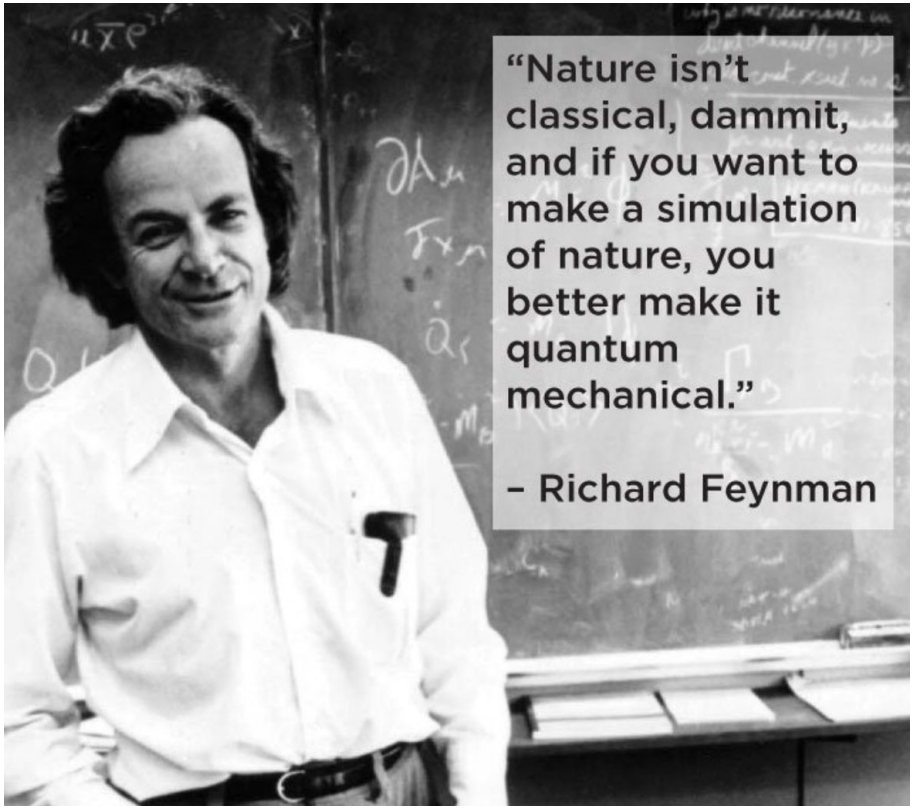
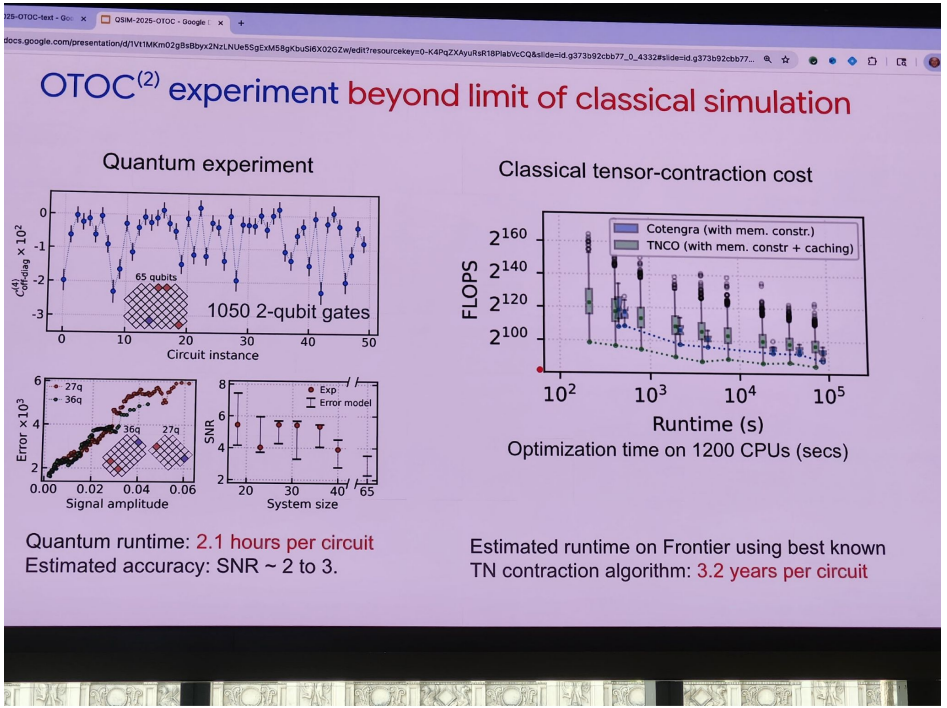
Quantum Algorithms for Quantum Chemistry

Shah Ishmam Mohtashim

Why Quantum Chemistry Needs Quantum Algorithms

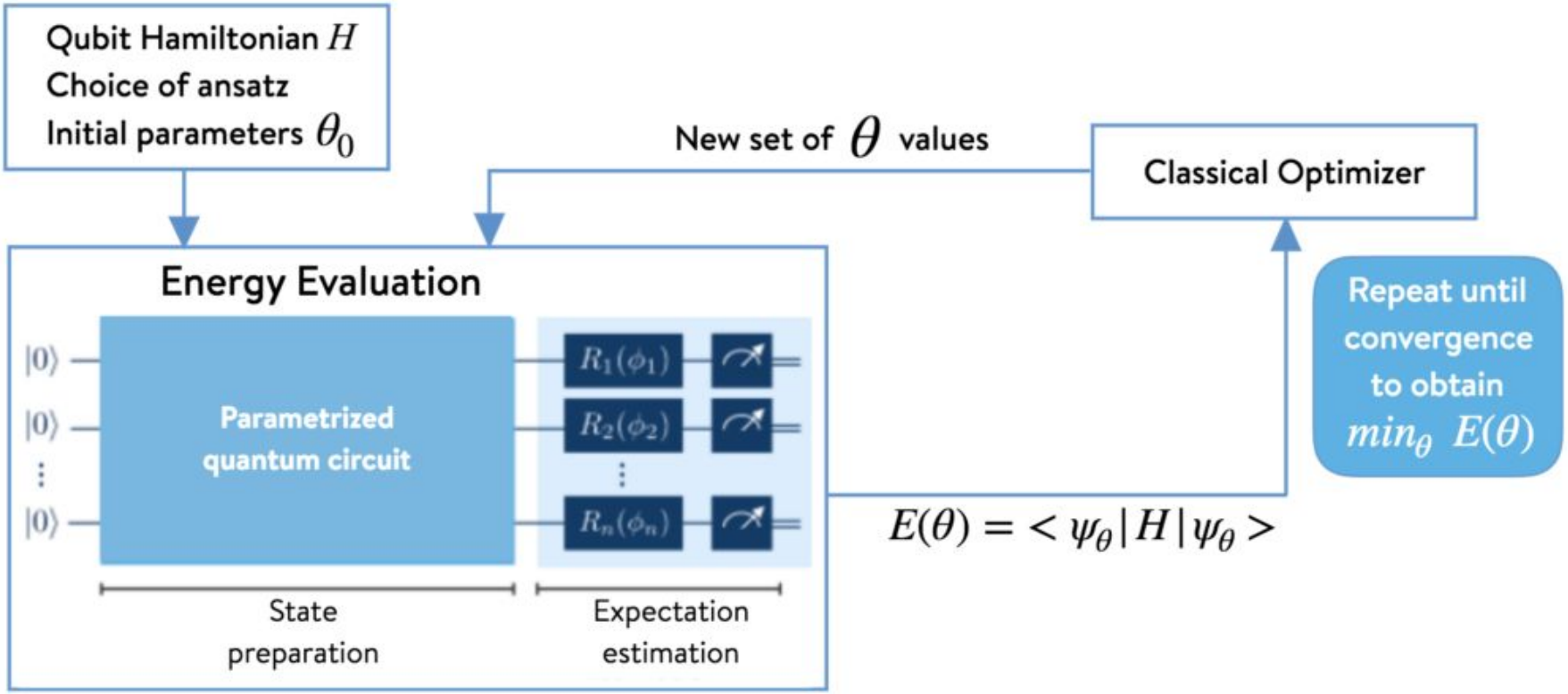




Overview

- **Variational Quantum Eigensolver** for ground-state molecular energies and Ising Model
- **Subspace Search VQE** for excited states.
- **Digital Continuous-Time Quantum Walks** → protein network centrality.
- **Hadamard test** + **Multi-fidelity Estimation**→ reaction probabilities.

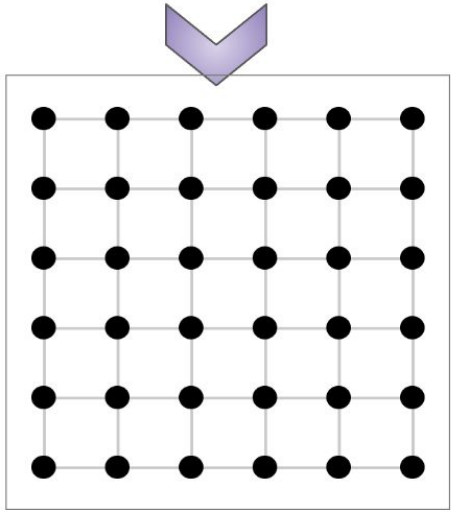
Variational Quantum Eigensolver



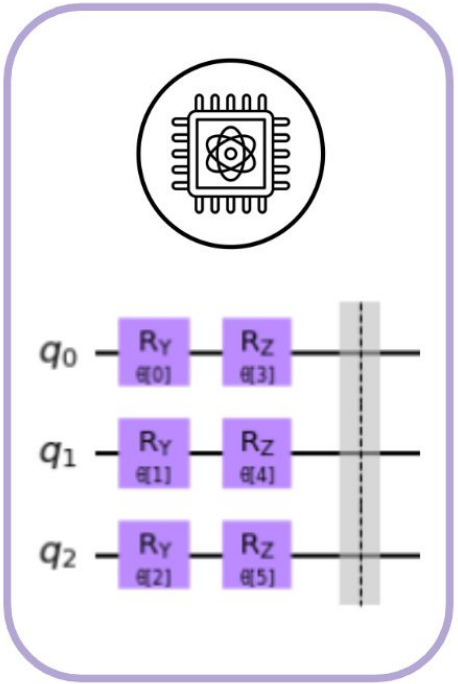
Simulating the Ising Model using VQE

$$\mathcal{H} = J \sum_i \sigma_i^z \sigma_{i+1}^z$$

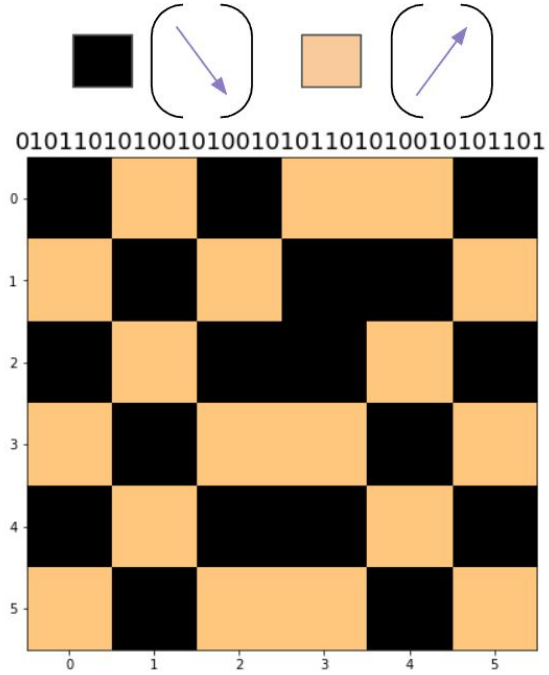
$$-B_x \sum_i \sigma_i^x - B_z \sum_i \sigma_i^z$$



6 x 6 lattice

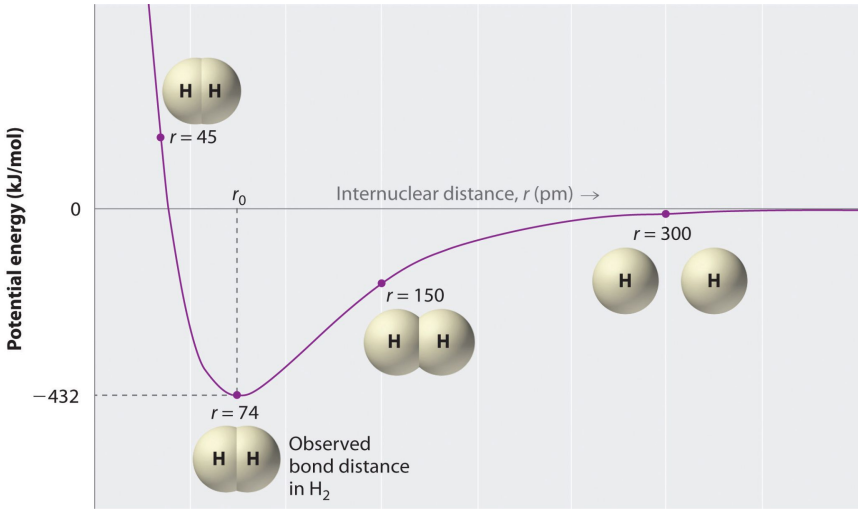


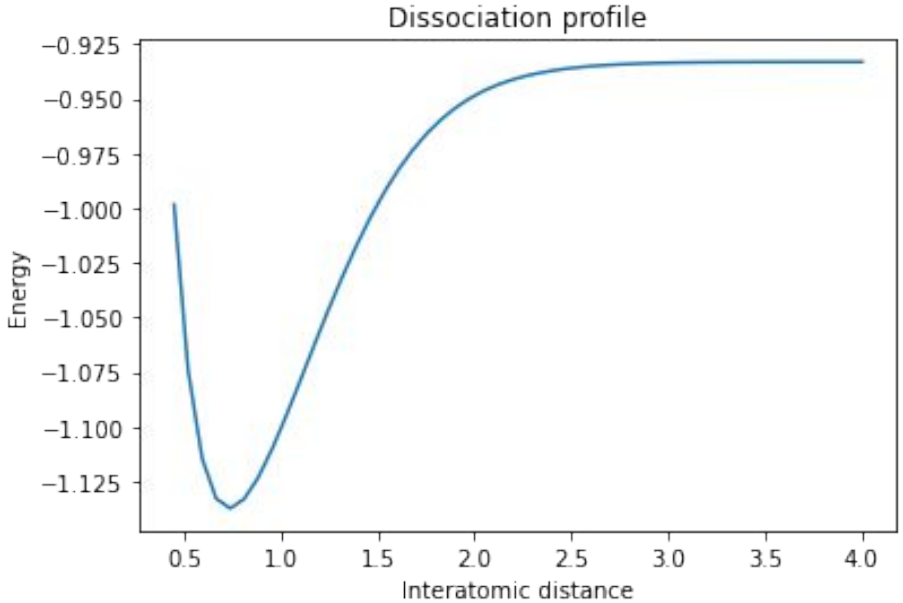
Quantum Simulator



Disordered State!

Molecular Energies using Variational Quantum Eigensolver





SubspaceSearch: Extracting Excited States

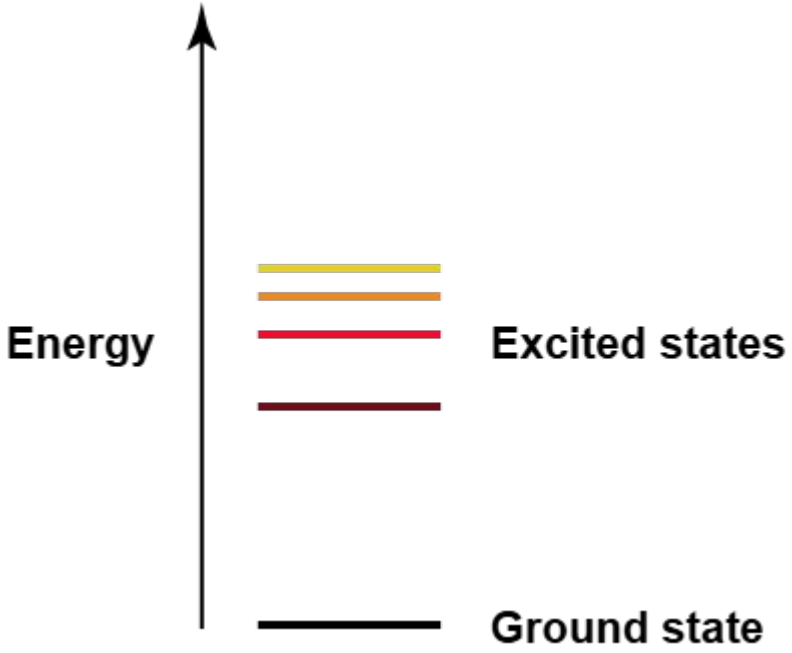
The procedures for SSVQE is as following:

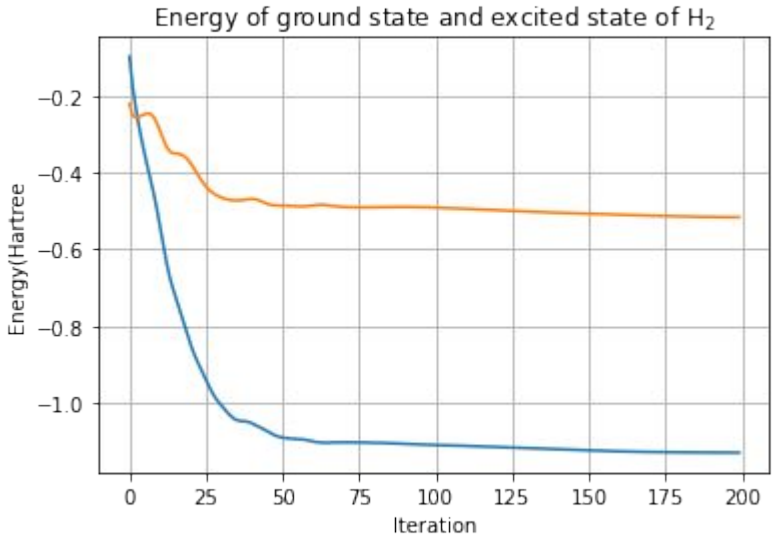
1) Preparation of k initial states $\{|\varphi_i\rangle\}_{i=0}^{k-1}$ orthogonal to each other.

2) Construct a parametrized quantum circuit $U(\theta)$

3) Minimize $L(\theta) = \sum_i w_i \langle\psi_i(\theta)|H|\psi_i(\theta)\rangle$. Here, w_i is the weight.

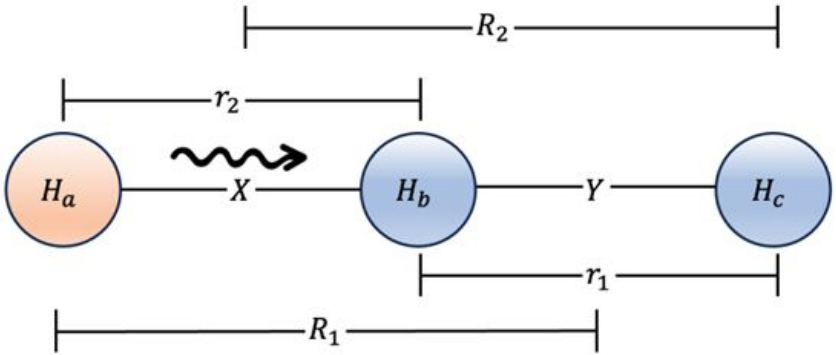
SubspaceSearch VQE

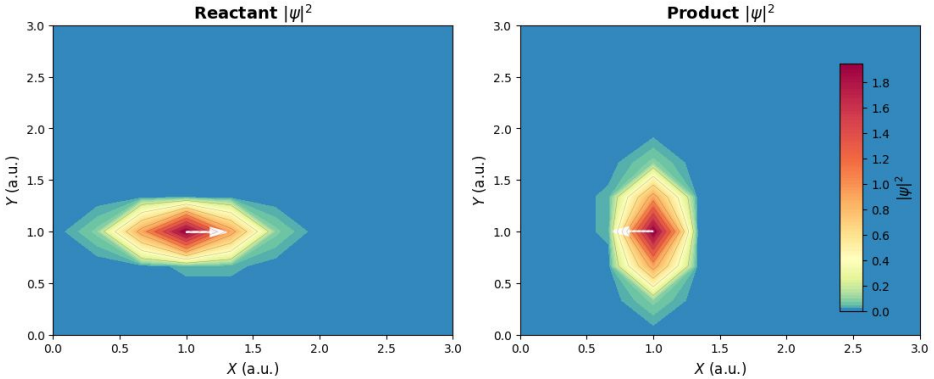


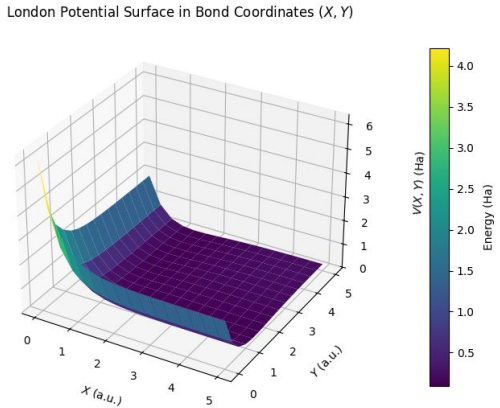


Quantum Simulation of Reaction Probabilities

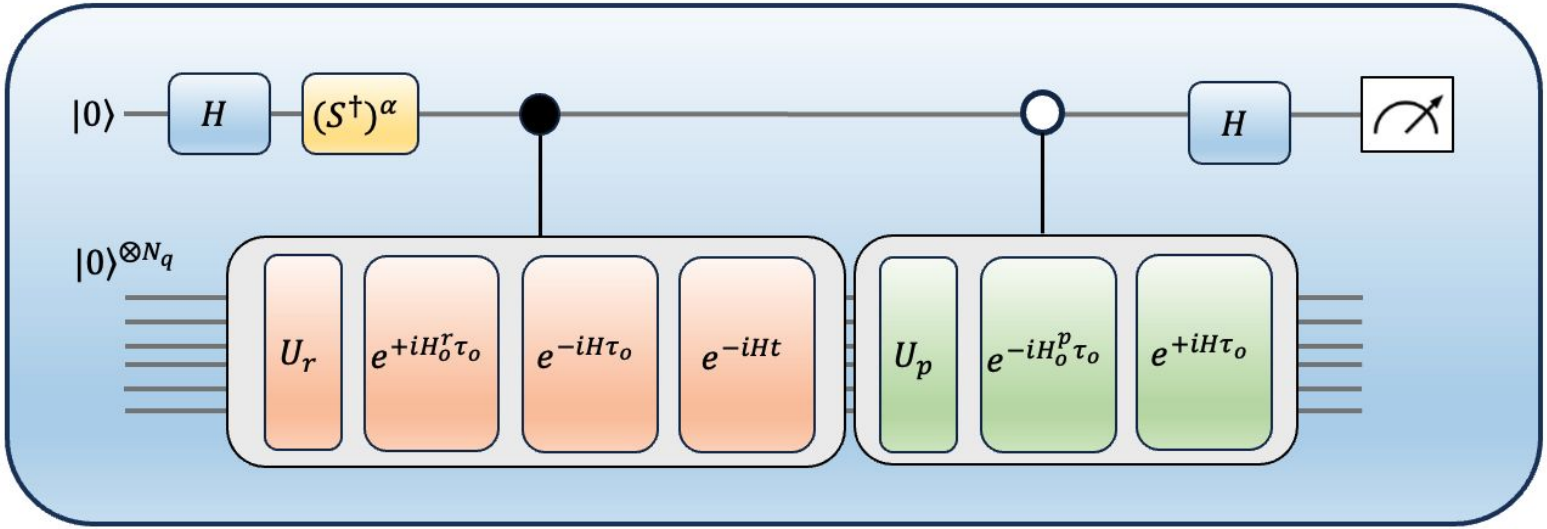
$$H_a + H_b H_c(v) \rightarrow H_a H_b(v') + H_c$$





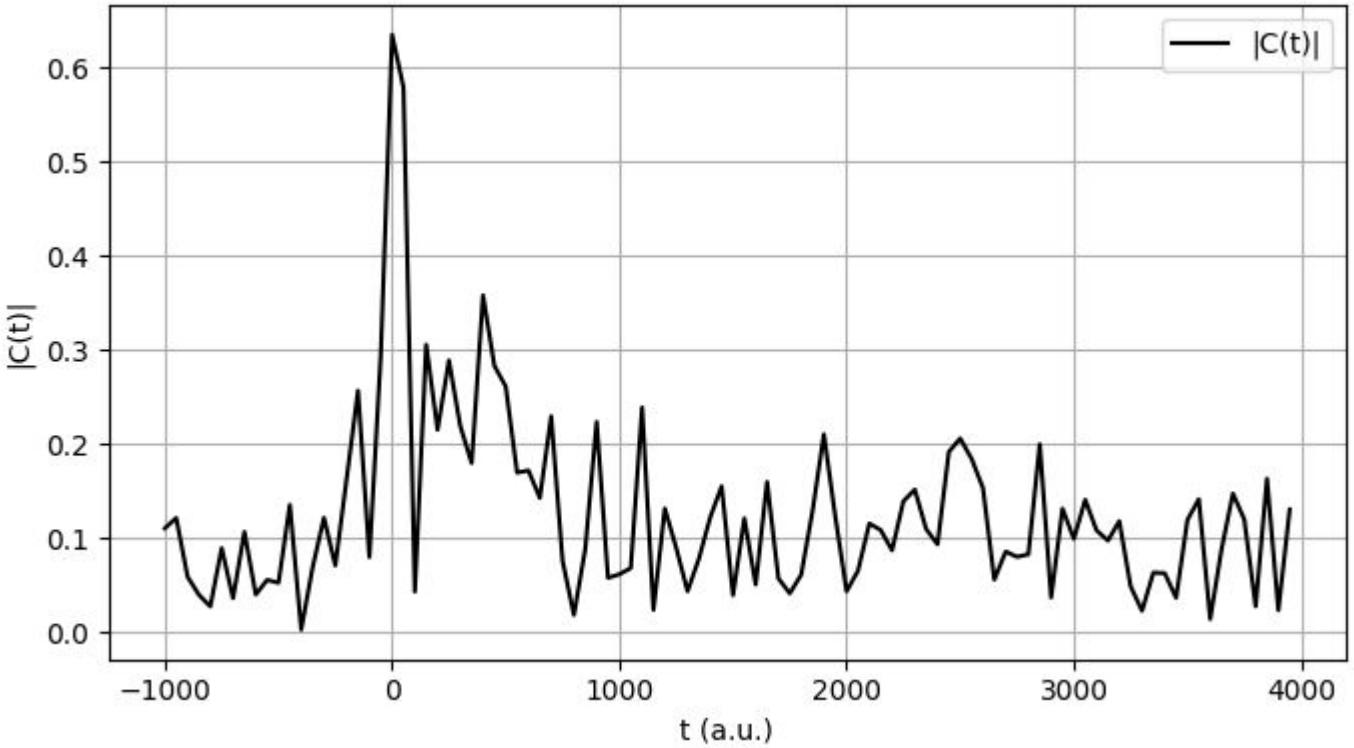


Quantum Simulation of Reaction Probabilities

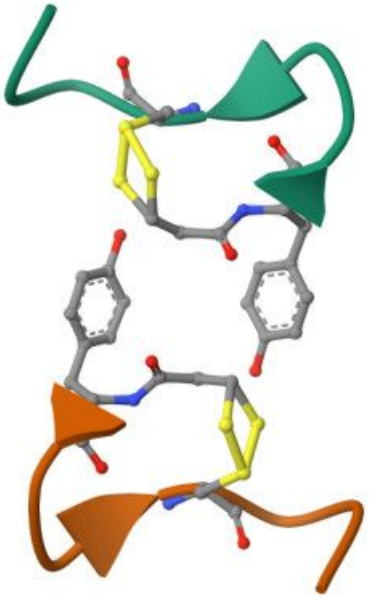


Quantum Simulation of Reaction Probabilities

$$C_{\gamma',\gamma}(t) = \langle \Psi^-_{\gamma'} | e^{-iHt} | \Psi^+_{\gamma} \rangle.$$



Continuous-Time Quantum Walks for protein centrality



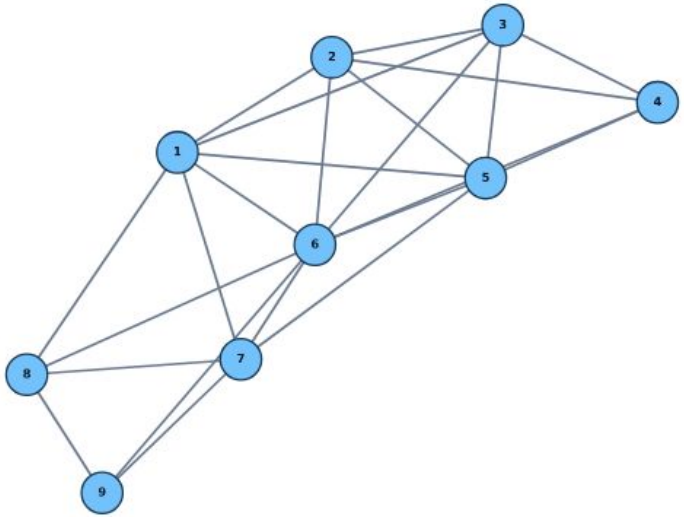


FIG. 1. Residue–interaction network for oxytocin (PDB ID: 1XY1). Nodes are residues; edges indicate C_α contacts under an 8 Å cutoff.

CTQW for protein centrality circuit

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle, \quad H = A$$

$$|\psi(t)\rangle = e^{-iAt} |\psi(0)\rangle$$

$$A_{ij} = \begin{cases} w_{ij}, & \text{if nodes } i \text{ and } j \text{ are connected,} \\ 0, & \text{otherwise.} \end{cases}$$

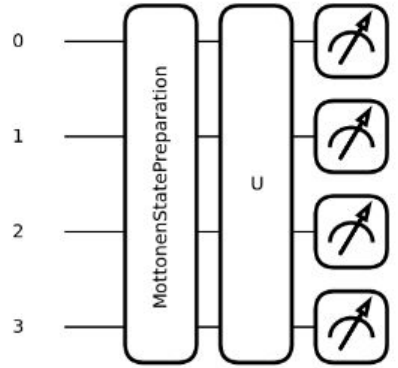


FIG. 3. CTQW Quantum circuit for oxytocin (PDB ID: 1XY1). Nodes are residues; edges indicate C_α contacts under an 8 Å cutoff.

CTQW probability plot

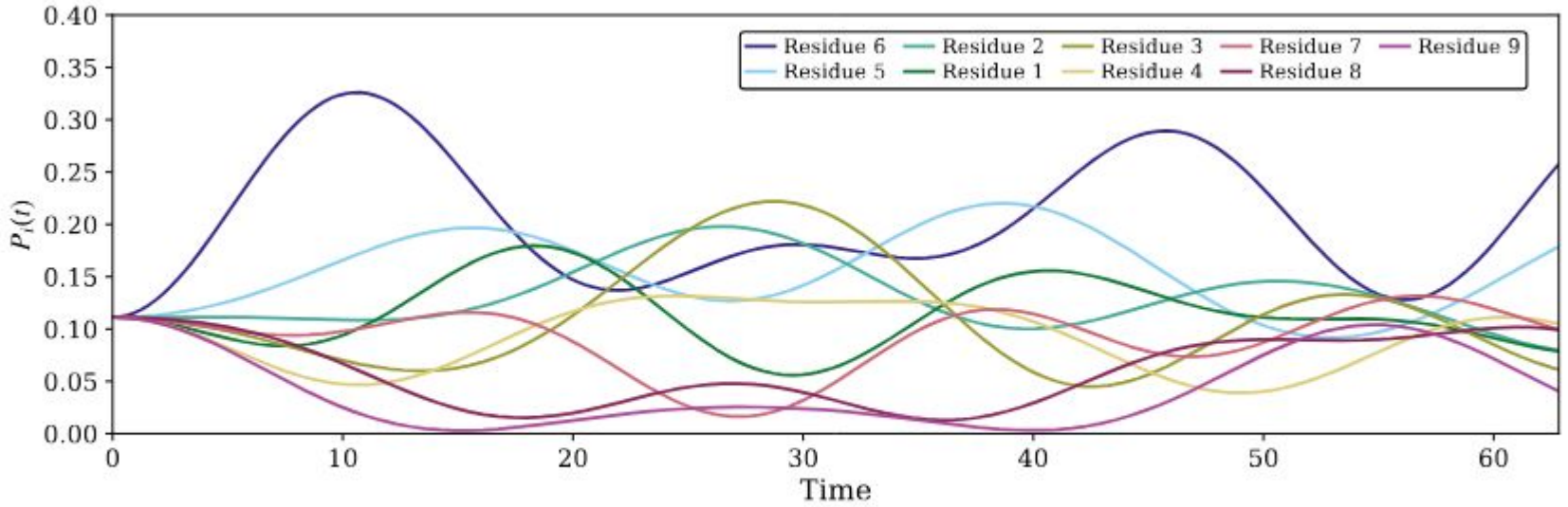
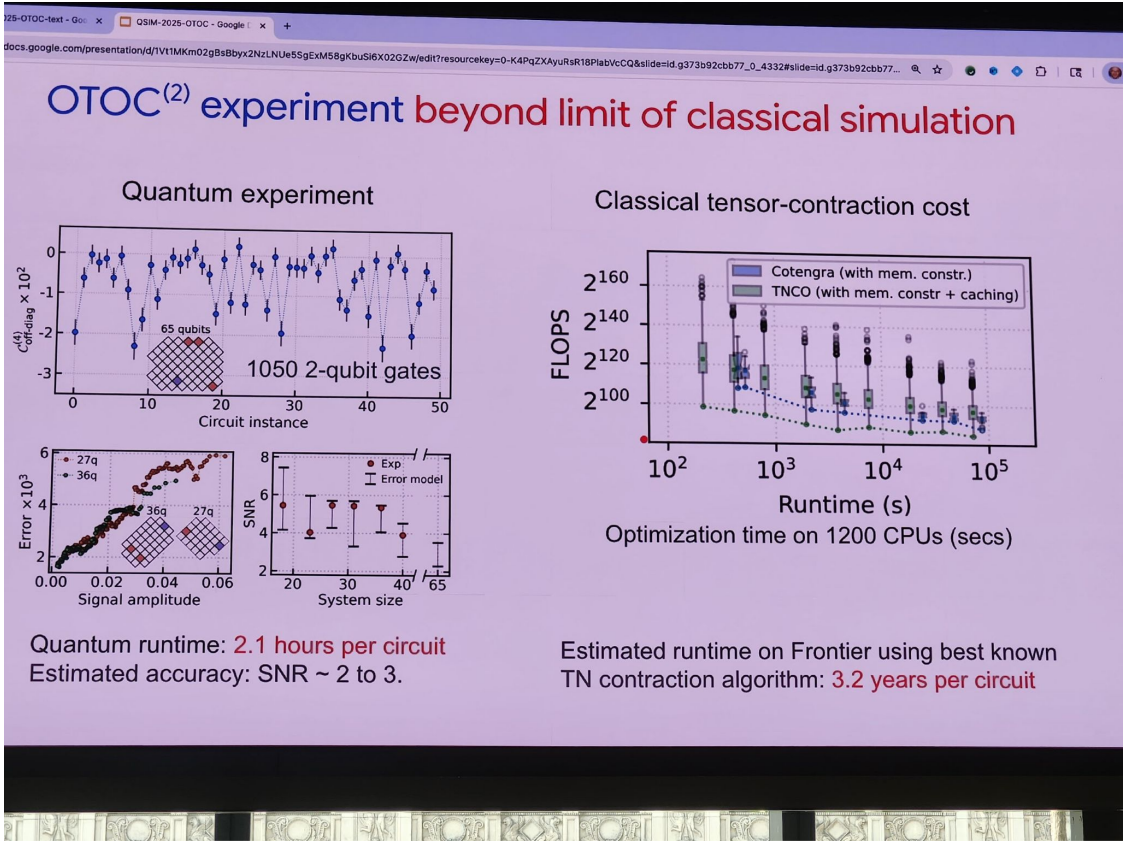


FIG. 2. Time evolution of node-occupation probabilities $P_i(t) = \left|\langle i|\psi(t)\rangle\right|^2$ for residues ranked by CTQW centrality.

Future!


OTOC(2) experiment beyond limit of classical simulation
Quantum experiment
65 qubits
1050 2-qubit gates
Circuit instance
27q
36q
Error ×10^3
Signal amplitude
Exp
Error model
SNR
System size
Classical tensor-contraction cost
Cotengra (with mem. constr.)
TNCO (with mem. constr + caching)
FLOPS
Runtime (s)
Optimization time on 1200 CPUs (secs)
Quantum runtime: 2.1 hours per circuit
Estimated accuracy: SNR ~ 2 to 3.
Estimated runtime on Frontier using best known
TN contraction algorithm: 3.2 years per circuit