

# Scalable Quantum Chemistry Simulation Using **DMET-VQE Framework with CUDAQ**

2024 NCHC Open Hackathon

Team 7 **NoLab**

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# Motivation



# Variational Quantum Eigensolver (VQE)

A powerful approach for simulating molecules and materials in the NISQ era.

## Energy Expectation Value

$$E(\theta) = \langle \psi(\theta) | H | \psi(\theta) \rangle$$

## Variation Principle

$$E_0 = \text{minimize} E(\theta)$$

# Challenge

## Real Quantum Computer

- Limited by noise, scalability, and measurement overhead.

## Simulation Challenges

- As qubit count increases, simulation complexity grows **exponentially**, making large systems challenging
- Examples:
  - **H<sub>2</sub> (4 qubits)** Easily simulable.
  - **H<sub>10</sub> (20 qubits)** Challenging for classical simulators.

## DMET iteration

Split molecular into  
different fragment

Use VQE compute the  
energy of each fragment

Compute total energy

# Our Approach

## GPU simulation via CUDA-Quantum

- Single-GPU simulation
- Multi-GPU simulation

## Density Matrix Embedding Theory (DMET)

Calculate the molecular **partially**

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**How Many  
Times We  
Speed Up**



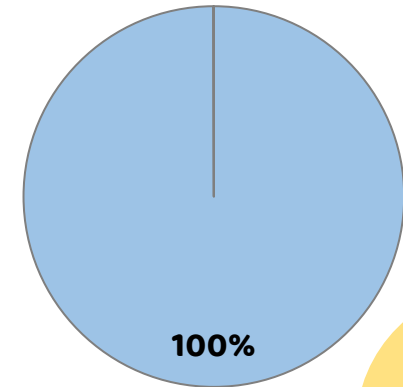
# Profiling (CPU)

	Total Time (sec.)	Each Iteration Time (sec.)
H <sub>2</sub> (4)	2658.8	8.1
H <sub>2</sub> O (14)	168225.3	841.2
CH <sub>4</sub> (18)	2037372.6	10186.8
H <sub>10</sub> (20)	3264852.7	16324.2
C <sub>2</sub> H <sub>6</sub> (32)	CAN'T RUN	CAN'T RUN

Blue: estimated time

## H<sub>2</sub> PROFILING

- Quantum Simulation
- Others



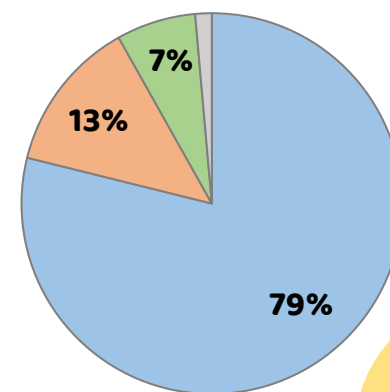
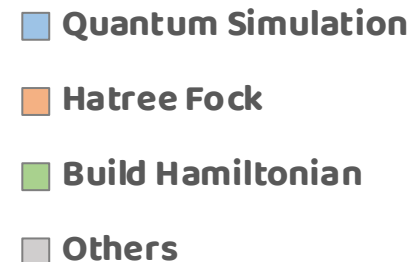
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# Profiling (Single-GPU)

	Total Time (sec.)	Each Iteration Time (sec.)
<b>H<sub>2</sub> (4)</b>	17.598	0.098
<b>H<sub>2</sub>O (14)</b>	497.401	2.487
<b>CH<sub>4</sub> (18)</b>	5518.200	27.591
<b>H<sub>10</sub> (20)</b>	11801.014	59.005
<b>C<sub>2</sub>H<sub>6</sub> (32)</b>	CAN'T RUN	CAN'T RUN

## H<sub>2</sub> PROFILING

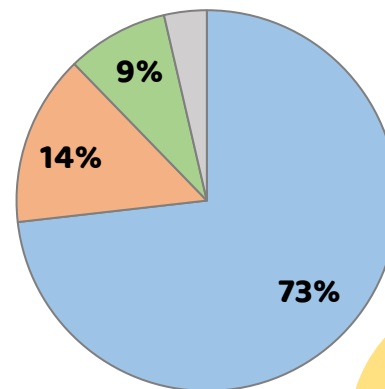
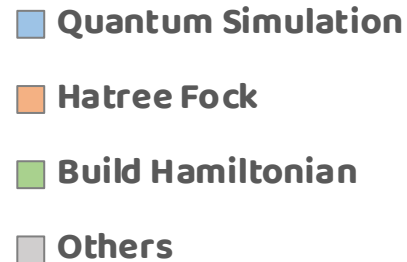


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# Profiling (Multi-GPU)

	Total Time (sec.)	Each Iteration Time (sec.)
<b>H<sub>2</sub> (4)</b>	12.784	0.065
<b>H<sub>2</sub>O (14)</b>	335.008	1.675
<b>CH<sub>4</sub> (18)</b>	4399.789	21.999
<b>H<sub>10</sub> (20)</b>	9868.743	49.344
<b>C<sub>2</sub>H<sub>6</sub> (32)</b>	CAN'T RUN	CAN'T RUN

## H<sub>2</sub> PROFILING



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# Profiling Tables

	CPU (sec.)	Single-GPU (sec.)	Multi-GPU (sec.)	Speed Up
<b>H<sub>2</sub> (4)</b>	8.165	0.098	0.065	125x
<b>H<sub>2</sub>O (14)</b>	841.275	2.487	1.675	502x
<b>CH<sub>4</sub> (18)</b>	10186.863	27.591	21.999	463x
<b>H<sub>10</sub> (20)</b>	16324.244	59.005	49.344	330x
<b>C<sub>2</sub>H<sub>6</sub> (32)</b>	CAN'T RUN	CAN'T RUN	CAN'T RUN	CAN'T RUN

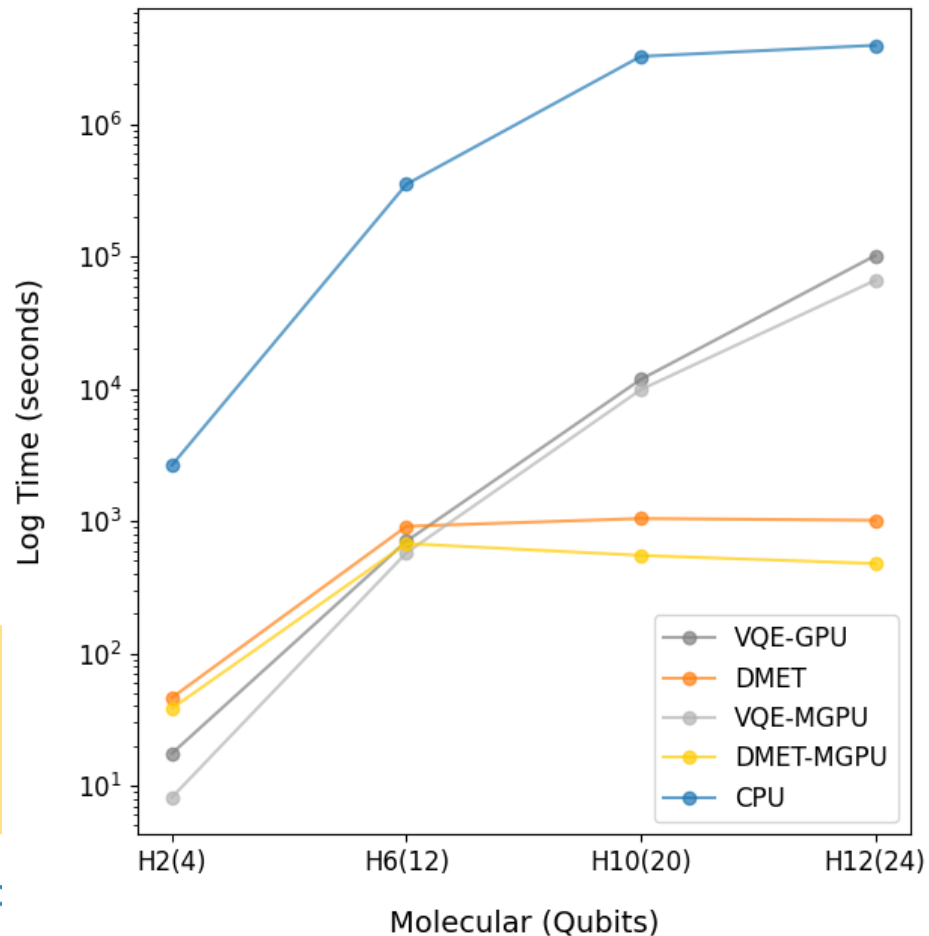
# DMET Profiling (Single-GPU)

	Total Time (sec.)	Each <b>DMET</b> Iteration Time (sec.)	Number of DMET iterations
<b>H<sub>2</sub>O (14)</b>	12370.513	1767.216	7
<b>CH<sub>4</sub> (18)</b>	11149.755	2229.950	5
<b>H<sub>10</sub> (20)</b>	1047.118	87.260	12
<b>H<sub>12</sub> (24)</b>	1015.835	101.584	10
<b>C<sub>2</sub>H<sub>6</sub> (32)</b>	83968.001	6997.333	12

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# Time Comparison

Total Time Comparison

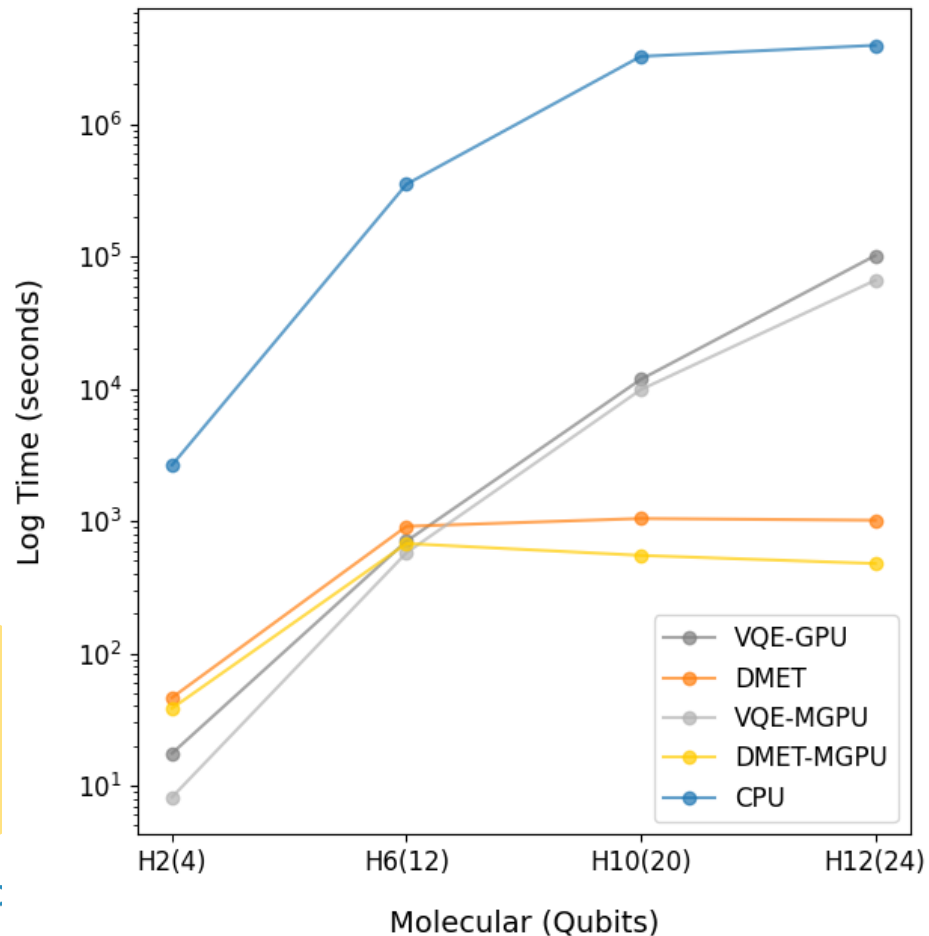


	VQE-GPU	DMET	VQE-MGPU	DMET-MGPU
<b>H<sub>2</sub> (4)</b>	151X	57X	324X	69X
<b>H<sub>6</sub> (12)</b>	499X	385X	611X	520X
<b>H<sub>10</sub> (20)</b>	277X	3118X	330X	5925X
<b>H<sub>12</sub> (24)</b>	39X	3898X	60X	<b>8282X</b>

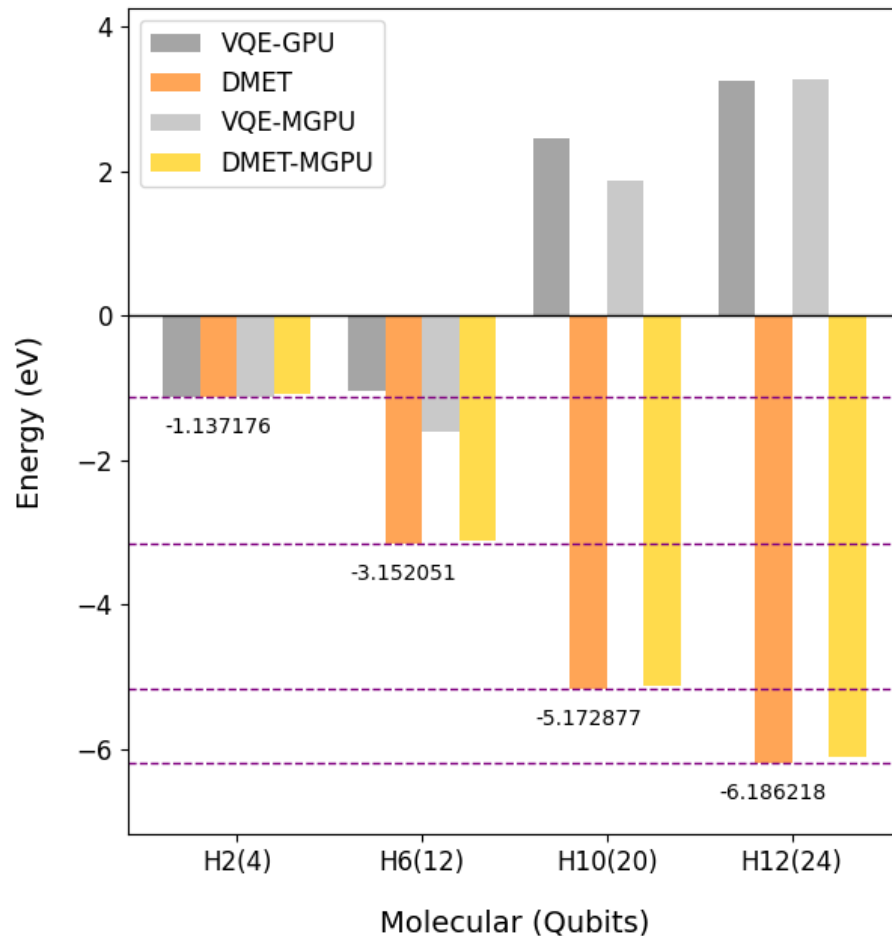
The acceleration factor is estimated, the actual speed up will be greater

# Time Comparison

## Total Time Comparison



## Energy Convergence Comparison



# Power Efficiency

	AMD Dual Rome 7742	3x A100 40GB	Power Savings
Compute Power (W)	189,796	6,500	183,296
Networking Power (W)	8,012	93	7,919
Total Power (W)	197,808	6,593	191,215
Compute Power (W)	189,796	6,500	183,296

**1188**

Metric tons of CO<sub>2</sub>



**256**

Gasoline cars driven for a year



**19632**

Trees growing for 10 years

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# DMET Benifit

- For large molecules, it can **accelerate convergence** to **accurate energy**.
- It enables rapid computation for a number of **qubits exceeding the GPU limit**.
- The computation time is lower, and the convergence effect is better.



# **Additional Highlights**

# Packages

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Cuda-Quantum

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OpenQemist (**Our Modified Version**)

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Qsharp

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Qiskit

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## Contribution to the community

- Bridged the CUDA-Q kernel to the OpenQEMIST package (DMET).
- Rewrote code to make it compatible with modern versions of packages.



# Problems encountered

1. Lack of rigorous comparison units due to constraints in computational resources, memory, and time.
2. Can't split one GPU into MQPU for some molecules. It would raise a memory error.

# Contribution

- **Enhanced scalability:** DMET-VQE surpasses the 32-orbital limit, simulating larger systems based on GPU resources.
- **CUDAQ-based DMET-VQE:** Facilitated systematic molecular comparisons, improving calculation accuracy and flexibility.
- Multi-GPU acceleration: Leveraged MGPU architectures for **scalable DMET-VQE** in high-dimensional systems.
- We shortened a **46-day task to just 17 minutes.**

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- DMET divides based on **orbitals** and the number of **qubits**, rather than by atomic species.
- DMET computations also utilize GPU processing.
- Experiment with **different partitioning methods**.
- **Multi Threading** to make calculation more efficient

## Future Work

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