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Quantum Assisted Optimization and Machine Learning for Coordinated Power and Hydrogen System

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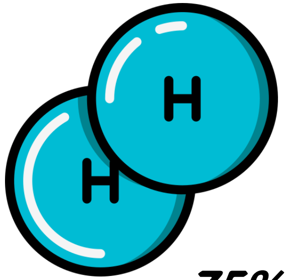
Content

Motivation

Why hydrogen?



75% of all is made up of hydrogen

Fossil fuel hydrogen	Black hydrogen	Blue hydrogen	Grey hydrogen
Renewable hydrogen	Green hydrogen		

What is Hydrogen

- Hydrogen's energy density is significantly higher than fossil fuels
- Hydrogen is an energy carrier and can be used as energy storage
- Hydrogen doesn't exist in nature by itself

Green hydrogen

- Green hydrogen is produced by electrolyzors using renewable energy
- Electrolysis is a process to split water into hydrogen and oxygen by a direct current
- Around 8GW of eletrolyzor capacity is installed

Electrolyzor

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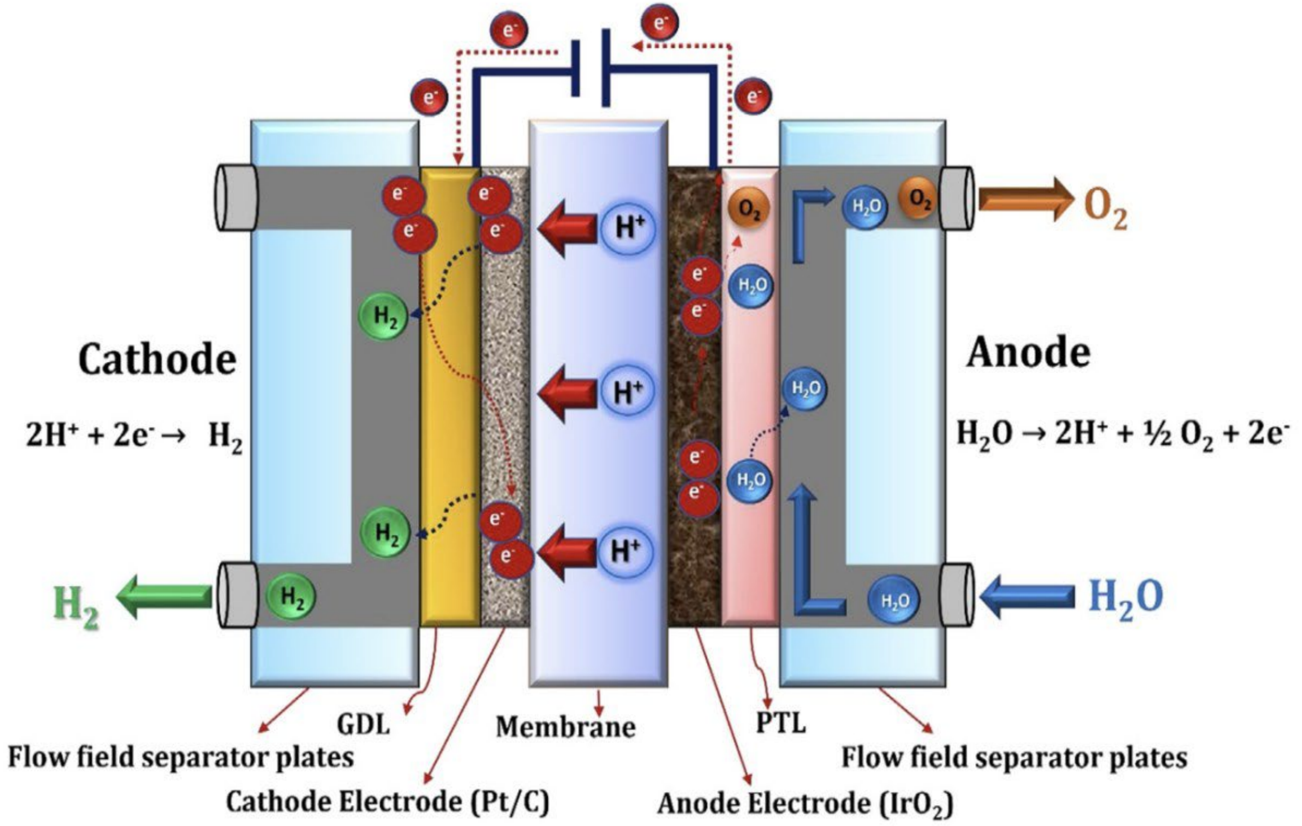
What is electrolyzor?

- **Use electricity to split water into hydrogen and oxygen**

  Can provide demand-side flexibility by
  - ✓ Adjusting hydrogen production to follow wind and solar generation profiles
  - ✓ Can provide grid balancing service

- There is a **trade-off between efficiency, cost and carbon emission**

- Great performance
  - High purity H_2 straight from the stack



Energy Flow of Hydrogen System

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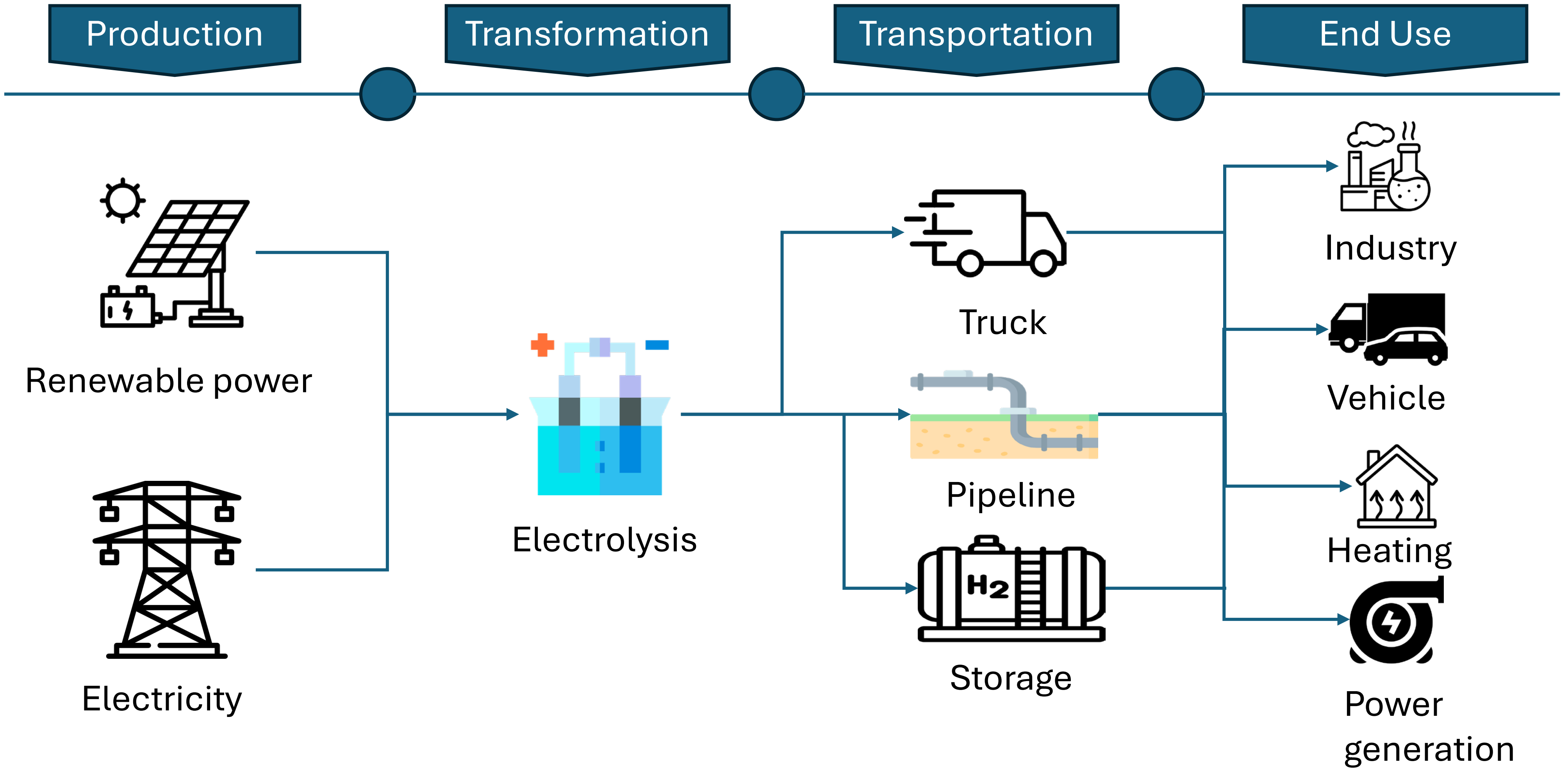
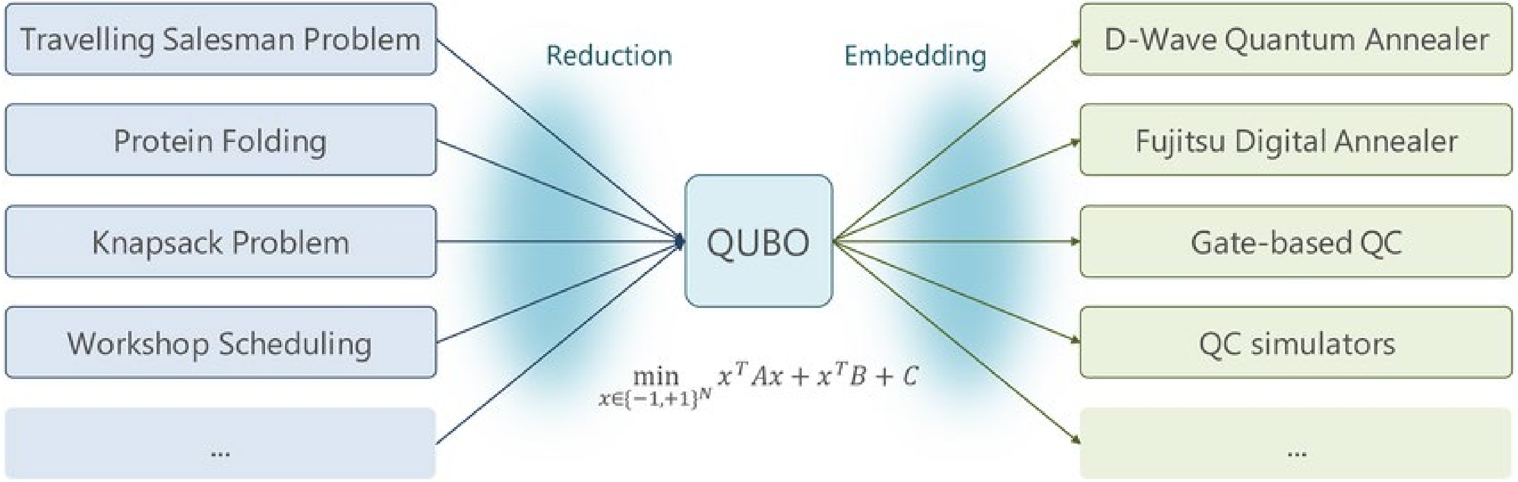


Quantum Tools

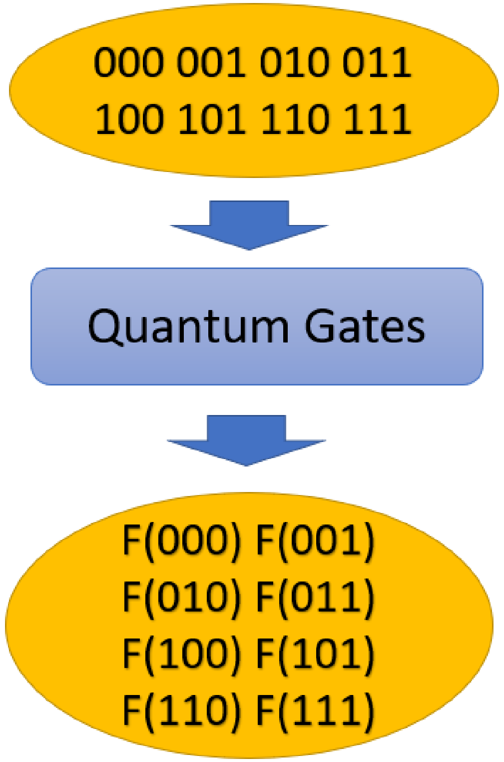


- Coordinated system is usually MILP or MINLP
- Both MILP and MINLP is **NP-Hard, can't** be solved in polynomial time
- We need **new tools** to solve complex problems

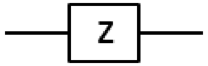
Divide the mixed-integer convex problem into two parts

- ❑ Pure integer part: solved by the quantum computer.
- ❑ Polynomial solvable continuous part: convex optimization algorithms.

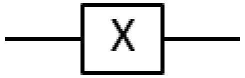
Gated Quantum Circuit



1 qubit gates

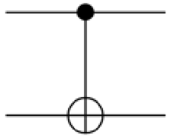


$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



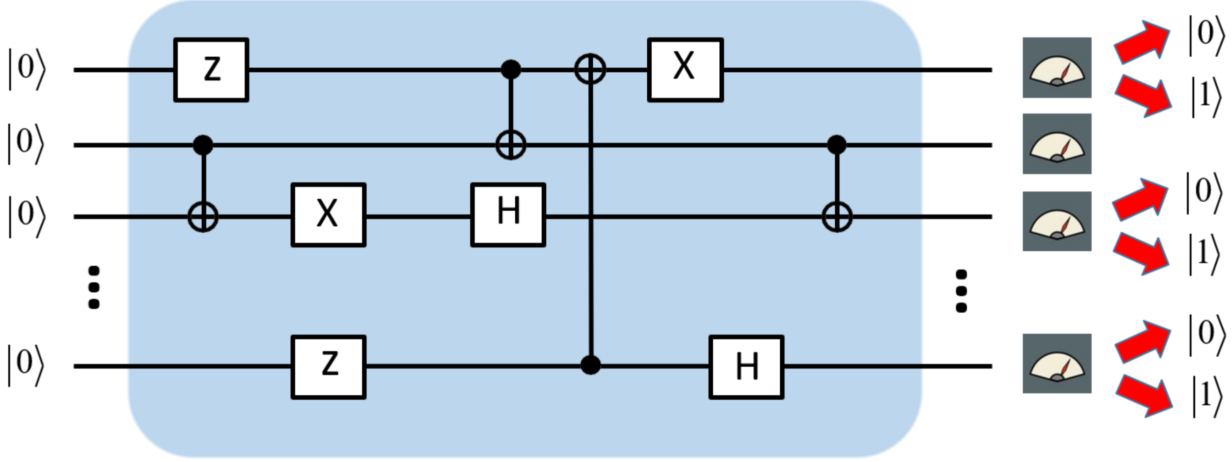
$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

2 qubit gates



$$U_{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Typically, a quantum circuit always looks like



Initial state is all qubits

Consist of 1 and 2 qubit gates

Measurement

- QML performs better than the classical NN under the **same level** of number of parameters
- The available qubits of Quantum computer are **limited**
- Quantum computing is unstable, easy to **lose information** while measurement

Quantum Annealing

Quantum Circuit

- Limited qubits
- Fit most problems that can be solved by classical machine learning
- Challenge: Commonly can NOT beat the classical computer because of limited qubits and noise

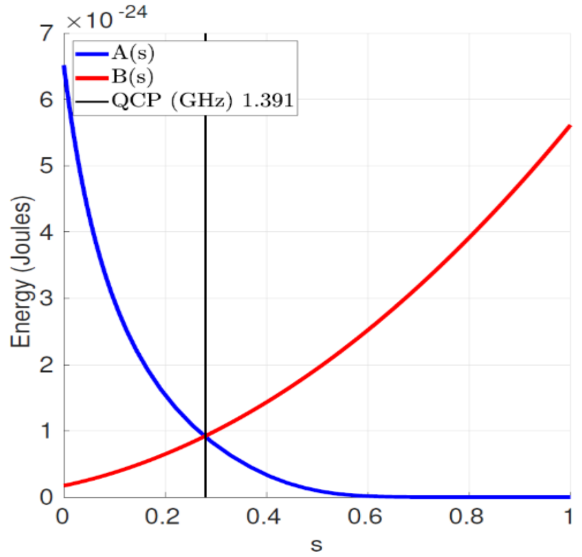
Quantum Annealing

- More qubits
- Fit a small part of problems like QUBO
- Faster than classical solver
- Challenge: Need additional algorithms to transform problem for quantum annealer

Quantum Hamiltonian

- **We work with only the problem Hamiltonian:**

$$H_{ising} = \underbrace{-\frac{A(s)}{2}\left(\sum_i \hat{\sigma}_x^{(i)}\right)}_{\text{Initial Hamiltonian}} + \underbrace{\frac{B(s)}{2}\left(\sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j}\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right)}_{\text{Final Hamiltonian}}$$



- **Goal (what the hardware does)**
  - Minimize $\sigma_i \in \{-1,+1\}$ subject to provided $J_{i,j} \in \mathrm{R}$ and $h_i \in \mathrm{R}$ coefficients
  - In other words, a quantum optimization program is merely a list of $J_{i,j}$ and h_i

Negative ($J_{i,j} = -5$)

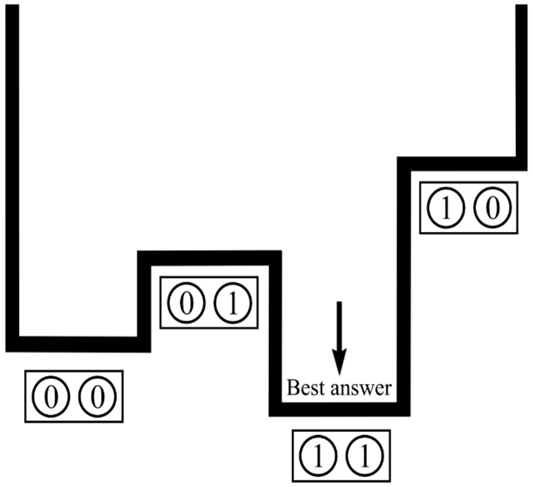
σ_i^z	σ_j^z	$J_{i,j}\sigma_i^z\sigma_j^z$
–1	–1	–5
–1	+1	+5
+1	–1	+5
+1	+1	–5

Zero

σ_i^z	σ_j^z	$J_{i,j}\sigma_i^z\sigma_j^z$
–1	–1	0
–1	+1	0
+1	–1	0
+1	+1	0

Positive ($J_{i,j} = +5$)

σ_i^z	σ_j^z	$J_{i,j}\sigma_i^z\sigma_j^z$
–1	–1	+5
–1	+1	–5
+1	–1	–5
+1	+1	+5



Content

Power-to-Hydrogen Pipeline System

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Objective: $\varphi_s = \sum_{t\in\mathcal{T}_s}\sum_{b\in\mathcal{B}_{root}} \hat{\lambda}_t p_{b,t}^{root} + \sum_{t\in\mathcal{T}_s}\sum_{i\in\mathcal{HR}} C_i^{\text{prd}} \cdot h_{i,t}.$ Minimize total cost

s.t.

$$\sum_{(b,n)\in\mathcal{L}} f_{b,n,t}^P - \sum_{(m,b)\in\mathcal{L}} f_{m,b,t}^P = 1_{b\in\mathcal{B}_{root}} \cdot p_{b,t}^{root} + \sum_{i\in\mathcal{W}^b} p_{i,t}^W - \sum_{i\in\mathcal{HE}_b} p_{i,t}^{HE} - p_{b,t}^D,\ \forall b\in\mathcal{B}, \forall t\in\mathcal{T}_s,$$

$$\sum_{(b,n)\in\mathcal{L}} f_{b,n,t}^Q - \sum_{(m,b)\in\mathcal{L}} f_{m,b,t}^Q = 1_{b\in\mathcal{B}_{root}} \cdot q_{b,t}^{root} + \sum_{i\in\mathcal{W}^b} q_{i,t}^W - \sum_{i\in\mathcal{HE}_b} q_{i,t}^{HE} - q_{b,t}^D,\ \forall b\in\mathcal{B}, \forall t\in\mathcal{T}_s,$$

Power balance

$$u_{m,t} - u_{n,t} = 2\left(r_{m,n}\cdot f_{m,n,t}^P + x_{m,n}\cdot f_{m,n,t}^Q\right),\ \forall (m,n)\in\mathcal{L}, \forall t\in\mathcal{T}_s,$$

$$f_{m,n,t}^{P\ 2} + f_{m,n,t}^{Q\ 2} \le S_{m,n}^2,\ \forall (m,n)\in\mathcal{L}, \forall t\in\mathcal{T}_s,$$

Voltage balance

$$h_{z,t}^{\text{pip dc}} - h_{z,t}^{\text{pip ch}} = \sum_{i|i=(m,z)\in\mathcal{P}} q_{i,t}^{\text{pip tail}} - \sum_{i|i=(z,n)\in\mathcal{P}} q_{i,t}^{\text{pip head}},$$

Pipeline transportation

$$\sum_{i\in\mathcal{HR}_z} h_{i,t} + \sum_{i\in\mathcal{HE}_z} \eta_i \cdot p_{i,t}^{HE} - \sum_{i|i=(z,n)\in\mathcal{P}} q_{i,t}^{\text{pip head}} + \sum_{i|i=(m,z)\in\mathcal{P}} q_{i,t}^{\text{pip tail}} = D_{z,t}^{\text{hyd}},$$

Zone level hydrogen balance

$$e_{i,t}^{\text{pip}} = e_{i,t-1}^{\text{pip}} + q_{i,t}^{\text{pip head}} - q_{i,t}^{\text{pip tail}}$$

Storage

Quantum Assisted Hydrogen System

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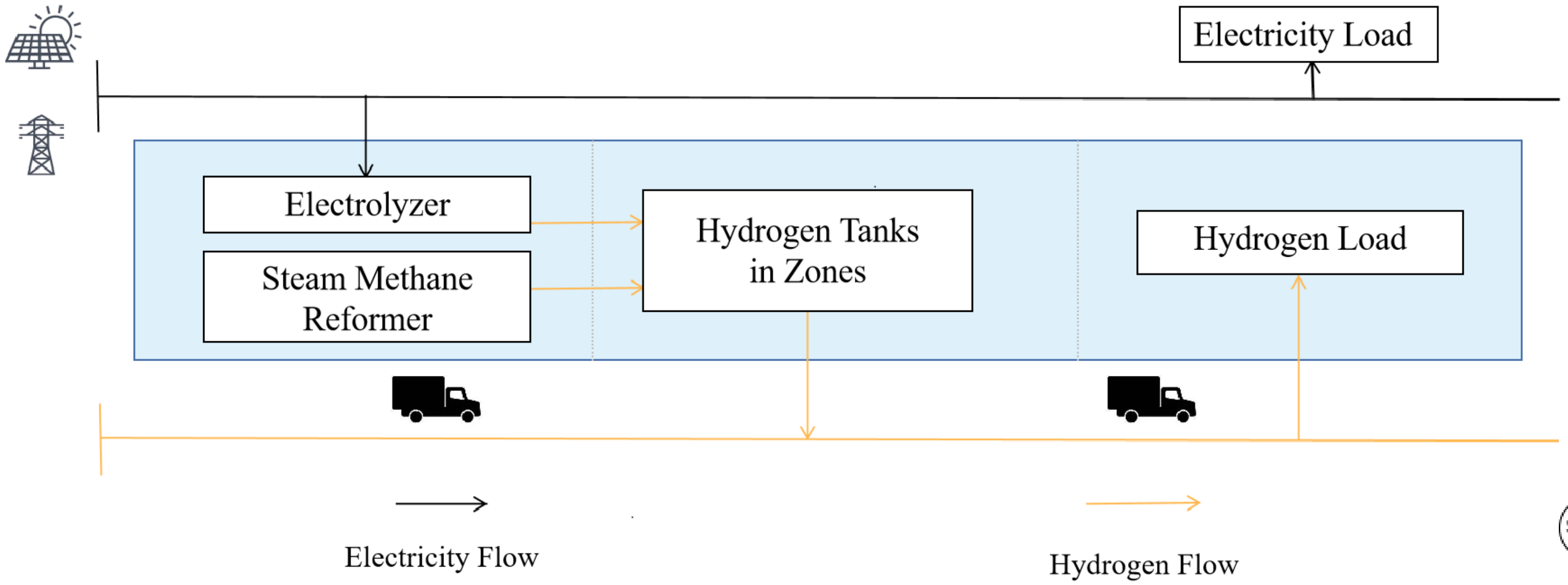

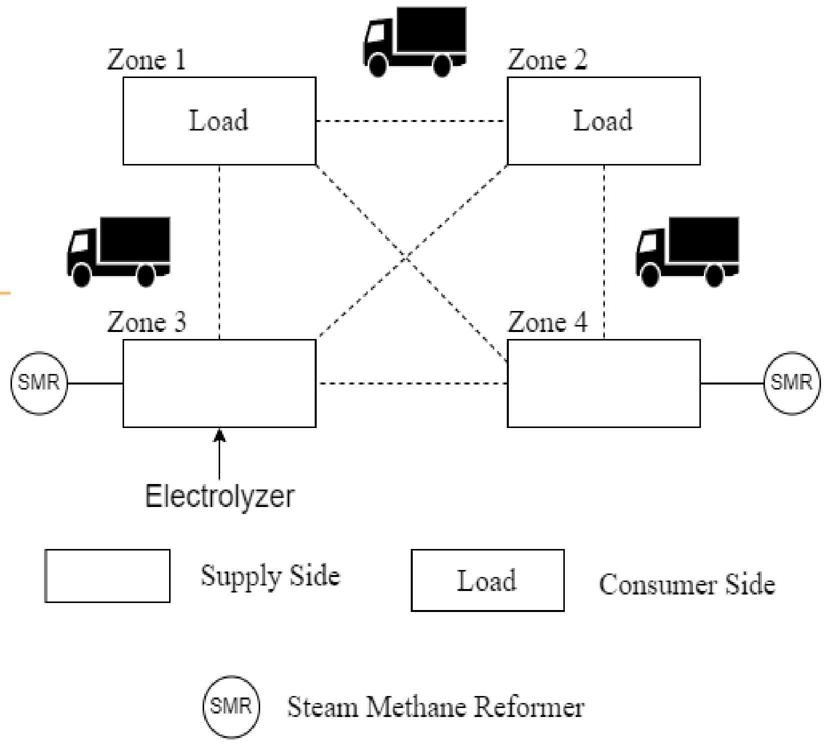

- In this model, we utilize trucks to transport hydrogen between zones
- Power can be generated by electricity or fossil fuels
- Hydrogen can be stored in the truck while transportation

Objective Functions

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Detailed Formulation

$$\min \ \varphi_s = C^{\text{h2prd}} + C_s^{\text{h2trs}} + C_s^{\text{ele}}.$$

The objective function: minimize the total cost of coordinated system.

$$C_s^{\text{h2prd}} = \sum_{t \in \mathcal{T}} \sum_{i \in \mathcal{HR}} c_i^{\text{prd}} \cdot h_{i,t}.$$

Hydrogen generation cost

$$C_s^{\text{ele}} = \sum_{t \in \mathcal{T}} \sum_{b \in \mathcal{B}_{root}} \hat{\lambda}_t p_{b,t}^{root}.$$

Cost of electricity production

$$C^{\text{h2trs}} = \sum_{t \in \mathcal{T}} \sum_{z \in \mathcal{Z}} \sum_{i \in \mathcal{TK}} (c_i^{\text{lding}} \cdot q_{i,z,t}^{\text{lding}} + c_i^{\text{unlding}} \cdot q_{i,z,t}^{\text{unlding}}) + \sum_{t \in \mathcal{T}} \sum_{i \in \mathcal{TK}} \sum_{z_{st} \in \mathcal{Z}} \sum_{z_{en} \in \mathcal{Z}} c^{\text{fuel}} \cdot d_{z_{st},z_{en}} \cdot x_{i,z_{en},t} \cdot x_{i,z_{st},t-1}.$$

Hydrogen transportation cost

Transportation cost has quadratic binary terms, difficult to solve

Need new ways to solve it!

Hydrogen System Constraints

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$$0 \le h_{i,t} \le \overline{H}_i \quad \forall i \in \mathcal{HR}, t \in \mathcal{T},$$
$$0 \le \eta_i \cdot p_{i,t} \le \overline{H}_i \quad \forall i \in \mathcal{HE}, t \in \mathcal{T}.$$

Hydrogen generation limit.

$$0 \le e_{z,0} + \sum_{\tau=1}^{t} \Bigg(\sum_{i \in \mathcal{HR}_z} h_{i,\tau} + \sum_{i \in \mathcal{HE}_z} \eta_i \cdot p^{HE}_{i,\tau} - \sum_{i \in \mathcal{TK}} q^{lding}{}_{i,z,\tau} + \sum_{i \in \mathcal{TK}} q^{unlding}_{i,z,\tau} - D^{\text{hyd}}_{z,\tau} \Bigg) \le \overline{E}_z, \forall z \in \mathcal{Z}, t \in \mathcal{T} \backslash \{|\mathcal{T}|\}.$$

$$e_{z,0} + \sum_{\tau \in \mathcal{T}} \Bigg(\sum_{i \in \mathcal{HR}_z} h_{i,\tau} + \sum_{i \in \mathcal{HE}_z} \eta_i \cdot p^{HE}_{i,\tau} - \sum_{i \in \mathcal{TK}} q^{lding}_{i,z,\tau} + \sum_{i \in \mathcal{TK}} q^{unlding}_{i,z,\tau} - D^{\text{hyd}}_{z,\tau} \Bigg) = e_{z,|\mathcal{T}|}, \forall z \in \mathcal{Z}.$$

$$e^{mhs}_{i,t+1} = e^{mhs}_{i,t} + \sum_{z \in \mathcal{Z}} q^{lding}_{i,z,t} - \sum_{z \in \mathcal{Z}} q^{unlding}_{i,z,t}, \forall i \in \mathcal{TK}, t \in \mathcal{T},$$

Balance of hydrogen storage

$$0 \le e^{mhs}_{i,t} \le \overline{C}_i, \forall i \in \mathcal{TK}, t \in \mathcal{T}.$$

$$0 \le q^{lding}_{i,z,t} \le \overline{C}_i \cdot x_{i,z,t}, \forall i \in \mathcal{TK}, \forall z \in \mathcal{Z}, t \in \mathcal{T},$$
$$0 \le q^{unlding}_{i,z,t} \le \overline{C}_i \cdot x_{i,z,t} \, \forall i \in \mathcal{TK}, \forall z \in \mathcal{Z}, t \in \mathcal{T},$$
$$\sum_{z \in \mathcal{Z}} x_{i,z,t} = 1, \forall i \in \mathcal{TK}, t \in \mathcal{T},$$
$$\sum_{i \in \mathcal{TK}} x_{i,z,t} \le NTK_{z,t}, \forall z \in \mathcal{Z}, t \in \mathcal{T},$$

Binary variables also exist in constraints, making it more difficult

Quantum Assisted Algorithms

Classical Linearization

$$\text{Cost} = \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}x_i x_j$$

A binary quadratic term can be linearized:

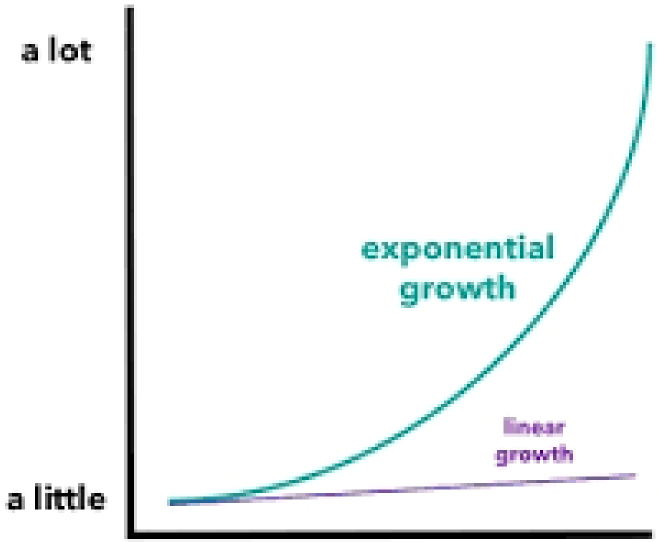
$$\text{Cost} = \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}z_{ij}$$

$$z_{ij} \leq x_i,$$
$$z_{ij} \leq x_j,$$
$$z_{ij} \geq x_i + x_j - 1,$$
$$z_{ij} \in \{0, 1\}.$$

- Though the quadratic term can be linearized, we have to introduce n^2 extra binary variables and $4n$ constraints

How about 10,000 variables or more?

- The complexity of classical solver to solve such a problem grows exponentially



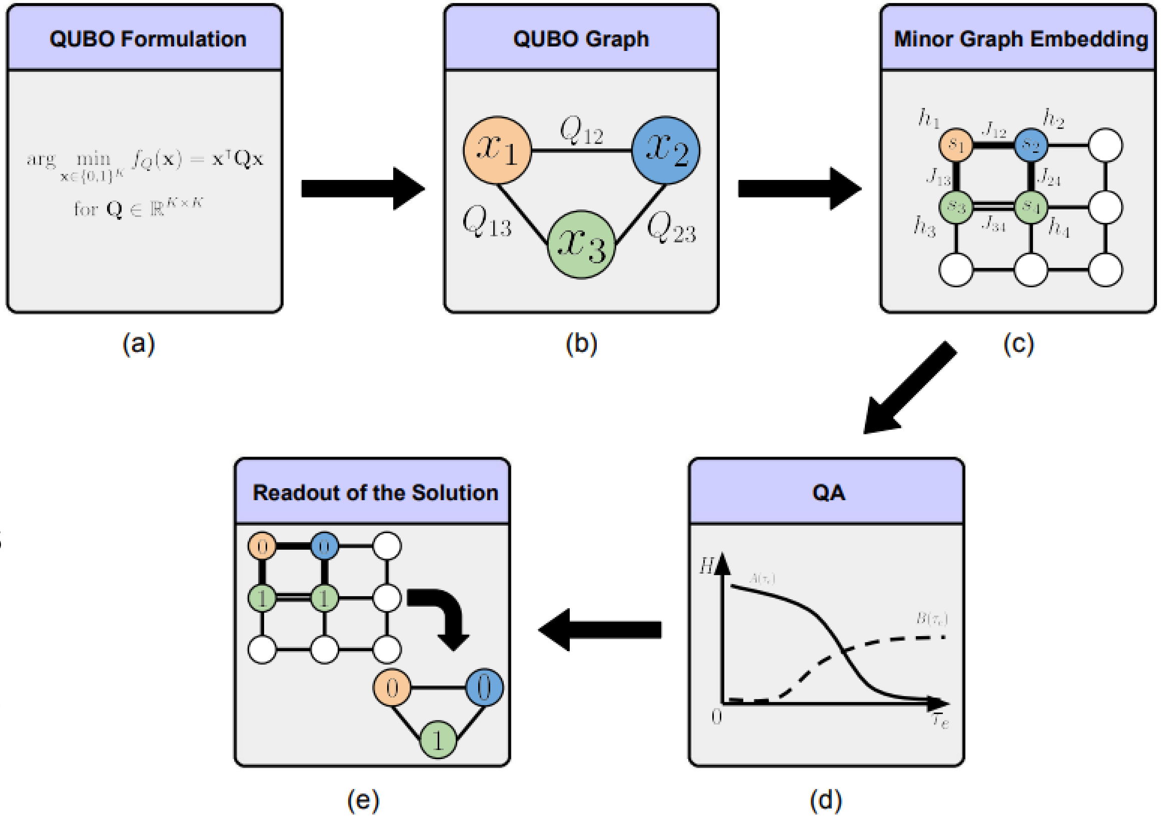
Quantum Annealing and QUBO

Quantum Annealing

$$\mathbf{Q}_{\text{obj}} = \sum_i x_i \mathbf{Q}_{i,i} x_i + \sum_i \sum_{i<j} \mathbf{Q}_{i,j} x_i x_j$$

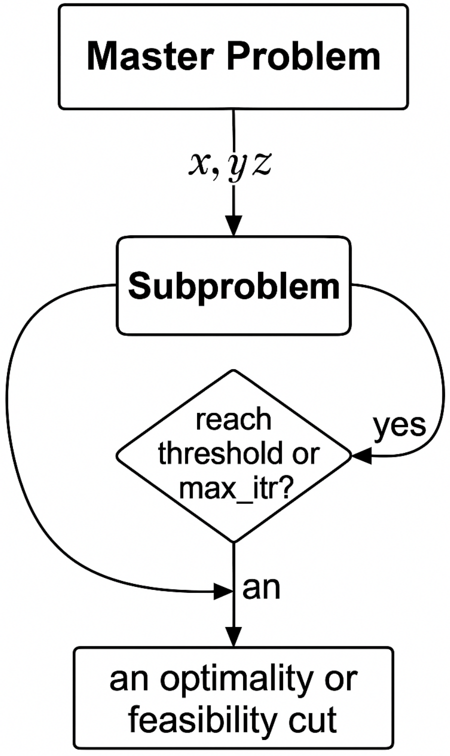
QUBO fits our problem well though need transformation

- Do not need extra variables for quadratic terms
- Need transform the problem into QUBO format



Benders' Decomposition

Classical Benders' decomposition



Benders' Decomposition

Master Problem

$$\begin{aligned} \min_{x,\theta} \quad & c^T x + \theta \\ \text{s.t.} \quad & \theta \geq \left(\pi^{(i)}\right)^T (b - Ax), \quad i \in I, \\ & 0 \geq \left(u^{(j)}\right)^T (b - Ax), \quad j \in J, \\ & x \in X \subseteq \mathbb{Z}^n, \quad \theta \in \mathbb{R}. \end{aligned}$$

Feasibility Cuts or Optimality Cuts ↑ ↓ Binary solution $\mathbf{x}$

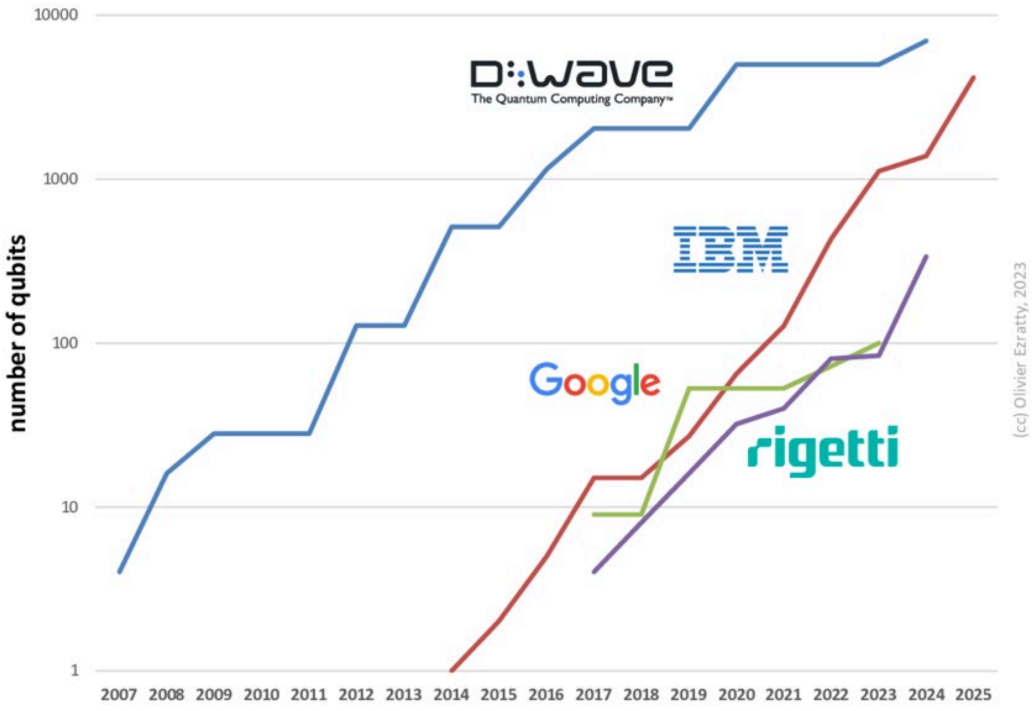
$$\begin{aligned} \min_{y} \quad & f^T y \\ \text{s.t.} \quad & By \geq b - A\hat{x}, \\ & y \geq 0. \end{aligned}$$

SUB

But still one problem!

Benders' Decomposition

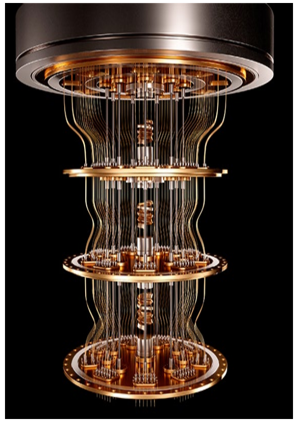
Quantum Machine still has limitation



For current stage, can we ask classical computer to give quantum a hand?

Continuous

Binary



Classical GPU/CPU Solver

Quantum Solver

Combinatorial Bender's Decomposition

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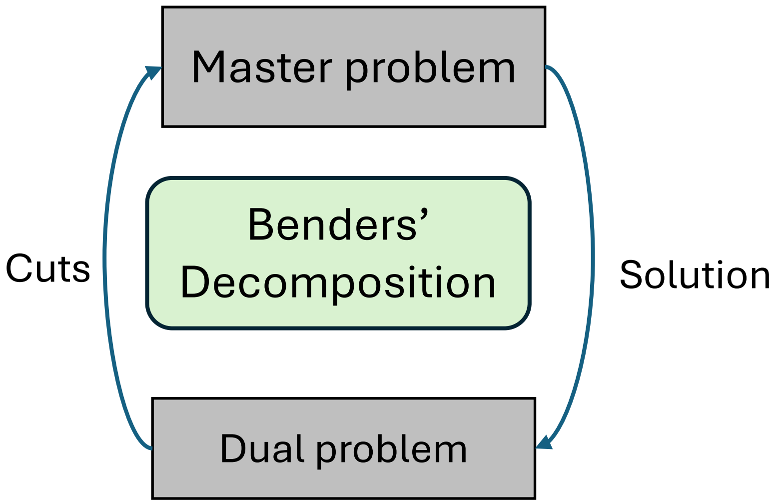
Original problem

$$
\begin{aligned}
\text{[P]: } & \min\ c^T x + d^T y \\
& \text{s.t. } Ax + Ey \geq b, \\
& x_i \in \{0,1\}, \\
& y_j \in \{0,1\} \quad \forall j \in B, \\
& y_j \text{ integer} \quad \forall j \in G, \\
& y_j \geq 0 \quad \forall j \in C,
\end{aligned}
$$



Master problem (MAP)

$$
\begin{aligned}
\text{[MP]: } & \min\ c^T x + \theta(x) \\
& \text{s.t. } x_i \in \{0,1\}.
\end{aligned}
$$

+

Subproblem (SUB)

$$
\begin{aligned}
\text{[SP]: } \theta(\bar{x}) = & \min\ d^T y \\
& \text{s.t. } Ey \geq b - A\bar{x}, \\
& y_j \in \{0,1\} \quad \forall j \in B, \\
& y_j \text{ integer} \quad \forall j \in G, \\
& y_j \geq 0 \quad \forall j \in C,
\end{aligned}
$$

- In Combinatorial Benders' Decomposition (CBD), we can split the binary variables into two sets, and assign them to MAP and SUBs freely.
  - ✓ MAP is a pure binary problem
  - ✓ The cuts are different from classical BD

Combinatorial Benders' decomposition

Master problem

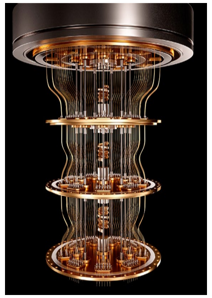
$$[\text{MP}]: \min c^T x + \theta(x)$$
$$\text{s.t. } x_i \in \{0,1\}.$$

solution $\mathbf{x}$

Feasibility Cuts / Optimality Cuts

Subproblem

$$\begin{aligned}[\text{SP}]: \theta(\bar{x}) = \min\ & d^T y \\ \text{s.t. } & Ey \geq b - A\bar{x}, \\ & y_j \in \{0,1\} \quad \forall j \in B, \\ & y_j \text{ integer} \quad \forall j \in G, \\ & y_j \geq 0 \quad \forall j \in C,\end{aligned}$$



1) Divide the original problem (**OP**) into master problem (**MAP**) and subproblem (SP).
2) Solve the **MAP** and obtain solution $\bar{x}$. if $\bar{x}$ leads to an infeasible SP. Add the corresponding feasibility cuts to MAP and return to MAP. (**Feasibility Cuts**).
3) If SP feasible , with optimal objective value $h^T y^v$. In that case an optimality cut is generate (**Optimality Cuts**)

Feasibility Cuts:

$$\sum_{i:x_i^v=0} x_i + \sum_{i:x_i^v=1} (1 - x_i) \geq 1,$$

Optimality Cuts:

$$M^v \sum_{i:x_i^v=0} x_i + M^v \sum_{i:x_i^v=1} (1 - x_i) + \theta \geq h^T y^v,$$

QUBO Transformation

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Reformulate the Final master problem (FMP)

$$\text{FMP:} \min_{\mathbf{x}} \ \mathbf{x}^\top U^\top \mathbf{x} + c^\top \mathbf{x} + \theta \tag{19a}$$

$$\text{s.t.} \sum_{z \in \mathcal{Z}} x_{i,z,t} = 1, \forall i \in \mathcal{TK}, t \in \mathcal{T}, \tag{19b}$$

$$\sum_{i \in \mathcal{TK}} x_{i,z,t} \le NTK_{z,t}, \forall z \in \mathcal{Z}, t \in \mathcal{T}, \tag{19c}$$

$$M^v \sum_{i:x_i^v=0} x_i + M^v \sum_{i:x_i^v=1} (1 - x_i) + \theta \ge d^T y^v \quad \forall v \in V^{\mathrm{P}}, \tag{19d}$$

$$\sum_{i:x_i^v=0} x_i + \sum_{i:x_i^v=1} (1 - x_i) \ge 1, \quad \forall v \in V^{\mathrm{R}}, \tag{19e}$$

$$x \in \mathbf{x}, x \in \{0,1\}^n. \tag{19f}$$

Reformulate the continuous variable:

$$\bar{\theta} = \sum_{i=-\underline{n}}^{\bar{n}_+} 2^i u_{i+\underline{n}} - \sum_{j=0}^{\bar{n}_-} 2^j u_{j+(1+\underline{n}+\bar{n}_+)}.$$

Constraint (19b) is transformed as:

$$\mathbf{H}_1 = P_1\Big(\sum_{z \in \mathcal{Z}} x_{i,z,t} - 1\Big)^2, \forall i \in \mathcal{TK}, t \in \mathcal{T},$$

Constraint (19c) is transformed as:

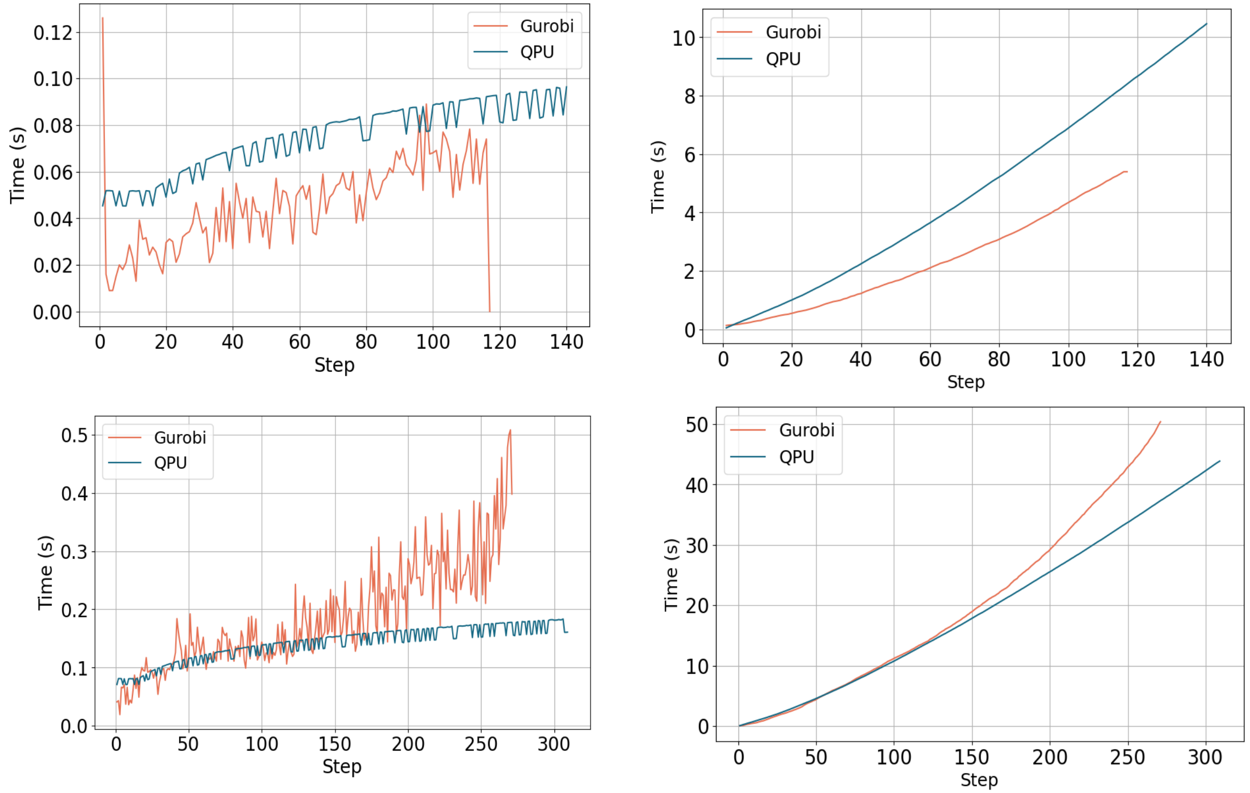
$$\mathbf{H}_2 = P_2\Big(\sum_{i \in \mathcal{TK}} x_{i,z,t} - NTK_{z,t} + s^1_{z,t}\Big)^2, \forall z \in \mathcal{Z}, t \in \mathcal{T},$$

Cuts (19d) and (19e) is transformed as

$$\mathbf{H}_3 = P_3\Big\{M^v \sum_{i:x_i^v=0} x_i + M^v \sum_{i:x_i^v=1} (1 - x_i) + \theta - d^\top y^v - s^2_{z,t}\Big\}^2$$

$$\mathbf{H}_4 = P_4\Big\{\sum_{i:x_i^v=0} x_i + \sum_{i:x_i^v=1} (1 - x_i) + \theta - 1 - s^3_{z,t}\Big\}^2.$$

Experiment Results

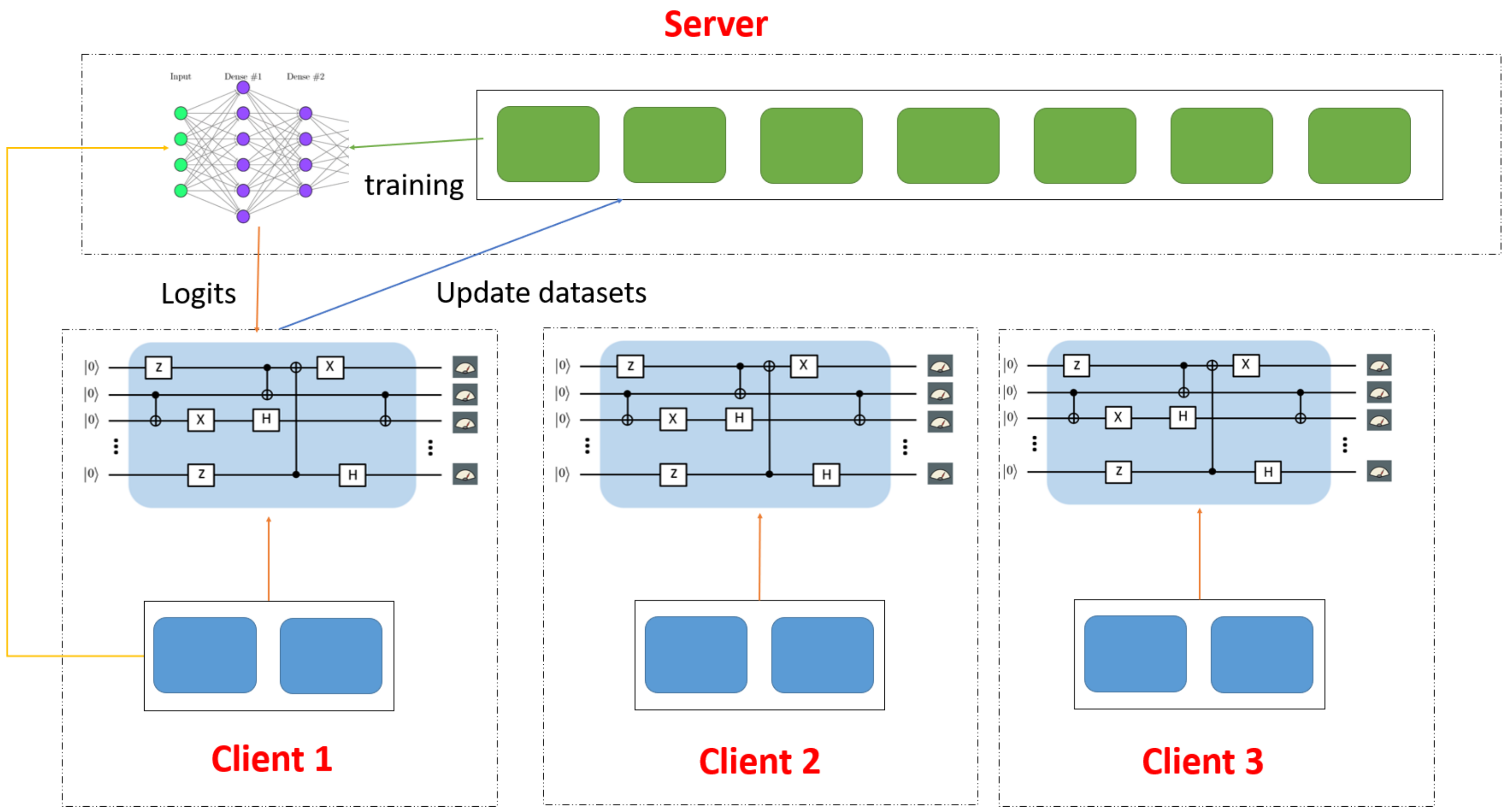


- Classical vs. Quantum
- Classical solver
  - ✓ Time consuming grows exponentially for each iteration
  - ✓ Quicker than quantum when the problem size is small
- Quantum annealer solver
  - ✓ Time consuming grows asymptotic linearly
  - ✓ Quicker than classical when the problem size is large

Content

- Motivation and Quantum Theory
- Application I: Quantum Assisted Combinatorial Benders' Algorithm for the Synergy of Hydrogen and Power Distribution Systems with Mobile Storage
- **Application II: Hybrid Quantum Classical Machine Learning with Knowledge Distillation**
- Application III: Quantum Hamiltonian Decent based Augmented Lagrangian Method for Constrained Nonconvex Nonlinear Optimization
- Conclusions and Future Work

Distributed Deep Learning



Advantage:

– QML performs better than the classical NN under the same level of number of parameters

Disadvantage:

– The available qubits of Quantum computer are limited
– Quantum computing is unstable, easy to lose information during measurement

Quantum Knowledge Distillation

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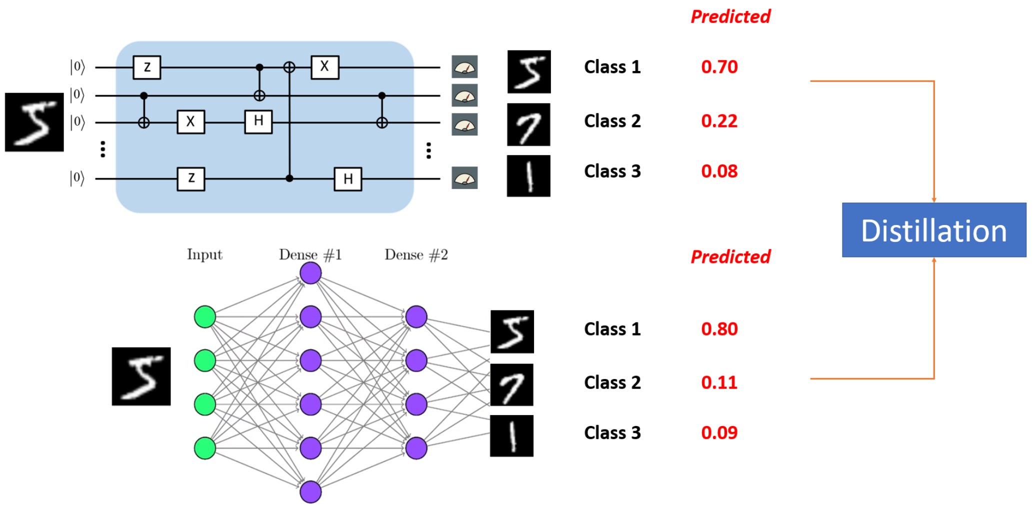


$T \to 0$ Less Attention on very negative logits

Student Loss

$$\mathcal{L}^C(y, \hat{y}) = -\sum_i y_i \log(\hat{y}_i),$$

Distilation Loss

$$\mathcal{L}_g^{KD} = -\tau^2 \sum_i KL(p_T^i, p_S^i).$$

Final Loss

$$\mathcal{L} = \alpha \mathcal{L}^C + (1-\alpha)\mathcal{L}_g^{KD}$$

$$y_i = 1(z_i = \max z_j)$$

↑ $T \to 0$

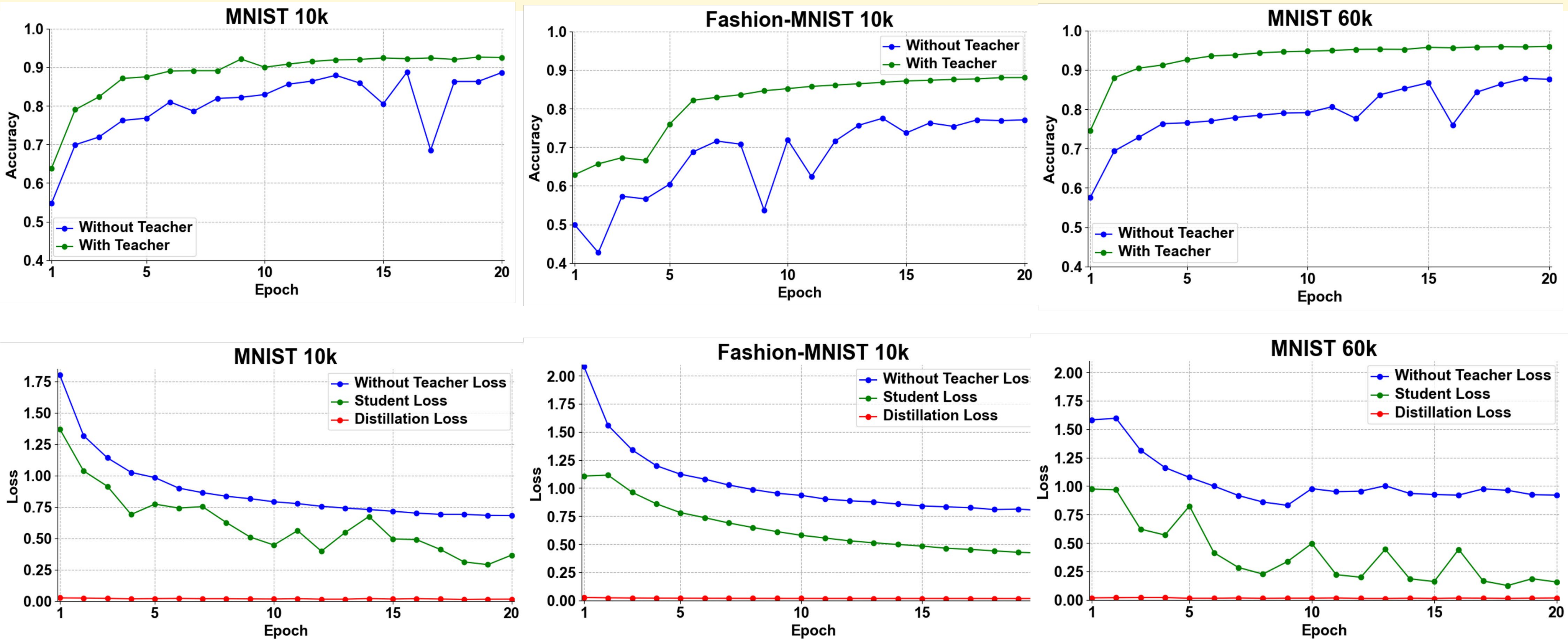
$$y_i = \frac{e^{(z_i/T)}}{\sum_j e^{(z_j/T)}}$$

↓ $T \to +\infty$

$$y_i = \frac{1}{J}$$

	Student	Teacher
Softmax with temperature (soft predictions)	$p = [0.25, 0.85\ \ldots\ 0.14]$	$q = [0.35, 0.92\ \ldots\ 0.1]$
Hard predictions	$p_{stu} = [0,1,0\ \ldots, 0]$	
Distillation Loss	$\text{CrossEntropy}(p, q)$	
Student Loss	$\text{CrossEntropy}(p_{stu}, y_{\text{true}})$	
Final Loss	$\alpha \cdot$ Student Loss $+ (1-\alpha) \cdot$ Distillation Loss	

Quantum Knowledge Distillation



Our approach can not only enhance the performance of inherently resource-constrained QNN but also increase the stability of the training process.

Content

- Motivation and Quantum Theory
- Application I: Quantum Assisted Combinatorial Benders' Algorithm for the Synergy of Hydrogen and Power Distribution Systems with Mobile Storage
- Application II: Hybrid Quantum Classical Machine Learning with Knowledge Distillation
- **Application III: Quantum Hamiltonian Decent based Augmented Lagrangian Method for Constrained Nonconvex Nonlinear Optimization**
- Conclusions and Future Work

Motivation of Work III

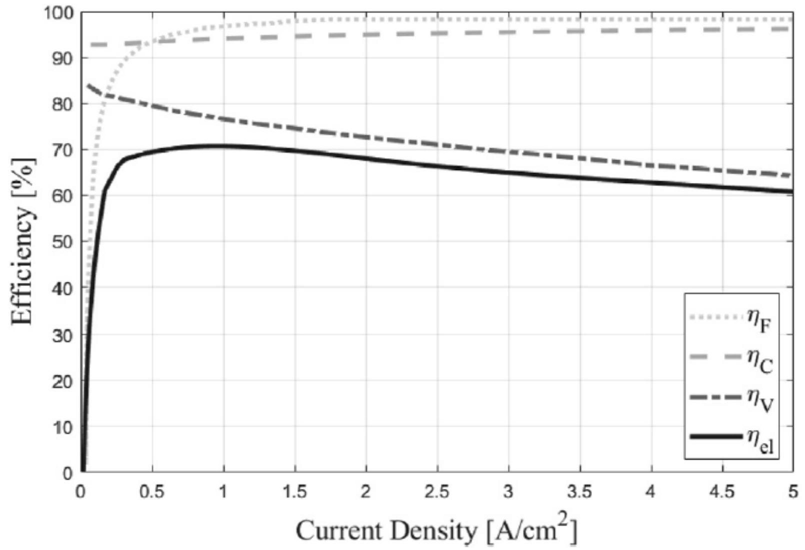
Current Electrolyzor Design

- Joint Planning of Power-to-hydrogen

  Find the minimum cost and satisfy demand by produce hydrogen by electricity via electrolyzor

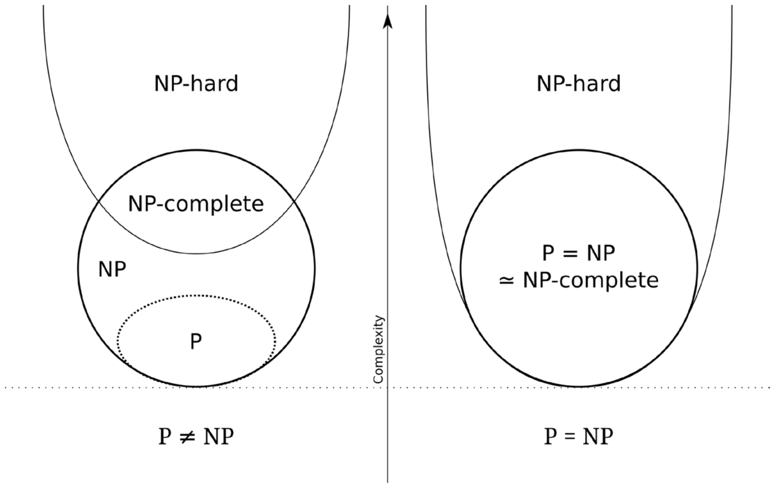
- Dynamic efficiency of electrolyzor [2]

  The efficiency of electrolyzor is affected by temperature and current density, with a nonlinear & nonconvex function



Problems

- Classical algorithms can only ensure local convergence for nonconvex problems
- The power balance equivalent function also increase difficulty to solve



[2] Benjamin Flamm, Christian Peter, Felix N. Büchi, John Lygeros, Electrolyzer modeling and real-time control for optimized production of hydrogen gas, Applied Energy, Volume 281, 2021, 116031, ISSN 0306-2619.

QHD Assisted Hydrogen System

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Detailed Formulation

$$\max C^{\text{hyo}}(e_N - e_0) - \sum_{t=0}^{N-1} C_t^{\text{power}} p_t^{\text{grid}},$$ maximize the total surplus

$$\text{s.t. } p_t^{\text{grid}} + p_t^{\text{Re}} = m^{\text{AC}} p_t^{\text{el}} + k^{\text{AC}},$$ Power transformation

$$e_{t+1} = e_t + e_t^{\text{el}} - E_t^{\text{d}},$$ Balance of hydrogen storage

$$E^{\min} \le e_t \le E^{\max},$$ Storage limit

$$0 \le p_t^{\text{el}} \le P^{\text{C,max}},$$ Power limit

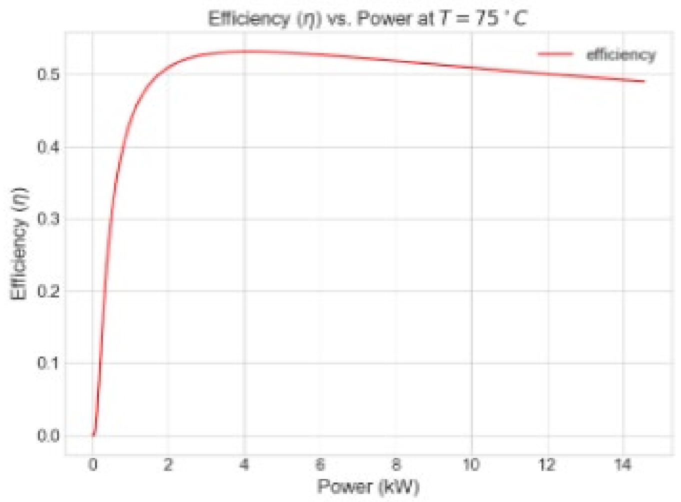
$$p_t^{\text{grid}} \ge 0,$$

$$e_t^{\text{el}} = \Delta t \cdot \frac{p_t^{\text{el}}}{HHV_{H_2}} \cdot \eta_{el}, \quad e_t^{\text{el}} \ge 0.$$

Production of electrolyzor

$$\eta_f = \text{B}_1 + \text{B}_2 \cdot \exp\left[\frac{\text{B}_3 + \text{B}_4 \cdot T + \text{B}_5 \cdot T^2}{I_{cell}}\right],$$

$$V_{cell} = V_{\text{rev}} + [(r_1 + d_1) + r_2 \cdot T + d_2 \cdot p] \cdot i + s \cdot \log\left[\left(t_1 + \frac{t_2}{T} + \frac{t_3}{T^2}\right) \cdot I_{cell} + 1\right].$$

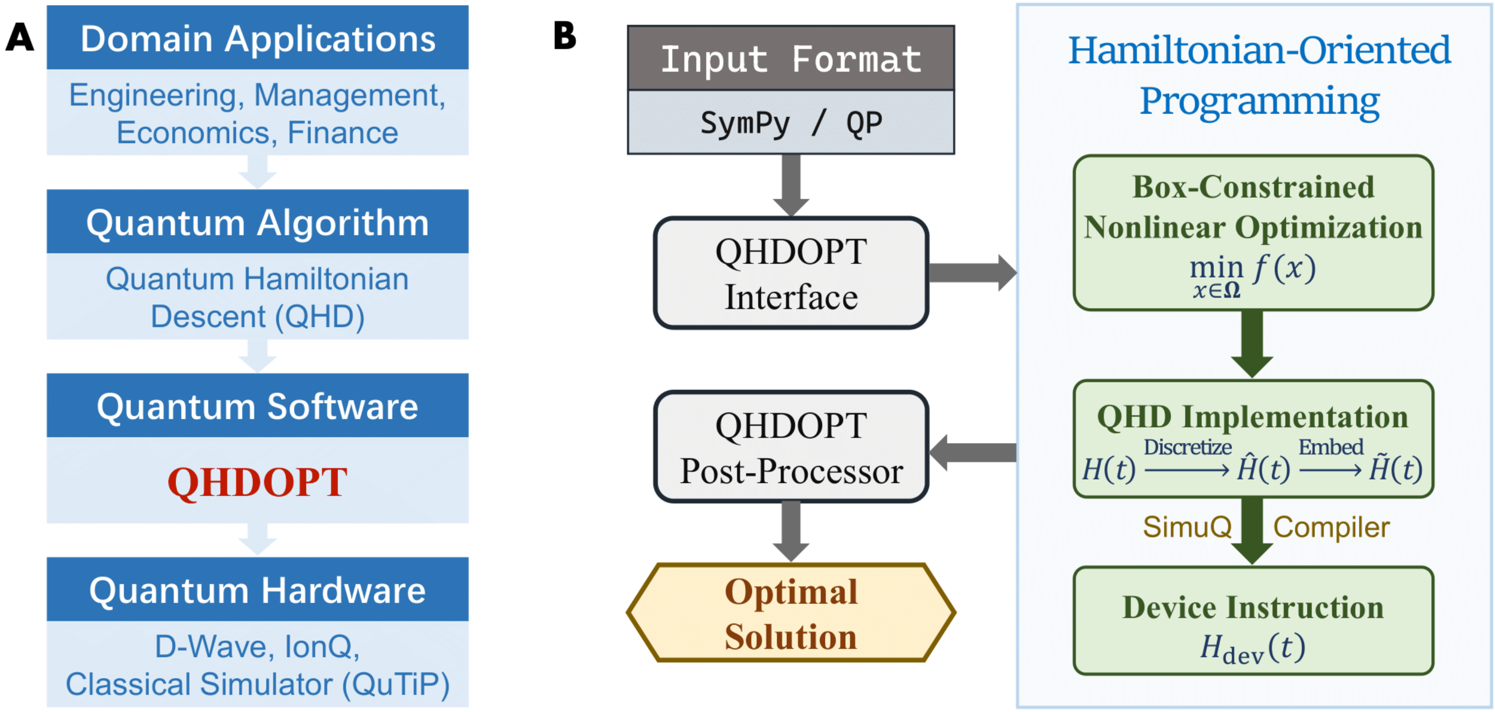


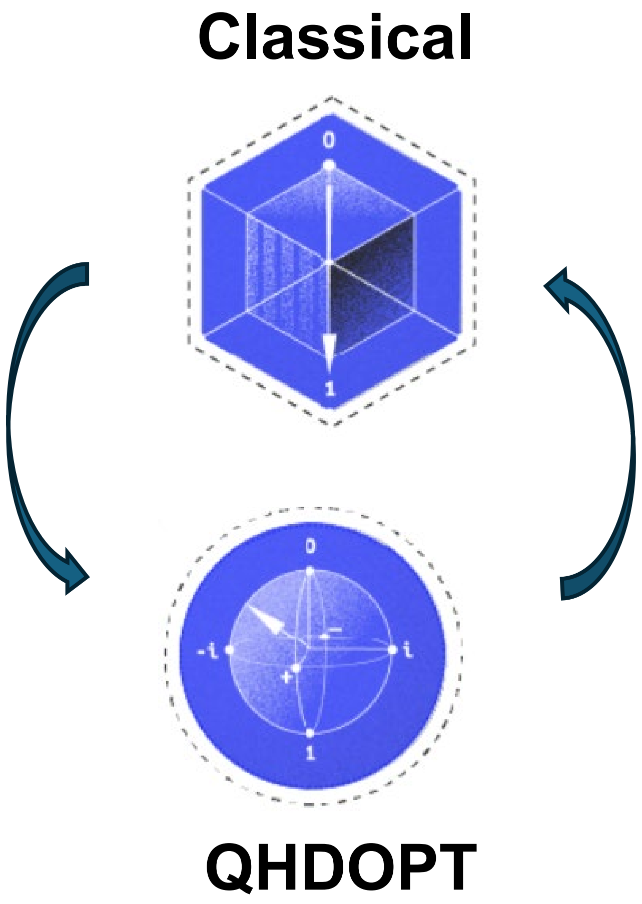
$$\eta_{el} \le a_1 + a_2 \cdot P^{\text{C,max}} + a_3 \cdot \exp\left(a_4 \cdot (100 \cdot p_t^{\text{el}} / P^{\text{C,max}})\right),$$

$$\eta_{el} \le \left(B_1 + B_2 \cdot \exp\left(\frac{B_3 + B_4 T + B_5 T^2}{\bar{I}_{cell}}\right)\right) / \bar{U}_{cell}.$$

Quantum Hamiltonian Descent-based OPTimizer (QHDOPT)

- QHDOPT is an open-source optimization solver that implements QHD to solve continuous NLP problems with box-constraints [3][4][5]
- Utilize QHDOPT to solve continuous problem





[3] J. Leng, J. Li, Y. Peng, and X. Wu, “Expanding Hardware-Efficiently manipulable Hilbert space via Hamiltonian embedding,” Jan. 2024.[Online].
[4] J. Leng, Y. Zheng, Z. Jia, L. Fan, C. Zhao, Y. Peng, and X. Wu, “Quantum Hamiltonian descent for non-smooth optimization,” Mar.2025. [Online].
[5] S. Kushnir, J. Leng, Y. Peng, L. Fan, and X. Wu, “QHDOPT: Asoftware for nonlinear optimization with quantum Hamiltonian descent,” INFORMS Journal on Computing, vol. 37, no. 1, pp. 107–124, Nov.2024.

Quantum Hamiltonian Descent-based OPTimizer (QHDOPT)

- With box constraints: $L_i \leq x_i \leq U_i, \quad \forall i = 1, \ldots, n$
- QHDOPT is designed to handle optimization problems of the form:

$$\min_{x \in \mathbb{R}^n} f(x) = \sum_{i=1}^{n} g_i(x_i) + \sum_{j=1}^{m} p_j(x_{k_j}) q_j(x_{\ell_j})$$

Univariate terms: $g_i(x_i)$

Bivariate terms: $p_j(x_{k_j}) q_j(x_{\ell_j})$

Quantum Annealing only for **BINARY** problems

- QHDOPT allows these constraints to be incorporated via penalty methods, making it flexible for a wide range of applications

Spatial Discretization

Encode the objective function into the Hamiltonian

Laplacian operator

$$H(t) = e^{\varphi t}\left(-\frac{1}{2}\Delta\right) + e^{\chi t} f(x),$$

Time-dependent scaling factors

QHDOPT applies spatial discretization to represent the continuous wavefunction over a finite grid:

$$\hat{H}(t) = e^{\varphi_t}\left(-\frac{1}{2}L_d\right) + e^{\chi_t} F_d$$

$$L_d = \sum_{i=1}^{n} I \otimes \cdots \otimes L \otimes D(g_i) \otimes \ldots I,$$

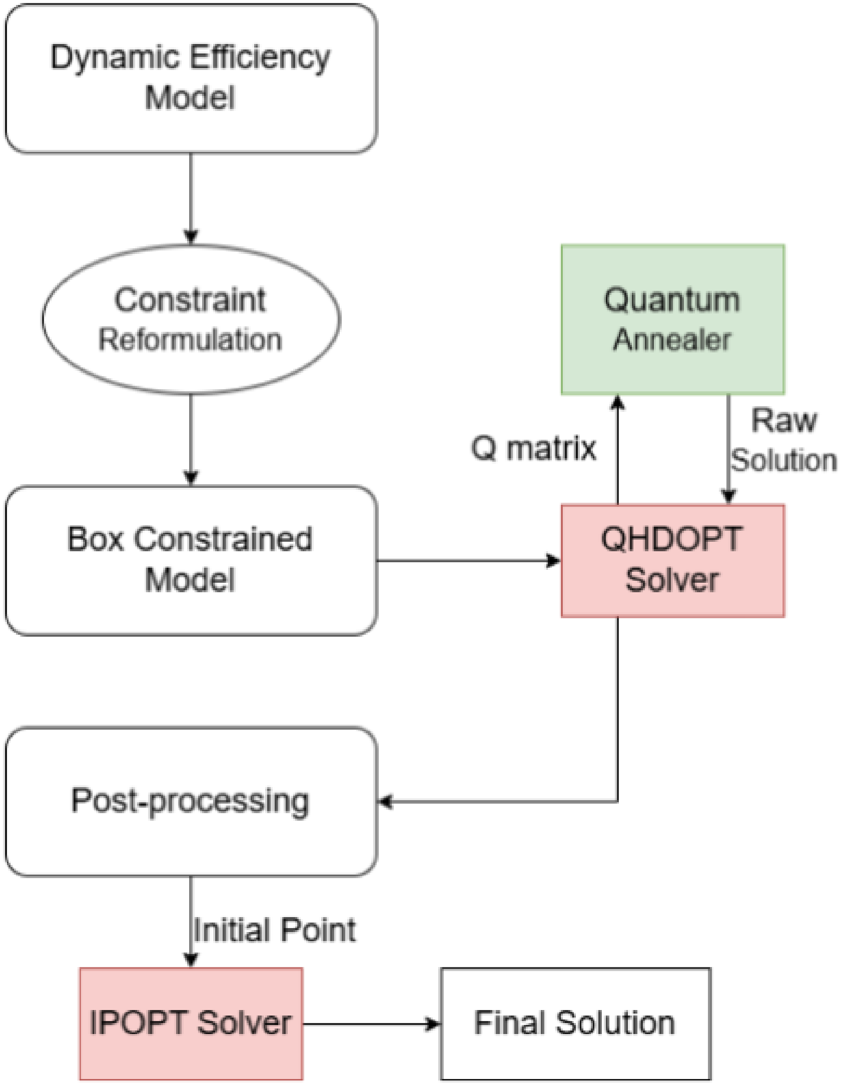
$$F_d = \sum_{i=1}^{n} I \otimes \cdots \otimes D(p_j) \otimes \sum_{j=1}^{m} I \otimes \cdots \otimes D(q_j) \otimes \ldots I.$$

I : N-dimensional identity operator
L, *D*: N-dimensional matrices

$$E(s) = \sum_{i<j} J_{ij} s_i s_j + \sum_i h_i s_i,$$

Now we can use quantum annealer

QUBO Transformation



Transform constraints to penalty terms in objective function

$$P_1 = (a_1 + a_2 \cdot P^{\mathrm{C,max}} + a_3 \cdot \exp\left(a_4 \cdot (100 \cdot p_t^{\mathrm{el}} / P^{\mathrm{C,max}})\right) - \eta_{el} - s_1)^2,$$

$$P_2 = \left((B_1 + B_2 \cdot \exp(\tfrac{B_3 + B_4 T + B_5 T^2}{\bar{I}_{cell}}))/\bar{U}_{\mathrm{cell}} - \eta_{el} - s_2\right)^2.$$

Too complex, penalty decides EVERYTHING

Case Study

			Optimal Objective Value				Computation Time	
Case	Decision Variables	Constraints	Pure-IPOPT (\$)	QHD+IP OPT (\$)	QHD (\$)	IPOPT 1k Samples (\$)	IPOPT 1k time (ms)	QHD+IP OPT (ms)
1	9	6	-4.63	**345.64**	107.68	**345.64**	263,93	45.032
2	12	8	-5.33	**465.37**	139	**465.37**	283,22	47.324
3	15	10	-5.53	**587.76**	156.62	**587.76**	308,92	44.406
4	18	12	-6.87	609.46	185.33	**713.31**	323,82	48.596

- Table shows that the IPOPT can not find optimal value efficiently
- QHD can find a better value but need to adjust penalty

Nonlinear Programming

General format of NLP:

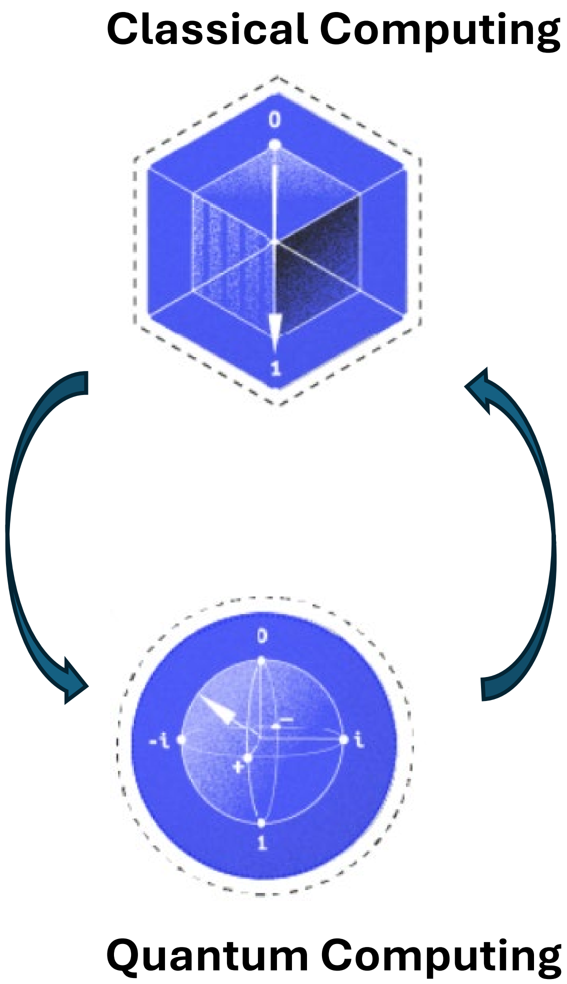
$$\min f(x) \quad \text{(Objective Function)}$$
$$s.t.\ g(x) = 0 \quad \text{(Equivalent Constraints)}$$
$$h(x) \le 0 \quad \text{(Inequivalent Constraints)}$$

- Large Scale NLP

  The objective function and constraints can be nonlinear and nonconvex, and the problem is usually large scale.

- Quantum Computing in NLP

  We propose a hybrid quantum Hamiltonian decent based Augmented Lagrangian Method for constrained optimization



Augmented Lagrangian Methods

Most quantum and quantum inspired algorithms are designed to solve unconstrainted or box-constrainted problems

$$\min f(x)$$
$$s.t.\ g(x) = 0$$
$$h(x) \leq 0$$

Add slack variables

$$\min f(x)$$
$$s.t.\ g(x) = 0$$
$$h(x) + s_j = 0$$

Augmented Lagrangian Functions

Lagrangian multipliers

$$\mathcal{L}_A(x, s, \lambda, \mu, \rho) = f(x) + \sum_{i \in \mathcal{E}} \lambda_i g_i(x) + \sum_{j \in \mathcal{I}} \mu_j (h_j(x) + s_j) + \sum_{i \in \mathcal{E}} \frac{\rho_i}{2} g_i(x)^2 + \sum_{j \in \mathcal{I}} \frac{\rho_j}{2} (h_j(x) + s_j)^2,$$

Penalty terms

Update multipliers

$$(x^{(k)}, s^{(k)}) = \arg\min_{x,s} \mathcal{L}_A(x, s, \lambda^{(k)}, \mu^{(k)}, \rho^{(k)}),$$

$$\lambda_i^{(k+1)} = \lambda_i^{(k)} + \rho_i^{(k)} g_i(x^{(k)}), \quad i \in \mathcal{E},$$
$$\mu_j^{(k+1)} = \mu_j^{(k)} + \rho_j^{(k)} (h_j(x^{(k)}) + s_j^{(k)}), \quad j \in \mathcal{I}.$$

Simulated Bifurcation

Ising Model:

$$E(s) = \sum_{i<j} J_{ij} s_i s_j + \sum_i h_i s_i,$$

Or

Quantum inspired algorithm

Each operator *a* is approximated by a complex amplitude $x_i + iy_i$

$$H_{\mathrm{SB}}(\mathbf{x}, \mathbf{y}, t) = \sum_{i=1}^{N} \frac{\Delta}{2} y_i^2 + \sum_{i=1}^{N} \left[\frac{K}{4} x_i^4 + \frac{\Delta - p(t)}{2} x_i^2 \right] - \frac{\xi_0}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} J_{ij} x_i x_j,$$

Quantum mechanical Hamiltonian

Kerr coefficient — amplitude — detuning

$$H_q(t) = \hbar \sum_{i=1}^{N} \left[\frac{K}{2} a_i^{\dagger 2} a_i^2 - \frac{p(t)}{2} (a_i^{\dagger 2} + a_i^2) + \Delta_i a_i^\dagger a_i \right] - \hbar \xi_0 \sum_{i=1}^{N} \sum_{j=1}^{N} J_{ij} a_i^\dagger a_j,$$

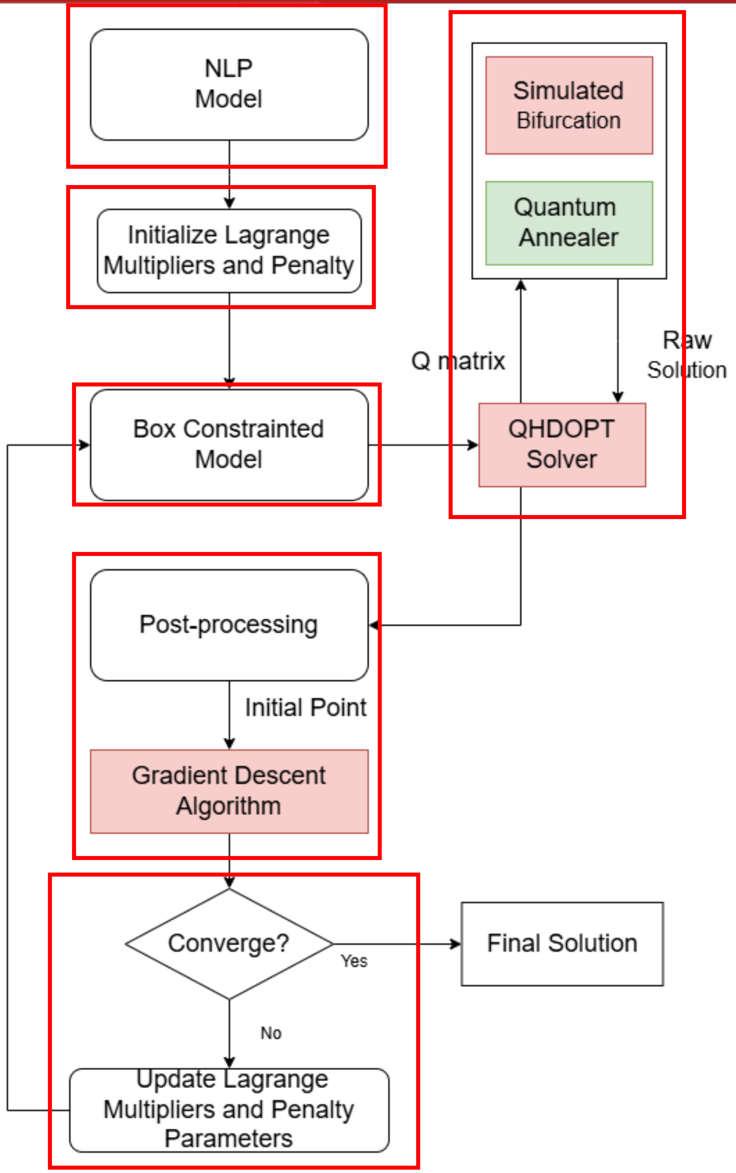
creation and annihilation operator

Update *x* and *y* by:

$$\dot{x}_i = \Delta y_i,$$

$$\dot{y}_i = -\left[K x_i^3 - (p(t) - \Delta) x_i + \xi_0 \sum_{j=1}^{N} J_{ij} x_j \right]$$

QHD-ALM



Algorithm 2 QHD-ALM Framework

Input: Nonlinear programming model with constraints
Step 1: Initialize
Set initial Lagrange multipliers $\lambda^{(0)}$ and penalty parameter $\rho^{(0)}$
Set iteration counter $k = 0$
repeat
    Step 2: Unconstrained Model Reformulation
    Construct the Augmented Lagrangian function:

$$\mathcal{L}(x, \lambda^{(k)}, \rho^{(k)}) = f(x) + \sum_i \lambda_i^{(k)} g_i(x) + \sum_i \frac{\rho_i^{(k)}}{2} g_i(x)^2$$

    Step 3: Solve with QHDOPT
    Formulate Q matrix from the unconstrained model
    Use QHDOPT with either Simulated Bifurcation or Quantum Annealer to obtain a raw solution
    Step 4: Post-processing
    Map the raw solution to original feasible space
    Use it as an initial point for IPOPT
    Step 5: Refinement with IPOPT
    Run IPOPT to solve the box constrained NLP from initial point
    Step 6: Check Convergence
    if convergence criteria is met **then**
        Output: Final solution
        Exit loop
    else
        Step 7: Update Parameters
        Update $\lambda^{(k+1)} = \lambda^{(k)} + \rho^{(k)} g(x)$
        Increase penalty $\rho^{(k+1)} > \rho^{(k)}$
        $k \leftarrow k + 1$
    end if
until convergence is achieved

QHD-ALM

$$\max\ C^{\text{hyo}}(e_N - e_0) - \sum_{t=0}^{N-1} C_t^{\text{power}} p_t^{\text{grid}},$$

$$\text{s.t.}\ p_t^{\text{grid}} + p_t^{\text{Re}} = m^{\text{AC}} p_t^{\text{el}} + k^{\text{AC}},$$

$$e_{t+1} = e_t + e_t^{\text{el}} - E_t^{\text{d}},$$

$$E^{\min} \le e_t \le E^{\max},$$

$$0 \le p_t^{\text{el}} \le P^{\text{C,max}},$$

$$p_t^{\text{grid}} \ge 0,$$

$$e_t^{\text{el}} = \Delta t \cdot \frac{p_t^{\text{el}}}{HHV_{H_2}} \cdot \eta_{el}, \quad e_t^{\text{el}} \ge 0.$$

ALM

$$\mathcal{L}_A = -C^{\text{hyo}}(e_N - e_0) + \sum_{t=0}^{N-1} C_t^{\text{power}} p_t^{\text{grid}}$$
$$+ \sum_{t=0}^{N-1} \lambda_{1,t} g_{1,t}(x) + \frac{\rho_1}{2} g_{1,t}(x)^2$$
$$+ \sum_{t=0}^{N-1} \mu_t (h_{1,t}(x) + s_{1,t}) + \frac{\rho_2}{2}(h_{1,t}(x) + s_{1,t})^2$$
$$+ \sum_{t=0}^{N-1} \mu_t (h_{2,t}(x) + s_{2,t}) + \frac{\rho_3}{2}(h_{2,t}(x) + s_{2,t})^2,$$

Subject to:

$$0 \le p_t^{\text{el}} \le P^{\text{C,max}}, E^{\min} \le e_t \le E^{\max}, p_t^{\text{grid}} \ge 0,$$

$$0 \le \eta_t \le 100, s_{1,t} \ge 0.$$

Case Study

Optimal Objective Value of Different Methods

Case	Pure-IPOPT ($)	IPOPT 1k Samples ($)	ALM ($)	QHD-ALM ($)
1	6.42	892.06	6.42	893.8
2	6.33	2312.92	6.33	2333.4
3	-760.23	14153.52	10124.05	13877
4	3040.31	19368.54	17423.74	18840.1

Computation Time of Different Methods

Case	Pure-IPOPT	IPOPT 1k Samples	ALM	QHD-ALM
1	0.089s	73s	1.31s	6.82s
2	0.289s	257s	3.18s	11.28s
3	1.767s	16 min	61.1s	78.2s
4	3.184s	52 min	351.58s	369.38s

- QHD-ALM achieves better solution when facing nonconvex problems than classical solver
- IPOPT 1k achieves best solution but cost much time
- Single IPOPT can not find the optimal solution

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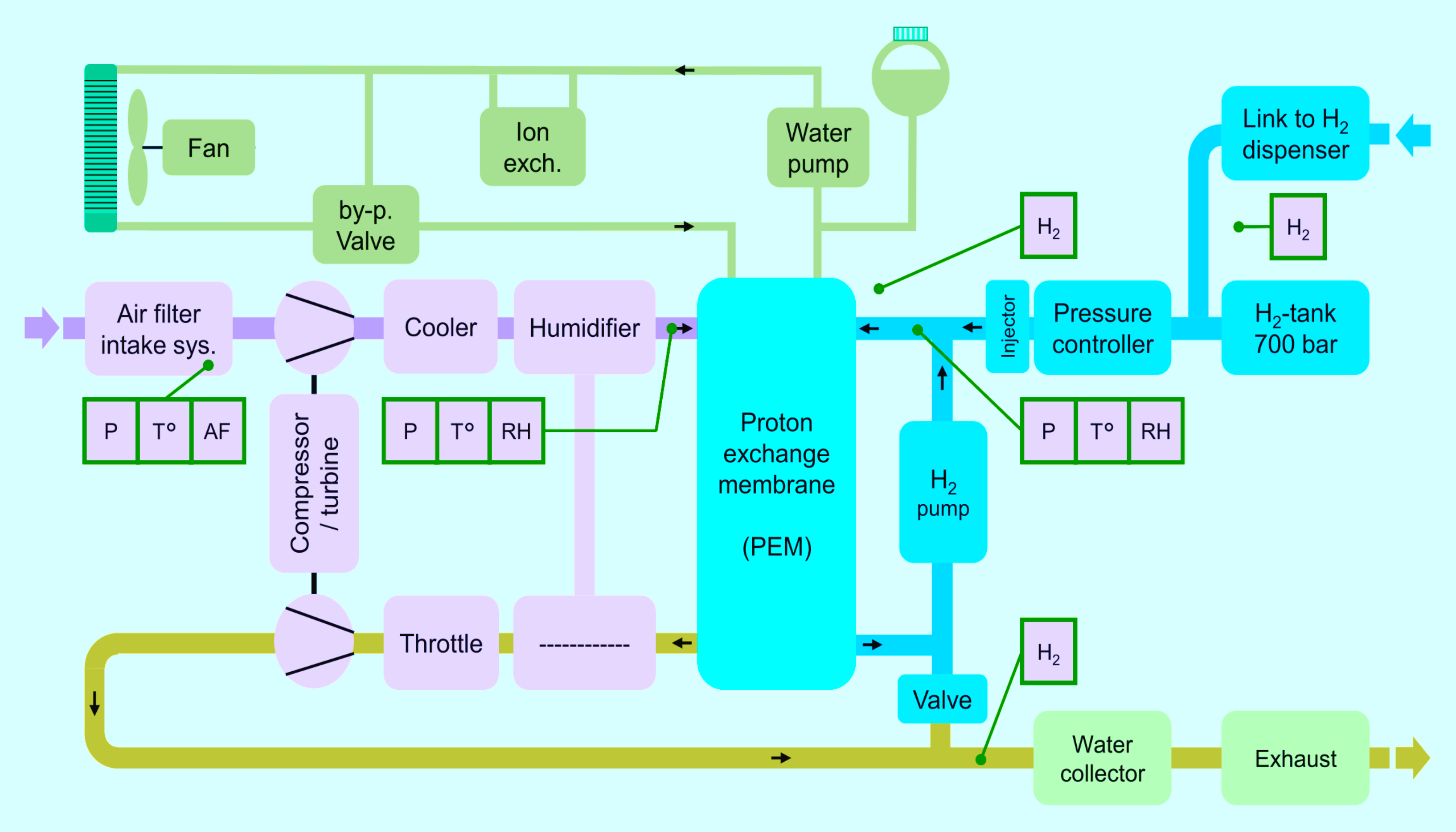
- **Conclusions and Future Work**

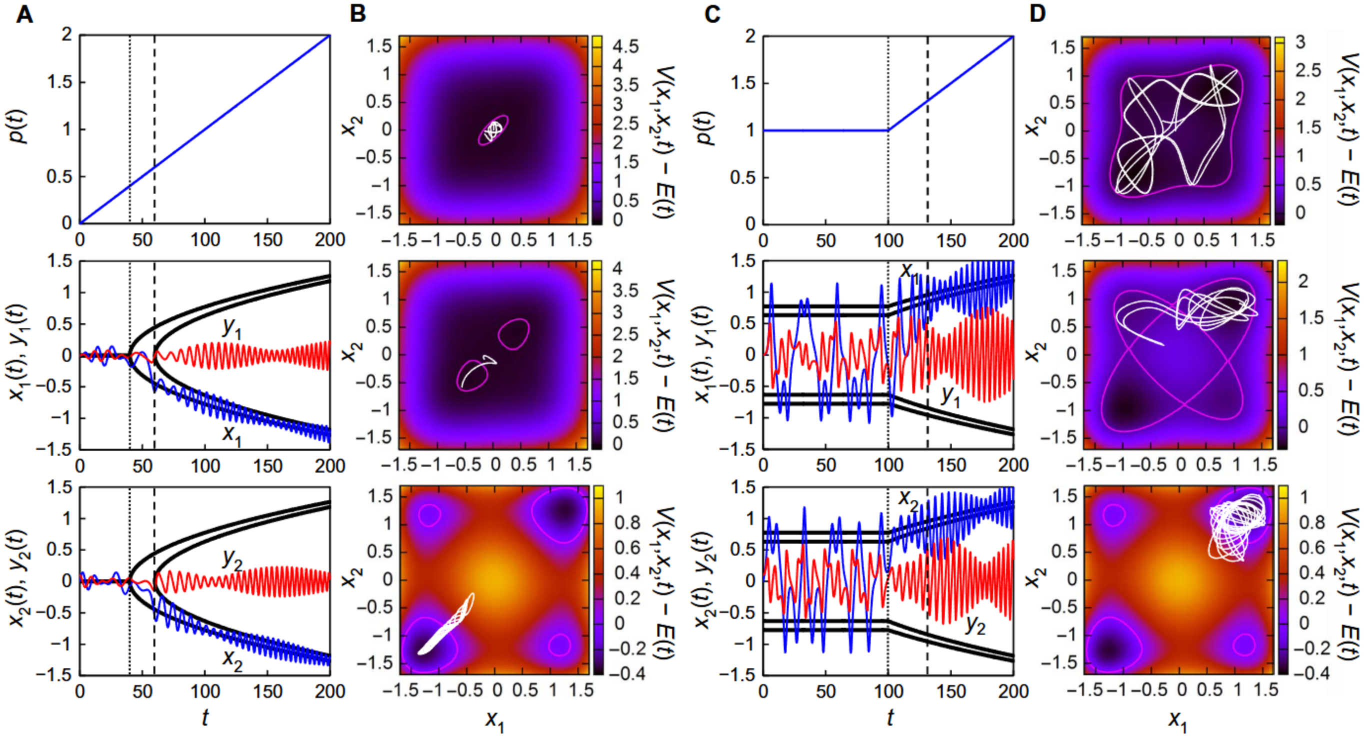
Future Work - I



1. Investigate a more complex electrolyzor model.
2. Investigate a large-scale power-to-hydrogen
3. Add the temperature variation into the modeling

Future Work - II

1. Develop different descent methods for Ising model.



2. Expand ALM-QHD to broader form of NLP

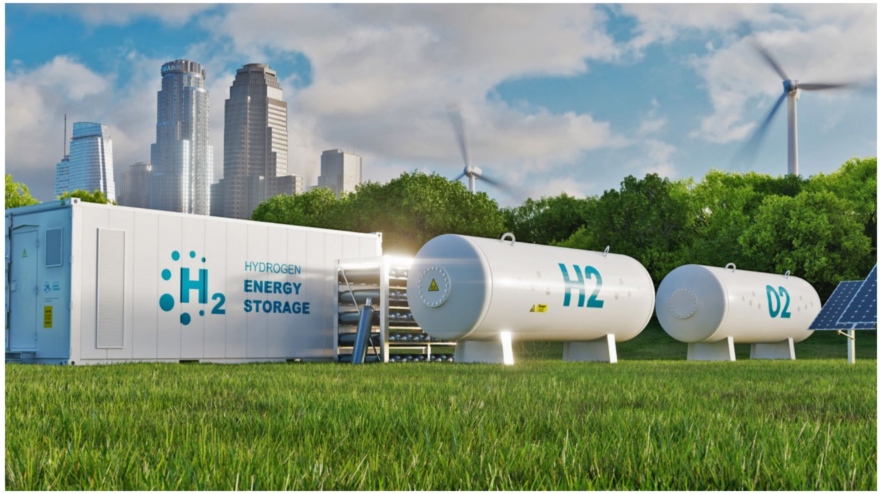
$$\min_{x\in\mathbb{R}^n} f(x) = \sum_{i=1}^{n} g_i(x_i) + \sum_{j=1}^{m} p_j(x_{k_j})q_j(x_{\ell_j})$$

↓

High-order formulations

Conclusion

- We developed a mixed-binary nonlinear programming (MBNLP) model for a hydrogen system integrated with a truck transportation network.
- To solve the MBNLP, we designed a Quantum Assisted Combinatorial Benders' Algorithm, using a quantum annealer for the binary master problem.
- Our latest advancement enhanced the electrolyzor model and employed QHDOPT to efficiently solve the resulting nonlinear problem using Quantum Hamiltonian Descent.



References

Published paper

Conferences

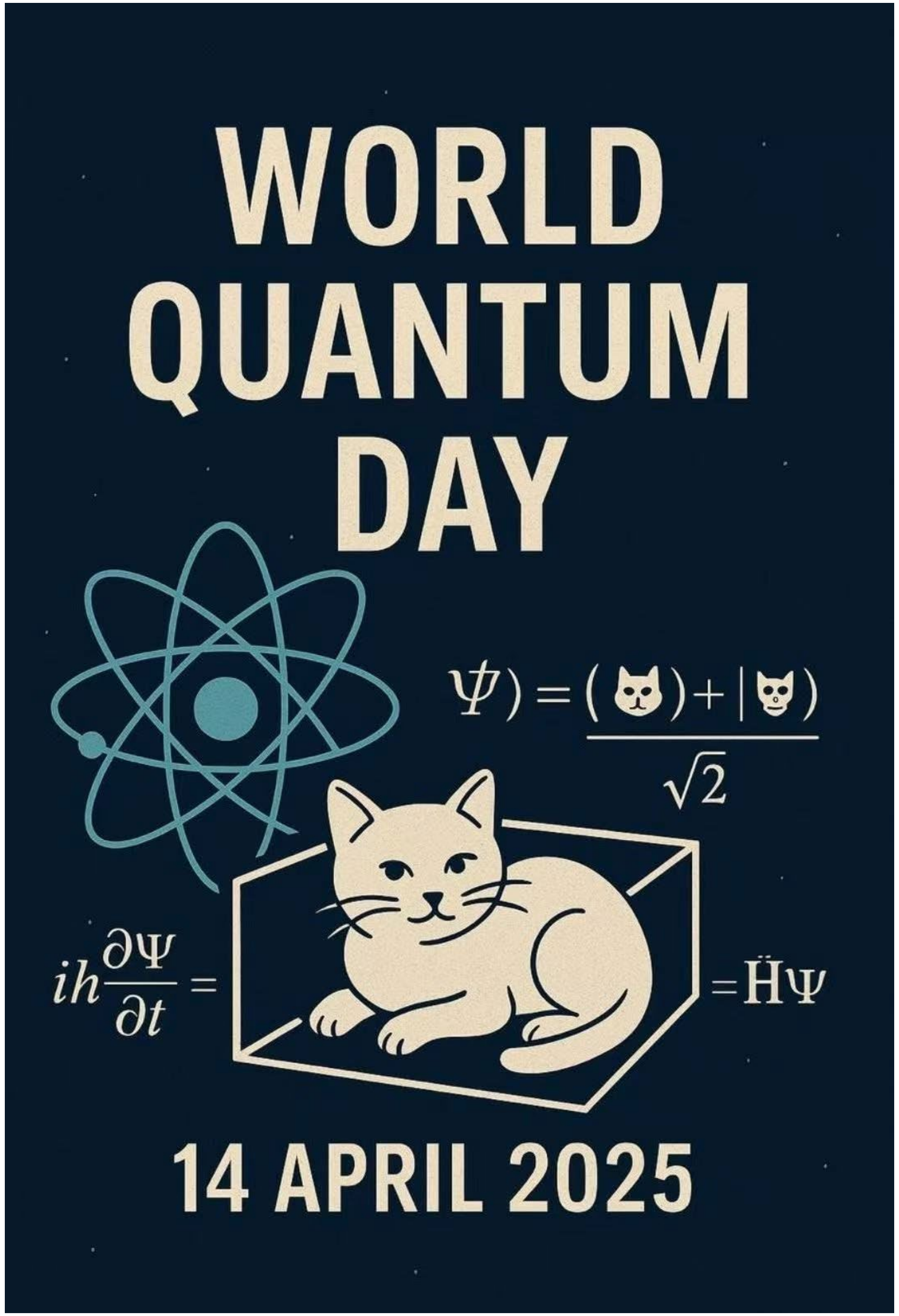
1. "Hybrid Quantum Classical Machine Learning with Knowledge Distillation", ICC 2024 - IEEE International Conference on Communications, Mingze Li, Lei Fan, Aaron Cummings, Xinyue Zhang, Miao Pan, and Zhu Han.
2. "A Generic Mixed-Integer Linear Model for Optimal Planning of Multi-Energy Hub",2023 North American Power Symposium (NAPS), Mingze Li, Siyuan Wang, Lei Fan, Jian Shi and Zhu Han.
3. "Coordinated Operations of Hydrogen and Power Distribution Systems", 2023 IEEE Power & Energy Society Innovative Smart Grid Technologies Conference (ISGT),Mingze Li, Siyuan Wang, Lei Fan, and Zhu Han
4. "A Quantum Feature Selection Method for Network Intrusion Detection," 2022 IEEE 19th International Conference on Mobile Ad Hoc and Smart Systems (MASS), Mingze Li, Hongliang Zhang, Lei Fan, and Zhu Han.
5. "Electricity Price Forecasting Enhancement Using Combined Model", 2024 North American Power Symposium , Eric Lu, Mingze Li.
6. "A Preprocessing Method for Security-Constrained Unit Commitment with AC Power Flows", IEEE Texas Power and Energy Conference, Mingze Li, Weihang Zhu, Lei Fan, Zhu Han.
7. "Integrated Quantum Hamiltonian Descent with Interior Point Method for Optimal Schedule of Hybrid Electricity-to-Hydrogen System", IEEE Kansas Power and Energy Conference, Mingze Li, Siyuan Wang, Lei Fan, and Zhu Han.

Journal

1. "Quantum Assisted Combinatorial Benders' Algorithm for the Synergy of Hydrogen and Power Distribution Systems with Mobile Storage", IEEE Transactions on Power System, Mingze Li, Siyuan Wang, Lei Fan, and Zhu Han.

Submitted paper

1. "Quantum Hamiltonian Decent based Augmented Lagrangian Method for Constrained Nonconvex Nonlinear Optimization", IEEE International Conference on Quantum Computing and Engineering, Mingze Li, Lei Fan, and Zhu Han



Thank you

Q & A