VQE for H_2 Simulation

VQE using Clifford Ansatz

Togan Tlimakhov Yusuf

Agenda

- VQA
- VQE
  - Structure & Ansatz
  - The Variational principle
  - Challenges
- Classical simulation of VQE
- CAFQA
  - Framework
  - H2 molecule ground state energy
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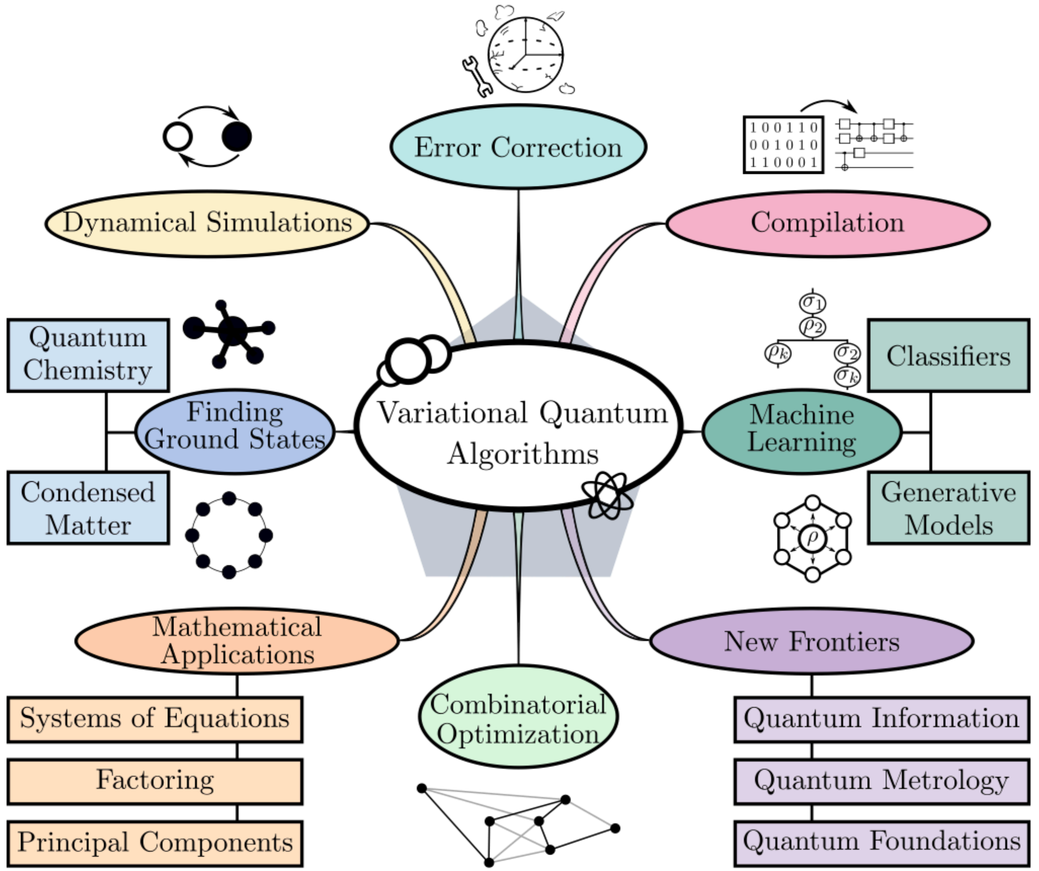
Variational Quantum Algorithms

Proposed to solve relevant computational problems on near term quantum devices

- VQAs are the leading proposal for achieving “quantum advantage” on the NISQ devices
- Their applications range form quantum chemistry to machine learning and optimization
- Uses much shallower circuits proposed by Peruzzo et al. that are executable by current hardware



*M. Cerezo, et al. "Variational quantum algorithms". Nature Reviews Physics 3. 9 (2021)

Variational Quantum Algorithms

- VQAs use parametrized quantum circuits to be run on the quantum hardware, and then outsource the parameter optimization to a classical optimizer
- Define a cost function that encodes the solution to the problem
- Proposes an ansatz; a quantum operation that depends on a set of parameters “θ” that can be optimized

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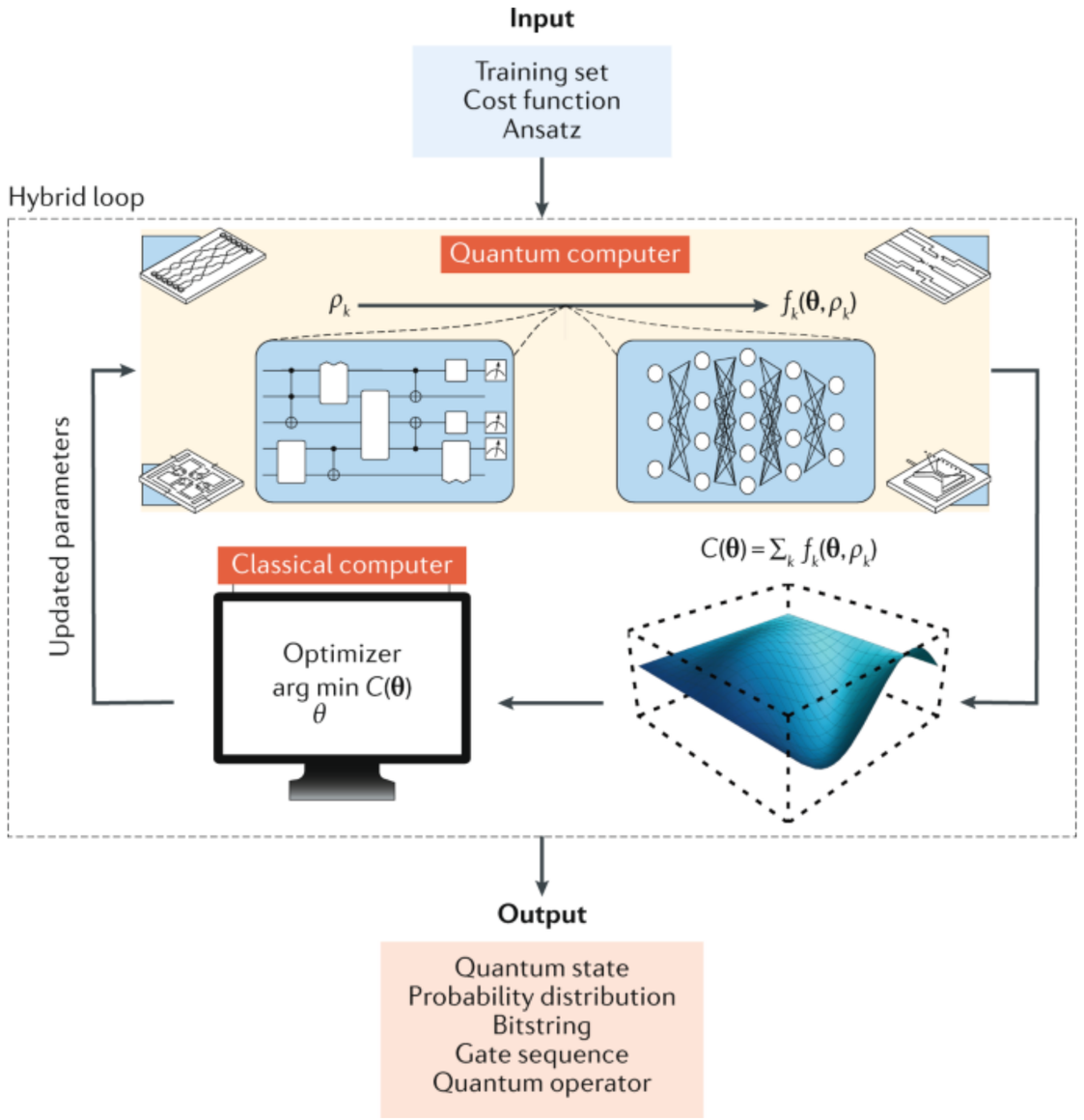

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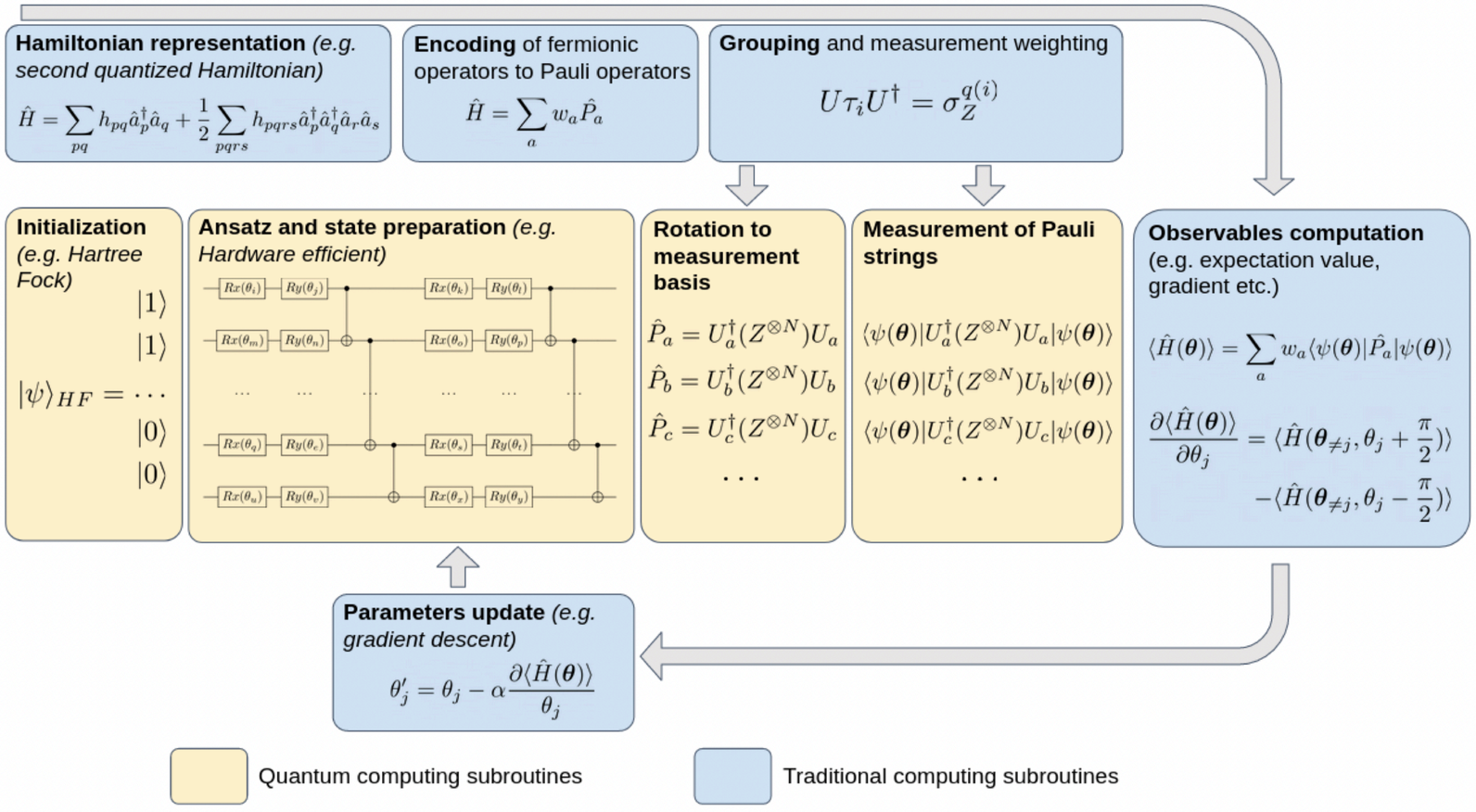
Variational Quantum Eigensolver

Searching for the ground state energy of quantum systems (Molecules, etc.)



*Tilly, Jules et al. "The Variational Quantum Eigensolver: a review of methods and best practices." (2021).

Ansatz

- In the NISQ era, it is imperative to choose a VQA's ansatz appropriately and its initial parameters to be as close to optimal as possible
- This would improve and accelerate the accurate convergence of the algorithm's execution on the quantum device
- The structure of an ansatz will generally depend on the task. However, some ansatz architectures are generic and can be used with no prior information

Method	Depth	Parameters	Entangling gates
Hardware Efficient Ansatz (HEA) [227]	$\mathcal{O}(L)$	$\mathcal{O}(NL)$	$\mathcal{O}((N-1)L)$
UCCSD [36, 392]	$\mathcal{O}\left((N-m)^2 m\tau\right)$	$\mathcal{O}\left((N-m)^2 m^2\tau\right)$	$\mathcal{O}\left(2(\tilde{q}-1)N^4\tau\right)$
UCCGSD [36, 60, 62]	$\mathcal{O}\left(N^3\tau\right)$	$\mathcal{O}\left(N^4\tau\right)$	$\mathcal{O}\left(2(\tilde{q}-1)N^4\tau\right)$
k-UpCCGSD [60]	$\mathcal{O}(kN\tau)$	$\mathcal{O}\left(k\tau N^2/4\right)$	$\mathcal{O}\left(k\tau(\tilde{q}-1)N^2/2\right)$
OO-UCCD [393]	$\mathcal{O}\left((N-m)^2 m\tau\right)$	$\mathcal{O}\left((N-m)^2 m^2\tau\right)$	$\mathcal{O}\left(2(\tilde{q}-1)N^4\tau\right)$

*Tilly, Jules et al. "The Variational Quantum Eigensolver: a review of methods and best practices." (2021).

The variational principle

- Given Hermitian matrix (Hamiltonian) with eigenstates and associated eigenvalues: $H|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle$
- We usually don't know what the eigenstate $|\psi_\lambda\rangle$ in order to calculate the value of the λ_{min}
- To obtain the energy value for state $|\psi\rangle$, we can calculate the expectation value of H: $\langle\psi|H|\psi\rangle = E(\psi)$
- For the eigenstate associated with the smallest eigenvalue: $\langle\psi\lambda_{min}|H|\psi\lambda_{min}\rangle = E\lambda_{min}$
- The variational principle: $\langle\psi\lambda|H|\psi\lambda\rangle >= E\lambda_{min}$

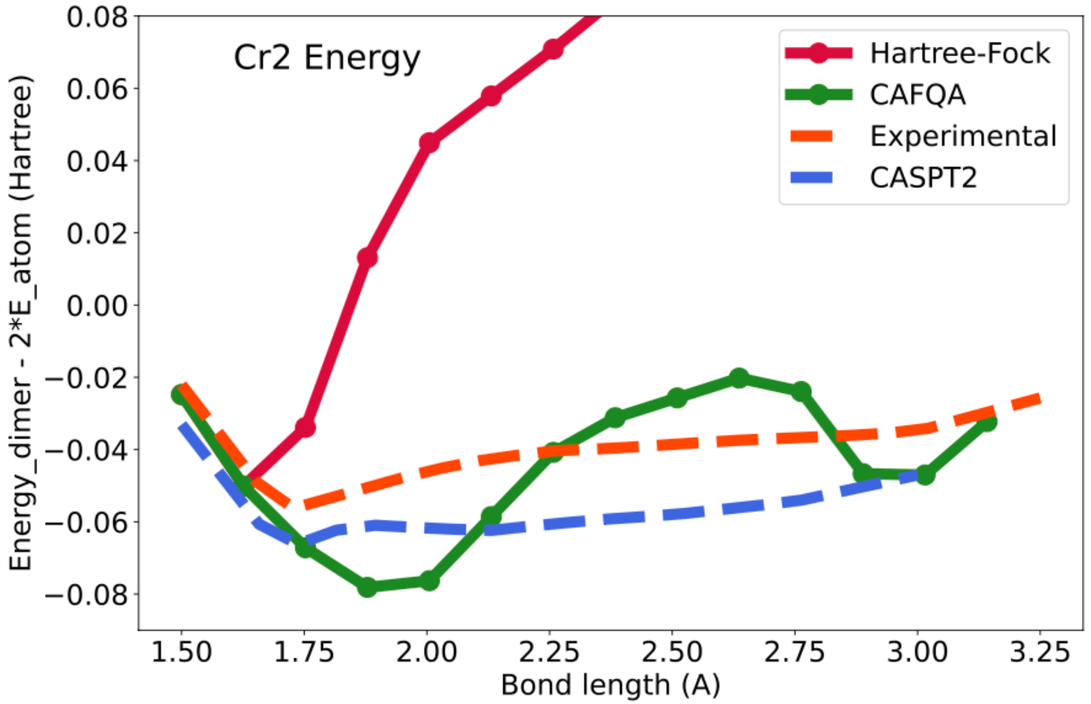
→ **By arbitrarily selecting a wave function $|\psi\rangle$ (Ansatz) as an initial guess approximating $|\psi_{min}\rangle$, calculating its expectation value and iteratively updating the wave function, arbitrarily tight bounds on the ground state energy of the Hamiltonian may be obtained**

Challenges for VQEs

- As the complexity of systems increases, a large number of shot becomes required to achieve accurate results
- Difficulties in optimizing the circuit parameters

→ **A relatively good Ansatz initialization is very crucial**

For HF, all non-diagonal Pauli terms have an expectation value of zero i.e., the state being found is a computational basis state. Only calculating the expectation values for the diagonal terms leads to ignoring the correlation energy, which is known to lead to serious errors for some larger molecules.



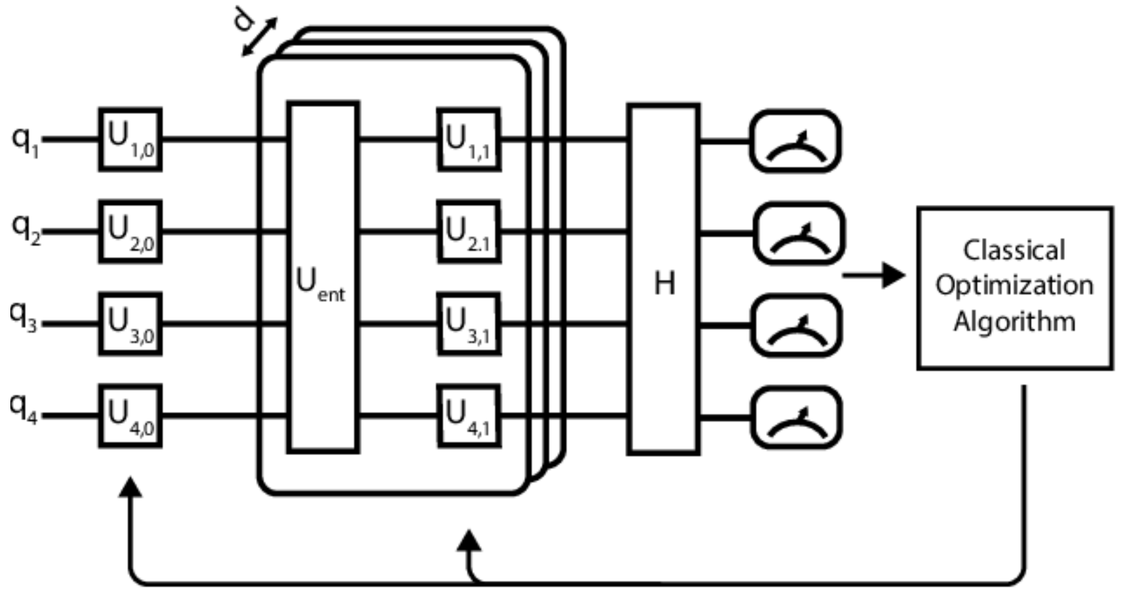
*Ravi, Gokul Subramanian et al. "CAFQA: Clifford Ansatz For Quantum Accuracy." (2022).

Classical simulation of VQE

Quantum optimization in NISQ era is expensive and noise sensitive

- It is plausible to do as much computation on the classical computer as possible
- In some cases, it is possible to simulate quantum circuits on classical circuits

→ **Clifford gates can be simulated classically in polynomial time****



*de Keijzer R, et al. *AVS Quantum Science*. 2022; 4(1):013803. doi:10.1116/5.0076435
**D. Gottesman, “The heisenberg representation of quantum computers,”, 1998.

CAFQA

Quantum circuits of Clifford gates can be perfectly simulated in polynomial time on classical computers and the discrete Clifford space, while scaling exponentially in the number of qubits

- The Clifford group do not provide a universal set of quantum gates, where the stabilizer states produced by Clifford-only circuits are limited in how effectively they can explore the quantum space of a given problem such as those targeted by VQAs.

✓ However, exploring the Clifford space of the VQA problem through classical simulation can potentially find useful initial states by identifying appropriate VQA parameters in a suitable parametrizable circuit.

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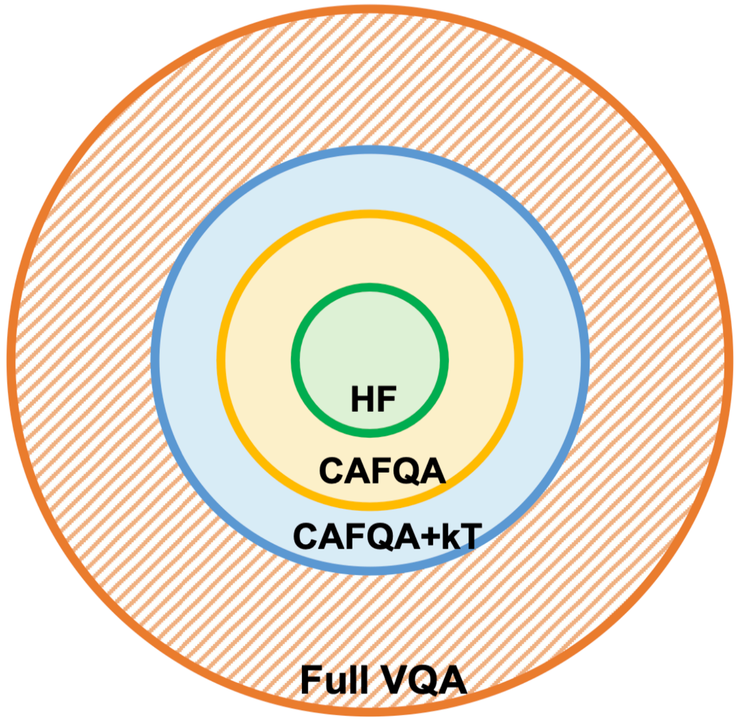

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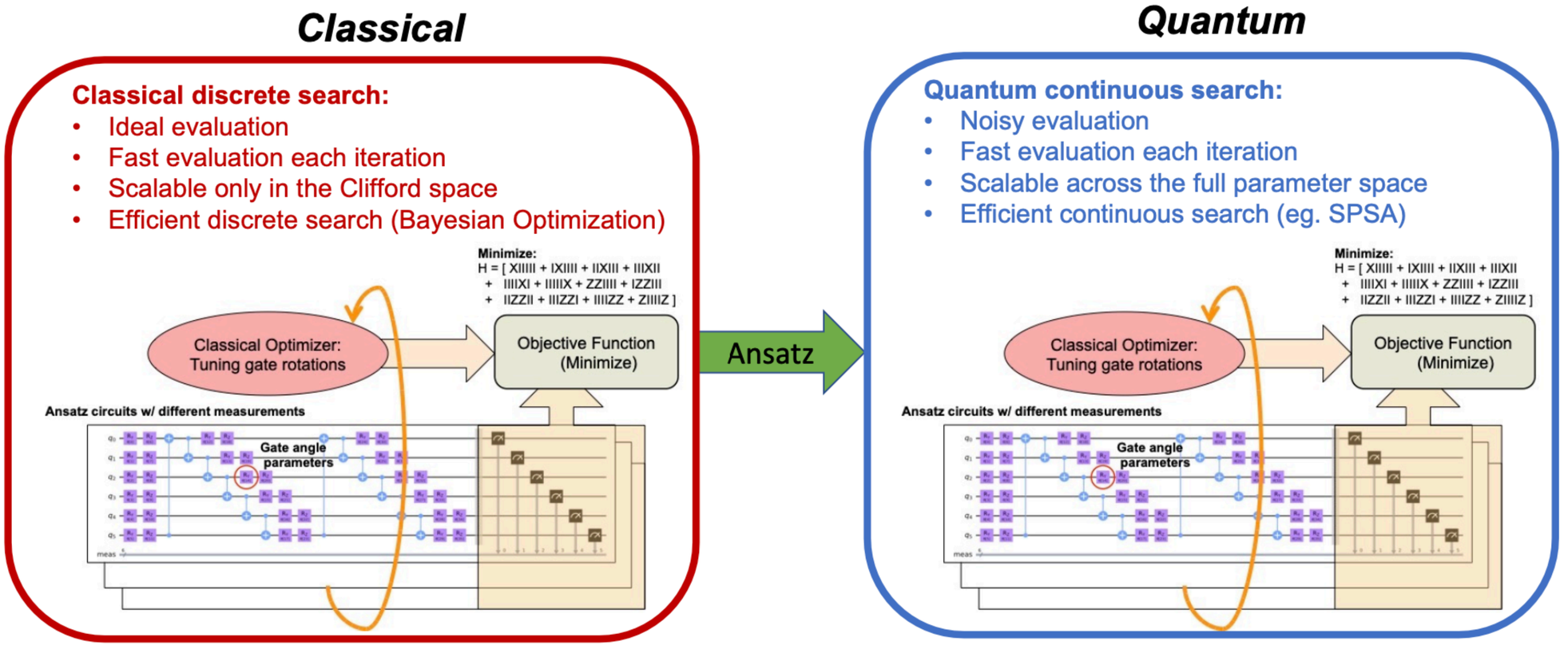
CAFQA framework

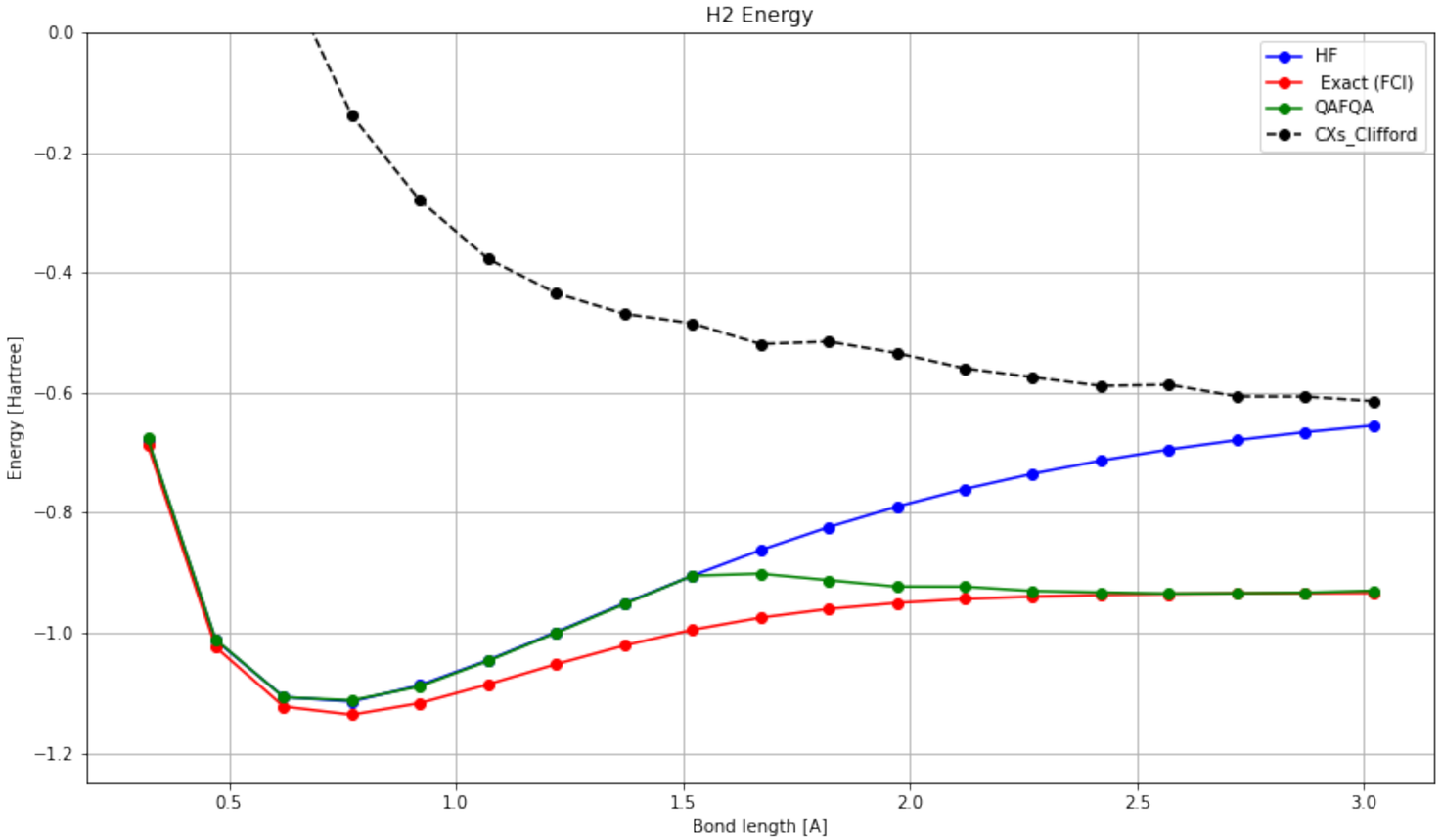
Perform parameter tuning on the ansatz which is suitable for classical computation



*Ravi, Gokul Subramanian et al. "CAFQA: Clifford Ansatz For Quantum Accuracy." (2022).

H_2 molecule ground state energy results

Comparisons to Exact (FCI) Chemical Accuracy, CXs Clifford, and Hartree-Fock



*Note that the number of Ansatz parameters is set to 4, which reduces the rotation gates to the Clifford group; theta[i]= {0, pi/2, pi, 3pi/2}

*FCI (full configuration interaction) can be considered the most accurate computation that can be performed for a given basis

CAFQA advantages

✓ CAFQA is classically simulatable

✓ It is a hardware-efficient Ansatz, providing fast convergence

✓ Accurate initialization, for up to 20 qubits, achieves accuracy of 99%

✓ Recovers over 99.99% of molecular correlation energy over HF

✘ **Scalable only in the Clifford and NOT across the full parameter space**

Simulation beyond Clifford gates

- Efficient classical simulation can be extended to constrained Clifford+T circuits wherein T refers to the single-qubit 45-degree phase shift*
- Some simulation overheads can be reduced by employing Hamiltonian term truncation techniques**
- Perturbative expansion of HF computational basis states by exploiting the classical simulability of Clifford circuits. Similar expansion to CAFQA produced stabilizer states can provide further improvements, benefiting from Clifford simulation***

*S. Bravyi and D. Gosset, “Improved classical simulation of quantum circuits dominated by clifford gates,” *Physical Review Letters*, vol. 116, no. 25, Jun 2016.
**G. Li, Y. Shi, and A. Javadi-Abhari, “Software-hardware co-optimization for computational chemistry on superconducting quantum processors,” 2021.
***K. Mitarai, Y. Suzuki, W. Mizukami, Y. O. Nakagawa, and K. Fujii, “Quadratic clifford expansion for efficient benchmarking and initializa- tion of variational quantum algorithms,” 2020.

If you want to make a simulation of nature, you'd better make it quantum mechanical.

- Richard Feynman

Thank you! Any questions?

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Appendix A

Clifford group gates

Single qubit Clifford	2 qubit Clifford
I (Identity)	CX
X	CY
Y	CZ
Z	SWAP
H	
S	
S†	

Appendix B

Clifford+T group gates

Type of Gate	Symbol	Matrix
NOT gate	N	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Hadamard gate	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
T gate	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i.\frac{\pi}{4}} \end{bmatrix}$
T gate Hermitian transpose	$T^\dagger$	$\begin{bmatrix} 1 & 0 \\ 0 & e^{-i.\frac{\pi}{4}} \end{bmatrix}$
Phase gate	S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
Phase gate Hermitian transpose	$S^\dagger$	$\begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix}$
CNOT gate	C	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

*Muñoz-Coreas, Edgard et al. "T-count and Qubit Optimized Quantum Circuit Design of the Non-Restoring Square Root Algorithm". (2017).

Appendix C

CXs Clifford circuit