CANOE:
Classically-Assisted Non-Orthogonal Eigensolver

WQI Colloquium

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Problem Setup

- Goal: Given a Hamiltonian of a molecule, find a good approximation of the ground state energy

$$H\,|\psi\rangle = \mathrm{E}_0\,|\psi\rangle$$

$$H = \sum_{p,q} h_{pq}\, a_p^\dagger a_q \;+\; \frac{1}{2}\sum_{p,q,r,s} h_{pqrs}\, a_p^\dagger a_q^\dagger a_s a_r$$

- 'Good' approximation: $\epsilon_c \approx 1.6\ \mathrm{mHa}$ (chemical accuracy)

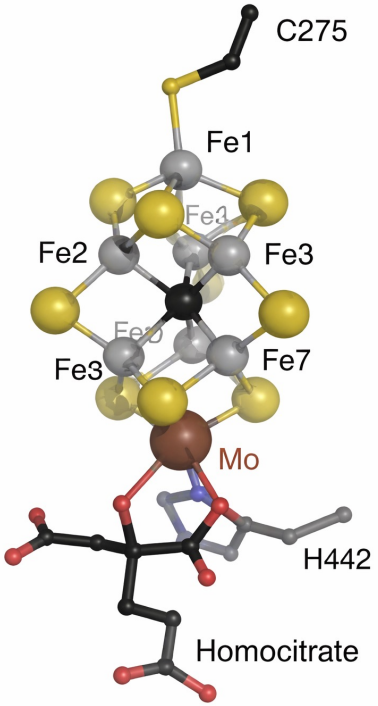
- Exact diagonalization (Full CI): feasible only up to

  (44 spin-orbitals, 22 electrons)

- Chemically important systems (e.g. FeMoco):

  (~108 spin-orbitals, ~50 electrons)

→ far beyond Full CI



Molecular structure of FeMoco

Spatzal et al., *Nat. Comm.* (2016)

Variational Principle & setting Ansatz

- Variational principle ensures

$$E_0 \leq \frac{\langle\psi(\theta)|H|\psi(\theta)\rangle}{\langle\psi(\theta)|\psi(\theta)\rangle}$$

with trial wavefunction, or ansatz $|\psi(\theta)\rangle$ with variational parameter θ

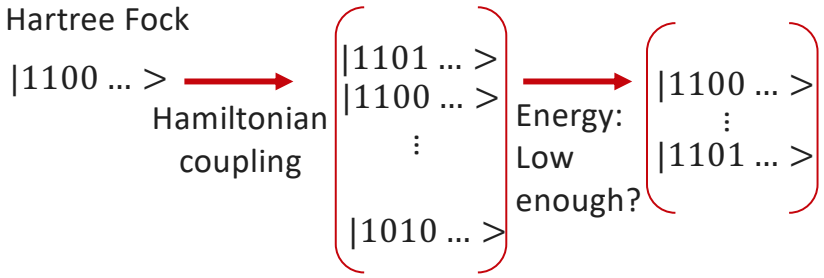
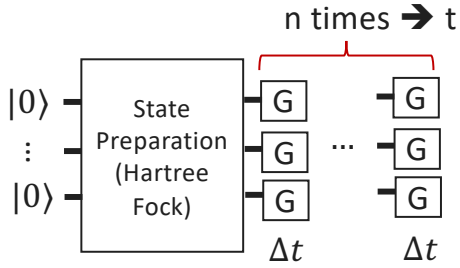
- Choose a restricted set of basis states($|\phi_i\rangle$)

→ trial wavefunction : $|\psi\rangle = \sum_{\mathrm{i}} c_i \, |\phi_i\rangle$

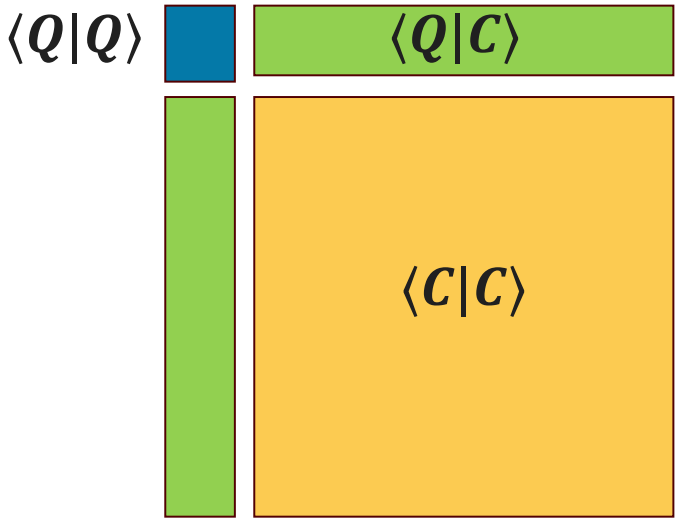
- Solving $H \, |\psi\rangle = \mathrm{E}_0 \, |\psi\rangle$ → variationally optimize c_i in the subspace of $\{|\phi_i\rangle\}$
- One interesting ansatz − **a superposition of both quantum and classical wavefunctions**:

$$|\psi\rangle = \sum_i c_i |\phi_i^C\rangle + \sum_j c_j |\phi_j^Q\rangle$$

Classical and Quantum States

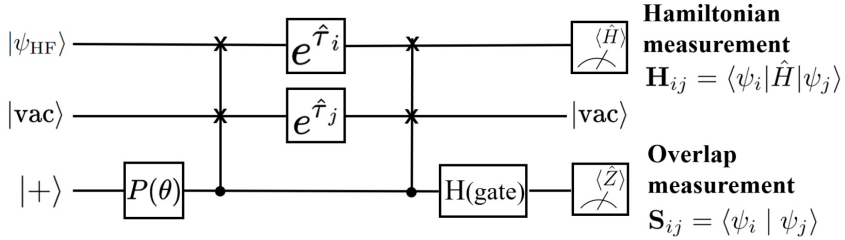
Classical states	Quantum states
Computational-basis processed on a classical computer	Prepared and measured on a quantum computer
SHCI  ➔ Determinants selected by SHCI (variational selection)	**Quantum Krylov states** $\|\psi(t)\rangle = e^{-iHt}\|\psi_0\rangle$ 
• Efficiently computed in classical computer → cheap • $\mathbf{10^4 \sim 10^6}$ classical are used in CANOE	• Represent entanglement and dynamics well • $\mathbf{10 \sim 100}$ quantum states are used in CANOE • Can be **non-orthogonal** ➔ we should solve Generalized Eigensolver $\boldsymbol{H}\|\boldsymbol{\psi}\rangle = \boldsymbol{\lambda S}\|\boldsymbol{\psi}\rangle$

Overlap matrix S



$$H|\psi\rangle = \lambda S|\psi\rangle$$

- Classical-Classical: easy to be done in classical computer, identity for determinants
- Quantum-Quantum: Hadamard test



https://arxiv.org/abs/2504.16008

- Quantum-Classical: Quantum tomography?
- After getting S, we can have H with tricks

Methods for $\langle Q|C\rangle$

Hadamard test

- Prepare $|C\rangle$ as a quantum state
- Do Hadamard test

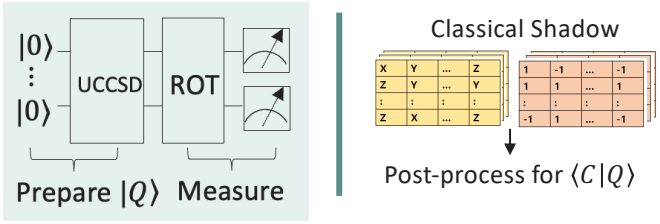
Direct measurement

- Think the role of $|C\rangle$ as a kind of operator
- Get the expectation value of the operator

Scale with the number of classical states

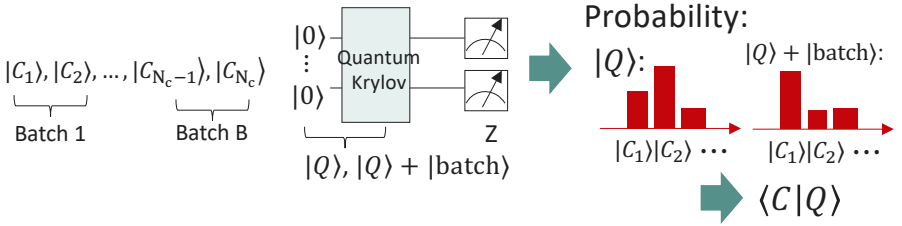
Classical shadow

- Think the role of $|C\rangle$ as a kind of operator
- Get the shadow of each quantum state
- Post-process classically for the operator

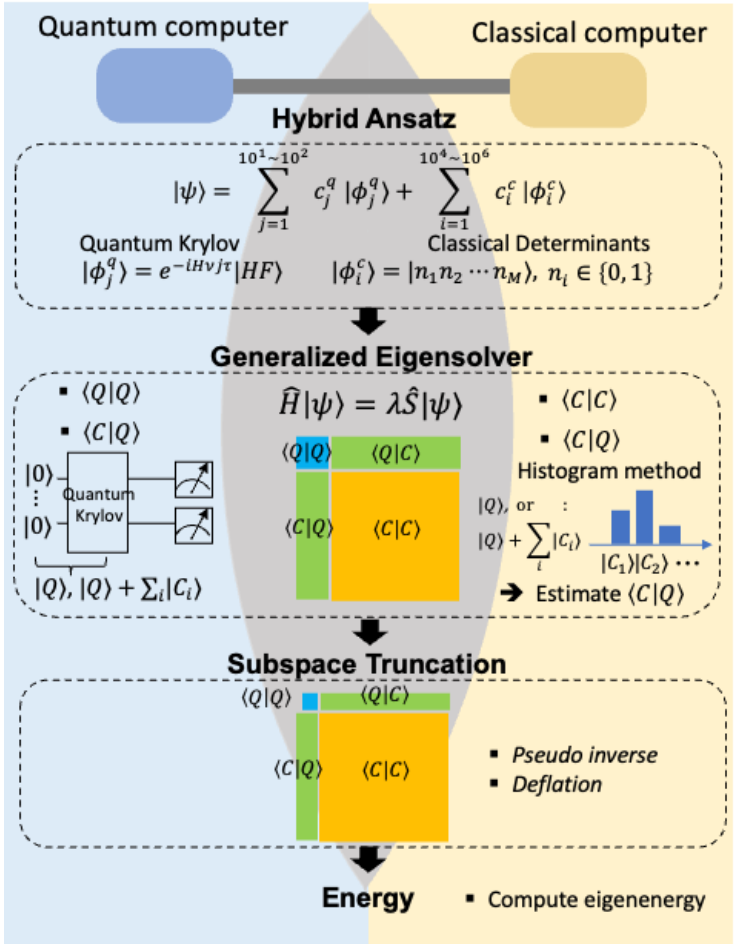


Histogram+batch

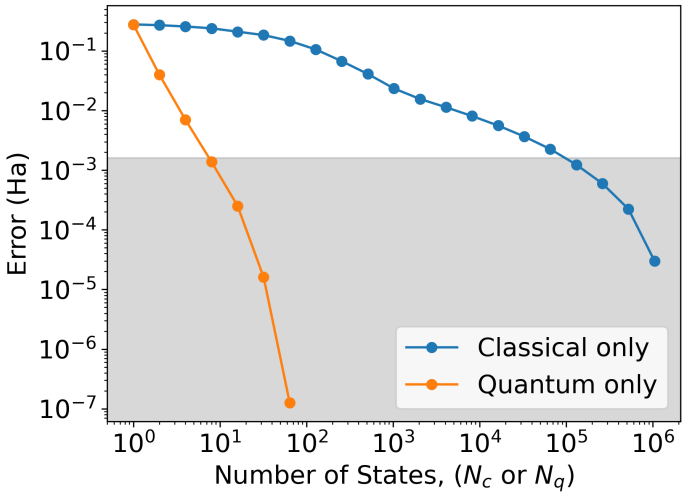
- Make B batches from the set of classical states
- Measure the probability of $|Q\rangle$ and $|Q\rangle + |\text{batch}\rangle$ to be classical determinants
- From the interference, get the phase of the overlap

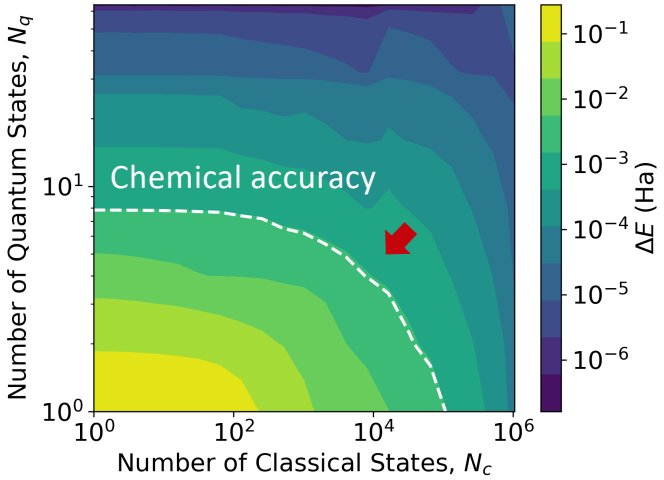


CANOE Workflow



CANOE results : Chromium atom (76so, 14e)

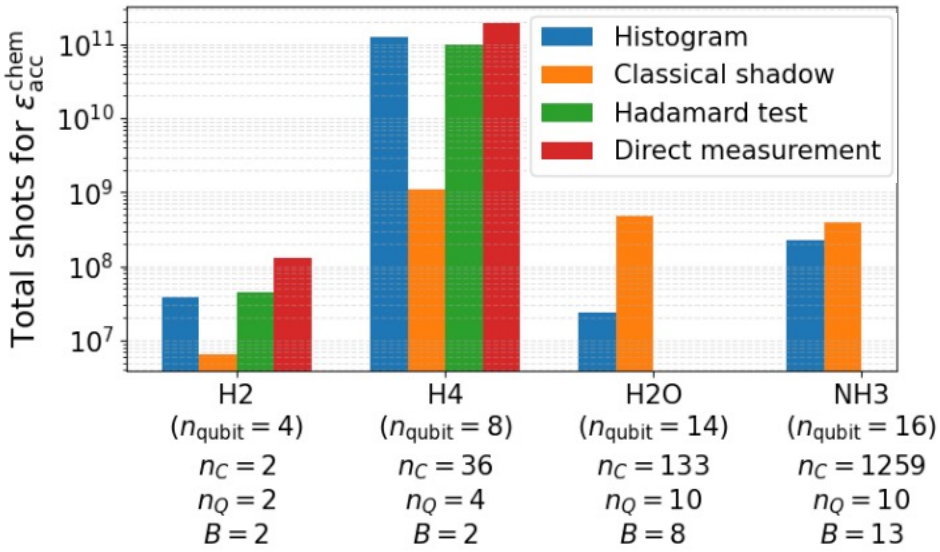




- 10 quantum Krylov states only or 10^5 selected determinants from SHCI only reach chemical accuracy

- The "elbow" at $n_q \approx 5, n_c \approx 10^4$ achieves chemical accuracy, halving the quantum state requirement
- Classical states improves the results from quantum states, and vice versa

CANOE results : Sampling



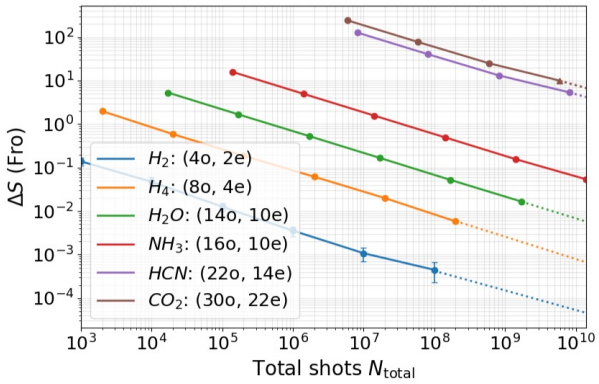
Method	Total shots
Hadamard Test	$\mathcal{O}\left(\frac{n_C n_Q n_H \|\mathbf{h}\|_{l_2}^2}{\epsilon^2}\right)$
Direct Measurement	$\mathcal{O}\left(\frac{n_C n_Q 2^{n_{qubit}} \|\mathbf{h}\|_{l_1}^2}{\epsilon^2}\right)$
Classical Shadow	$\mathcal{O}\left(n_Q \log(n_C) \frac{\|\mathbf{h}\|_{l_2}^2 \cdot 2^{n_{qubit}}}{\epsilon^2}\right)$
Histogram+Batch	$\mathcal{O}\left(\frac{n_Q B \|\mathbf{h}\|_{l_1}^2}{\epsilon^2} \log\left(\frac{2^{n_{qubit}} \cdot n_Q B}{\delta}\right)\right)$

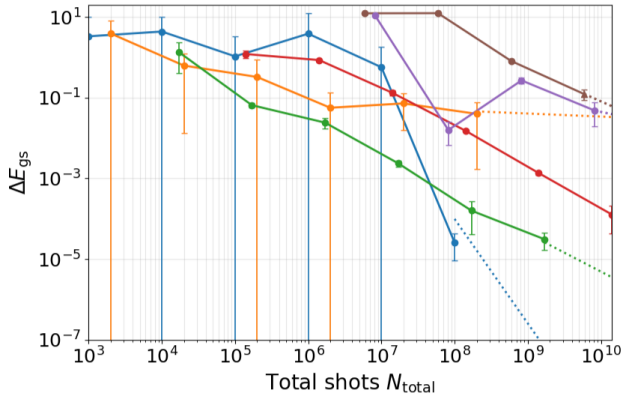
n_C: number of classical states
n_Q: number of quantum states
n_{qubit}: number of qubits
n_H: number of Pauli terms in Hamiltonian

B: number of batches in histogram method
$||h||_{li}$: the norm of Hamiltonian coefficients
ϵ: the error of an entry of Hamiltonian matrix
δ: precision

- Histogram sampling outperforms classical shadows as system size increases
- Direct measurement and Hadamard test do not scale to larger molecular systems
- H_4 is sample-intensive due to ill-conditioned S, not qubit count

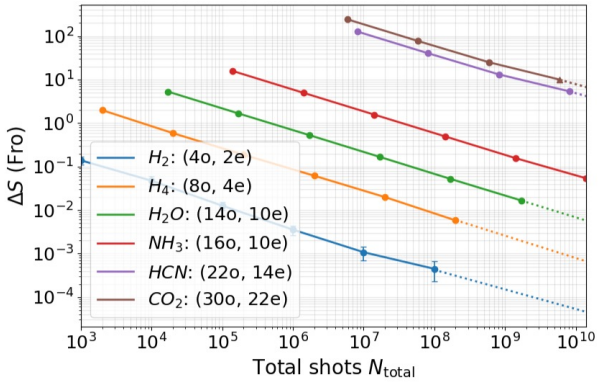
CANOE results : Histogram+batch method

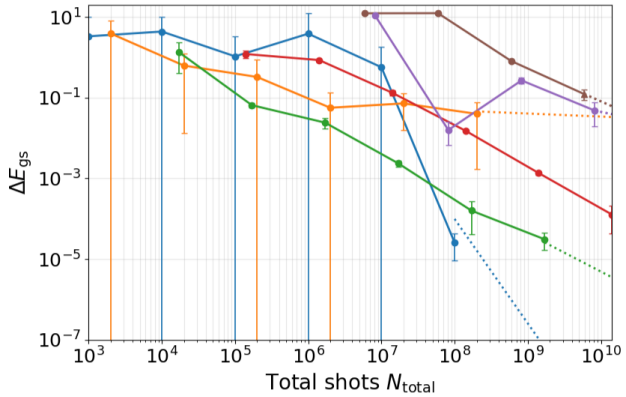




- ΔS(Frobenius norm) and ΔH decrease with total shots roughly as $1/\sqrt{N_{shot}}$
- For ΔS , ΔH, larger molecules require more shots to reach the same accuracy
- ΔEgs doesn't necessarily track Frobenius errors because of sensitivity of conditioning S

CANOE results : Histogram+batch method





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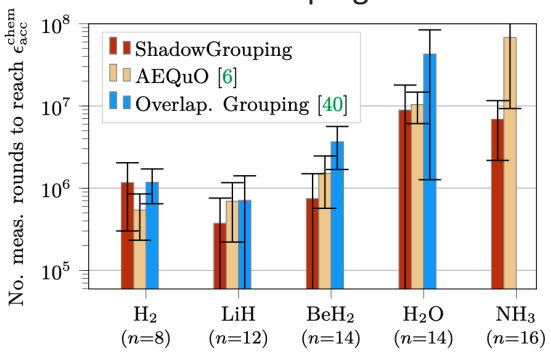
- E.g. H2O: ShadowGrouping vs CANOE

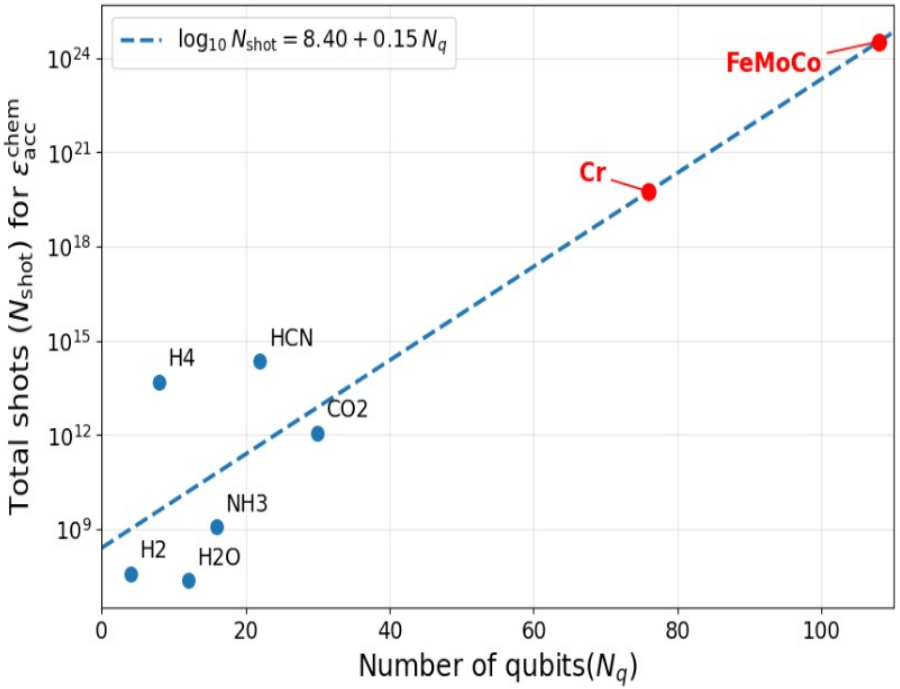
ShadowGrouping measures the energy of an **already-prepared** ground state, CANOE **finds** the ground state with the similar cost (~10^7)

ShadowGrouping result



https://arxiv.org/abs/2301.03385

CANOE results: extrapolation for larger systems



- Histogram-based estimation shows exponential shot scaling with qubit count : $\log_{10}\mathrm{N}_{\mathrm{shot}} \approx 8.4 + 0.15\mathrm{N}_{\mathrm{q}}$
- Small systems (H_2–NH_3) are accessible but FeMoCo-scale systems are infeasible
- The bottleneck for larger systems is measurement efficiency (sampling cost)

Conclusion

- CANOE is **an early fault-tolerant quantum** algorithm designed for chemistry, avoiding variational loops (VQE) while requiring much shallower circuits than full QPE
- CANOE offers the potential to augment quantum computers with extra classical power (or, alternately, augment classical computers with extra quantum power)
- Histogram+batch method shows the best fit for CANOE, but a huge sampling cost is still the main bottleneck for middle and large system sizes
- Fault-tolerant gadgets, like double factorization and amplitude amplification, can reduce shot costs. E.g. amplitude amplification : $O(\frac{1}{\epsilon^2}) \rightarrow O(\frac{1}{\epsilon})$

arXiv:2507.23074 (2025)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