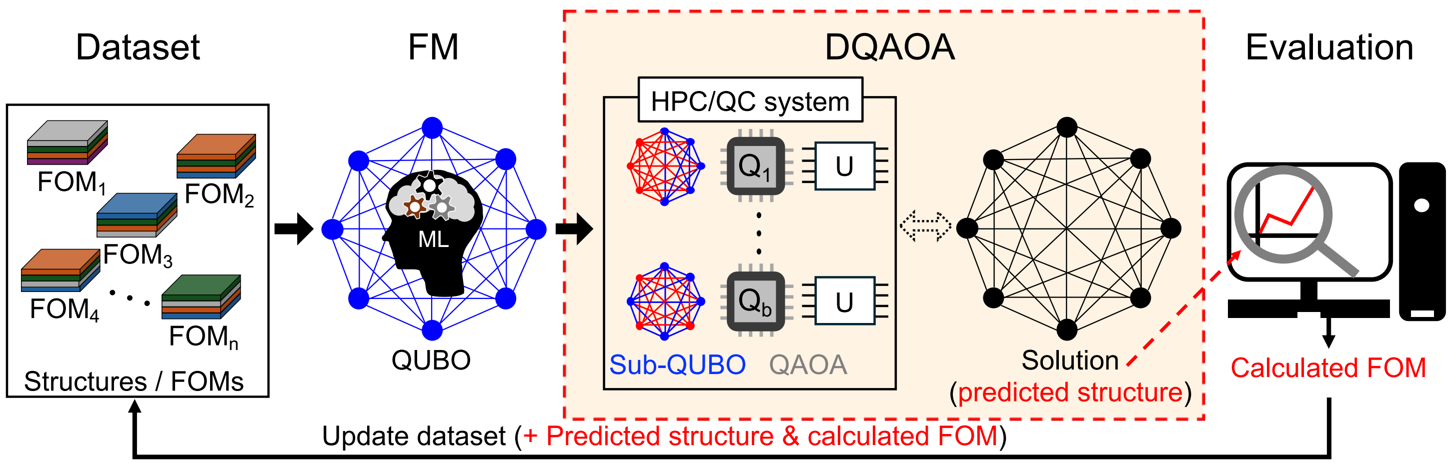
- DQAOA running on multi-cores/nodes can solve large QUBO problems (size: up to 1,000) with high accuracy and low time-to-solution
- DQAOA shows the highest accuracy and shortest time-to-solution (>7 times than dq-QAOA, and >160 times than QAOA)
- DQAOA not only addresses the limitations of current quantum techniques but also sets a foundation for future advancements as quantum technology continues to evolve

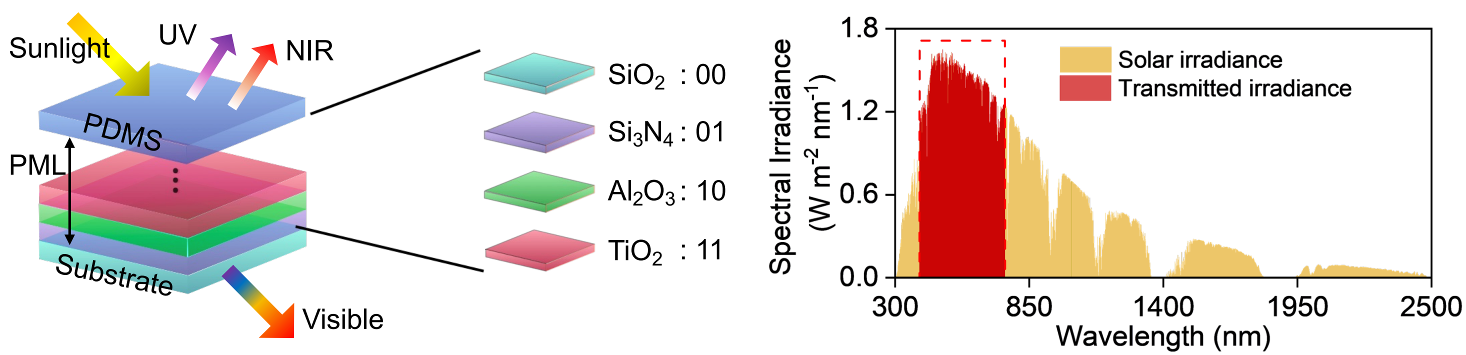
DQAOA on Quantum-Centric Supercomputer Architecture



- DQAOA on QCSC (IBM-Strasbourg & IBM-Kyiv) achieves a high approximation ratio (~0.97) for a problem of size *22*
- It also successfully solves a larger problem (size: 100) with a high approximation ratio (~0.94)
- Increasing the number of iterations is expected to further improve the approximation ratio

Active Learning using DQAOA (AL-DQAOA) for Material Design





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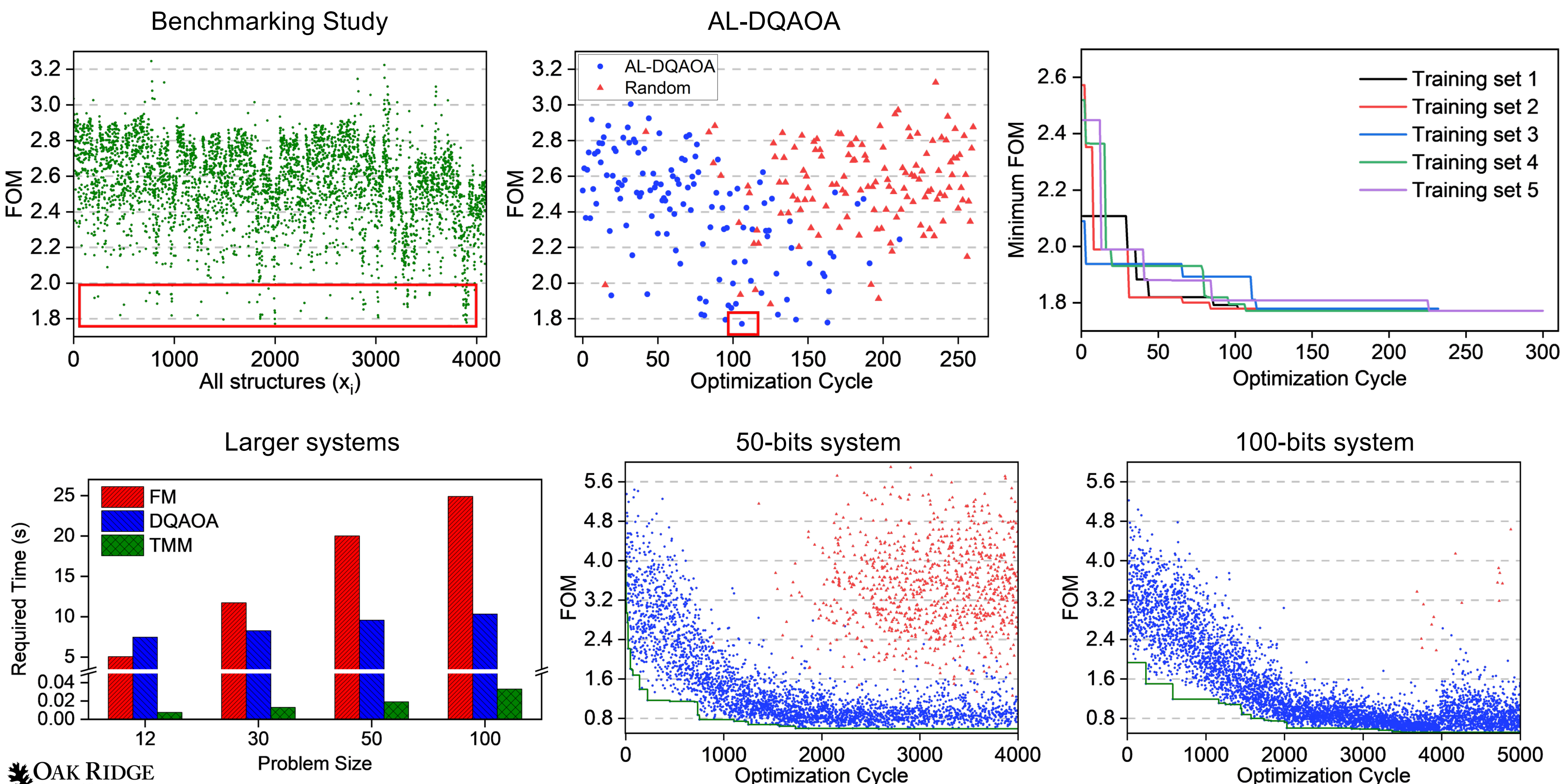
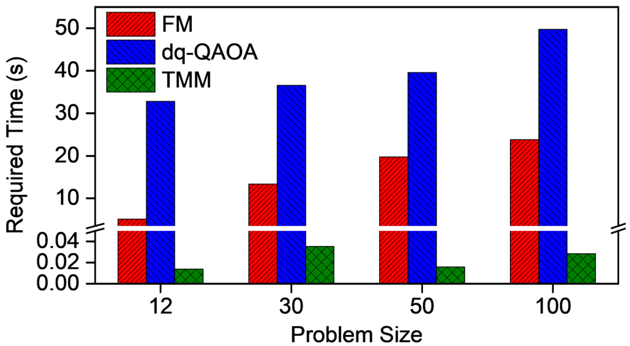
Optimization Results

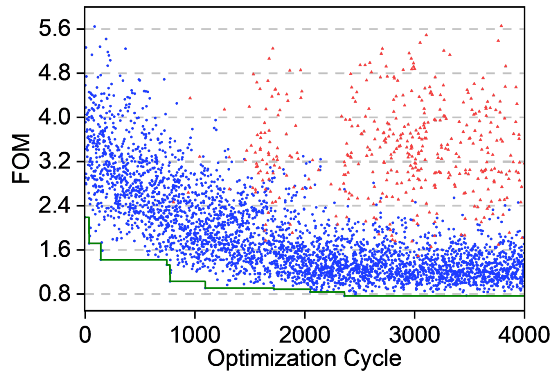


Optimization Results

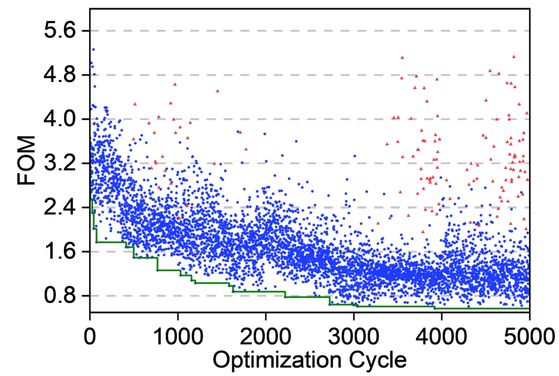
AL-dq-QAOA



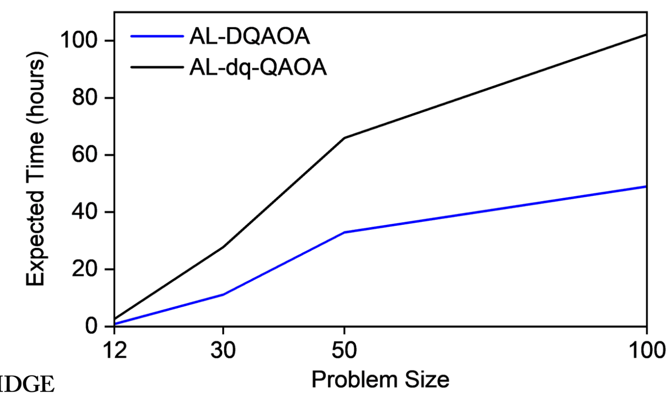
50-bits system

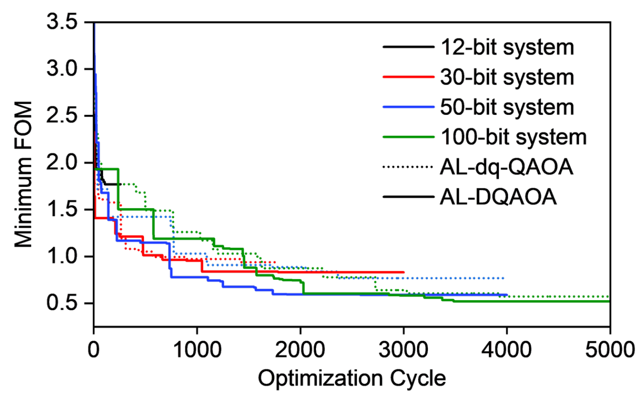


100-bits system



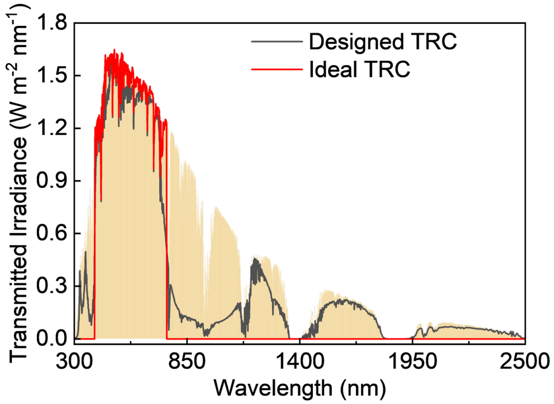
Comparison between AL-DQAOA and AL-dq-QAOA

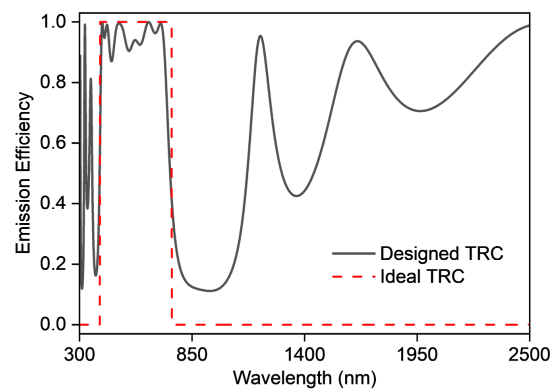


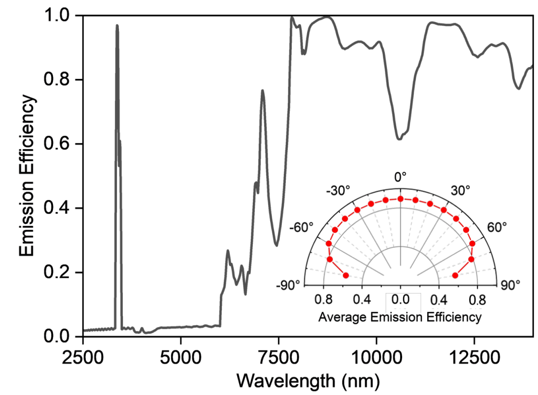


Optimization Results

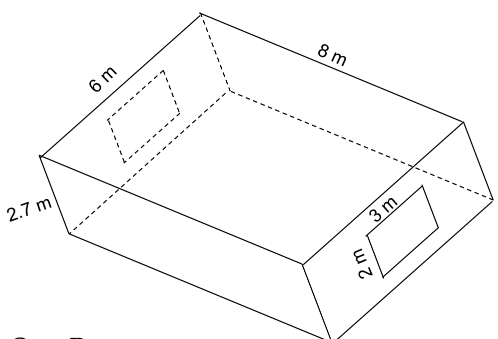
Optical Properties

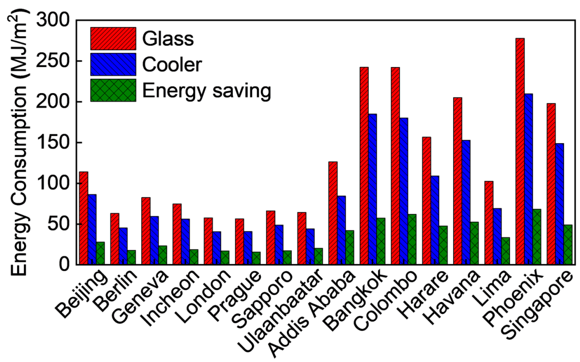


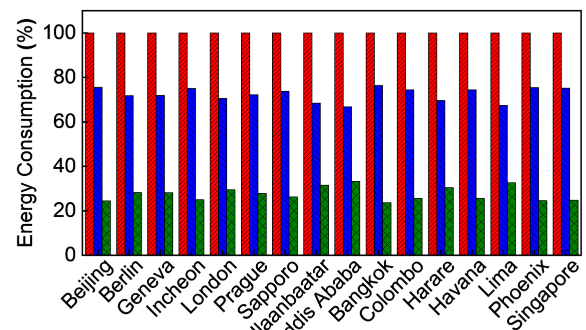




Energy-Saving Capability

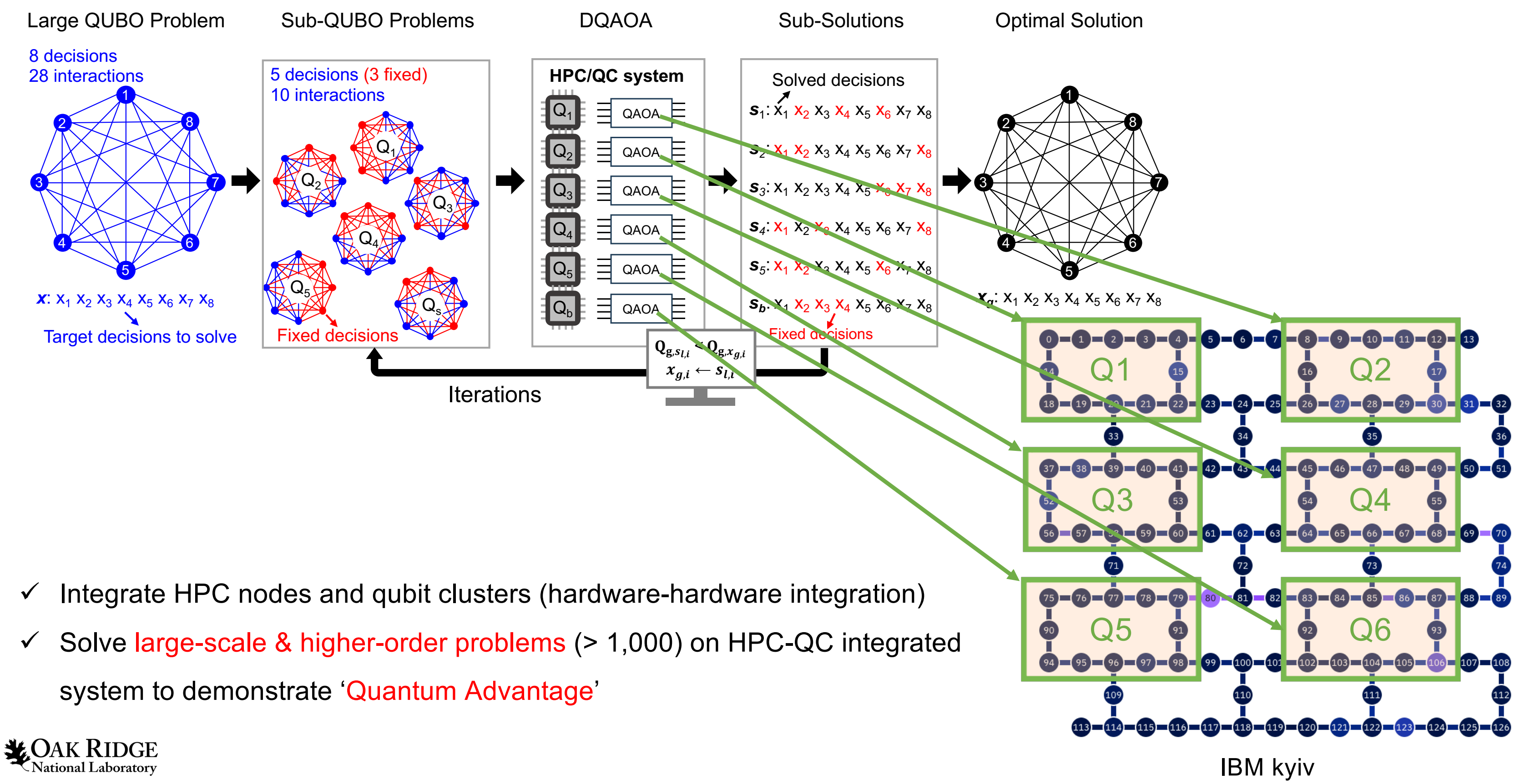






Future Work

DQAOA with Quantum Devices



- ✓ Integrate HPC nodes and qubit clusters (hardware-hardware integration)
- ✓ Solve large-scale & higher-order problems (> 1,000) on HPC-QC integrated system to demonstrate 'Quantum Advantage'

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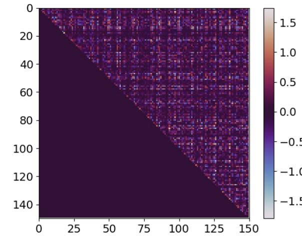
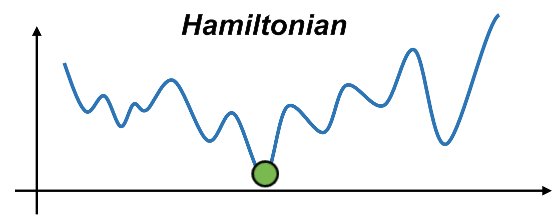
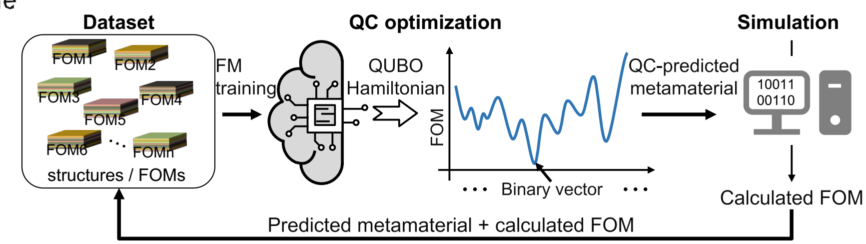
Conclusion

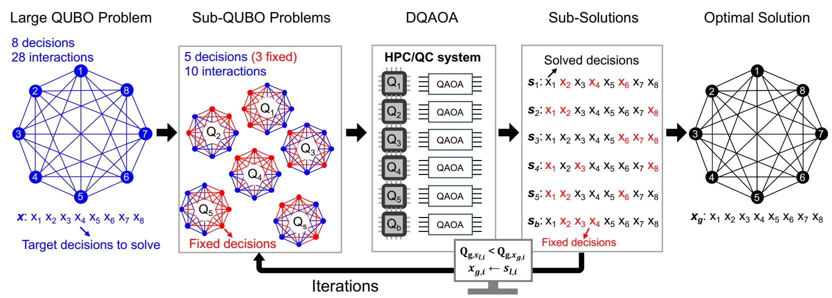
- QUBO surrogates can be generated using Factorization Machine
- Quantum computing (annealing) can be used to solve QUBO problems
- Functional materials (metamaterials) are designed and fabricated using the proposed active learning algorithm
- Efficiency of the active learning algorithm is demonstrated
- Performance of the designed materials is experimentally demonstrated
- DQAOA algorithm working on the HPC-QC integrated system is proposed to tackle large-scale optimization problems using the current quantum computing systems
- Active learning algorithm with DQAOA can solve large-scale real-world optimization problems







Papers, Profile



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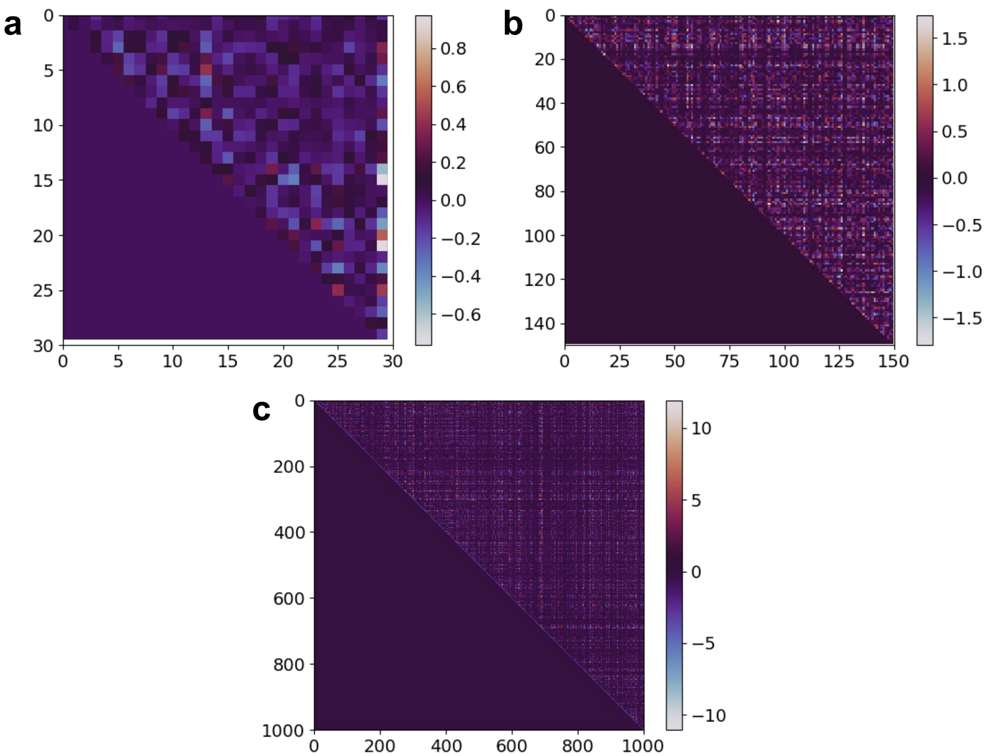
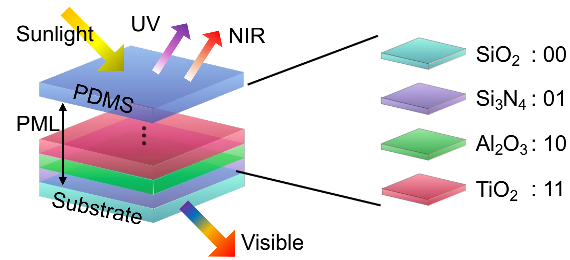
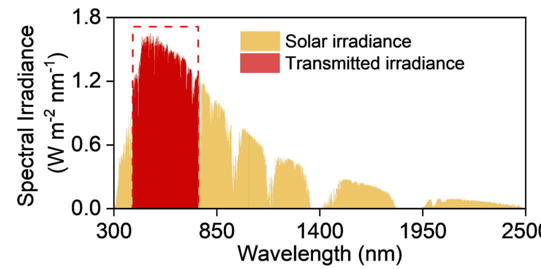
Thank you!

Questions?

Appendix







Solar transmission efficiency	0.6738
Solar reflection efficiency	0.3262
Visible transmission efficiency	0.9196
Visible reflection efficiency	0.0804
IR transmission efficiency	0.3908
Hemispherical emission efficiency	0.5343

Appendix

a Initialization

Fixed decisions

Sub-QUBO$_{init,1}$: x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8

Sub-QUBO$_{init,2}$: x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8

Sub-QUBO$_{init,3}$: x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8

...

Sub-QUBO$_{init,n\text{-}k+1}$: x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8

Target decisions

b Iteration

Sub-QUBO$_{iter,1}$: x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8

Sub-QUBO$_{iter,2}$: x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8

Sub-QUBO$_{iter,3}$: x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8

...

Sub-QUBO$_{iter,b}$: x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8

Abstract

In this tutorial, we provide an overview of distributed variational optimization algorithms designed to harness the power of integrated quantum–HPC ecosystems for solving large-scale combinatorial optimization problems. We focus on the Distributed Quantum Approximate Optimization Algorithm (DQAOA), a scalable quantum-classical hybrid algorithm that distributes quantum workloads across multiple QPUs or simulators, coordinated via classical HPC infrastructure.

A key of the tutorial is the application of DQAOA to materials optimization problems, which are naturally formulated as large and densely connected quadratic unconstrained binary optimization (QUBO) problems. These QUBO instances often exceed the capacity of current quantum hardware or simulator. We will present real-world case studies involving high-dimensional materials design problems, showcasing how distributed quantum resources can accelerate the search for optimal material configurations.