Hybrid classical/quantum algorithms

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Variational Quantum Eigensolver (VQE)

- VQE was the first variational algorithm

Problem:

Find the ground energy of a Hamiltonian that describes a molecule or solid state system

- Solution: use variational principle on QC

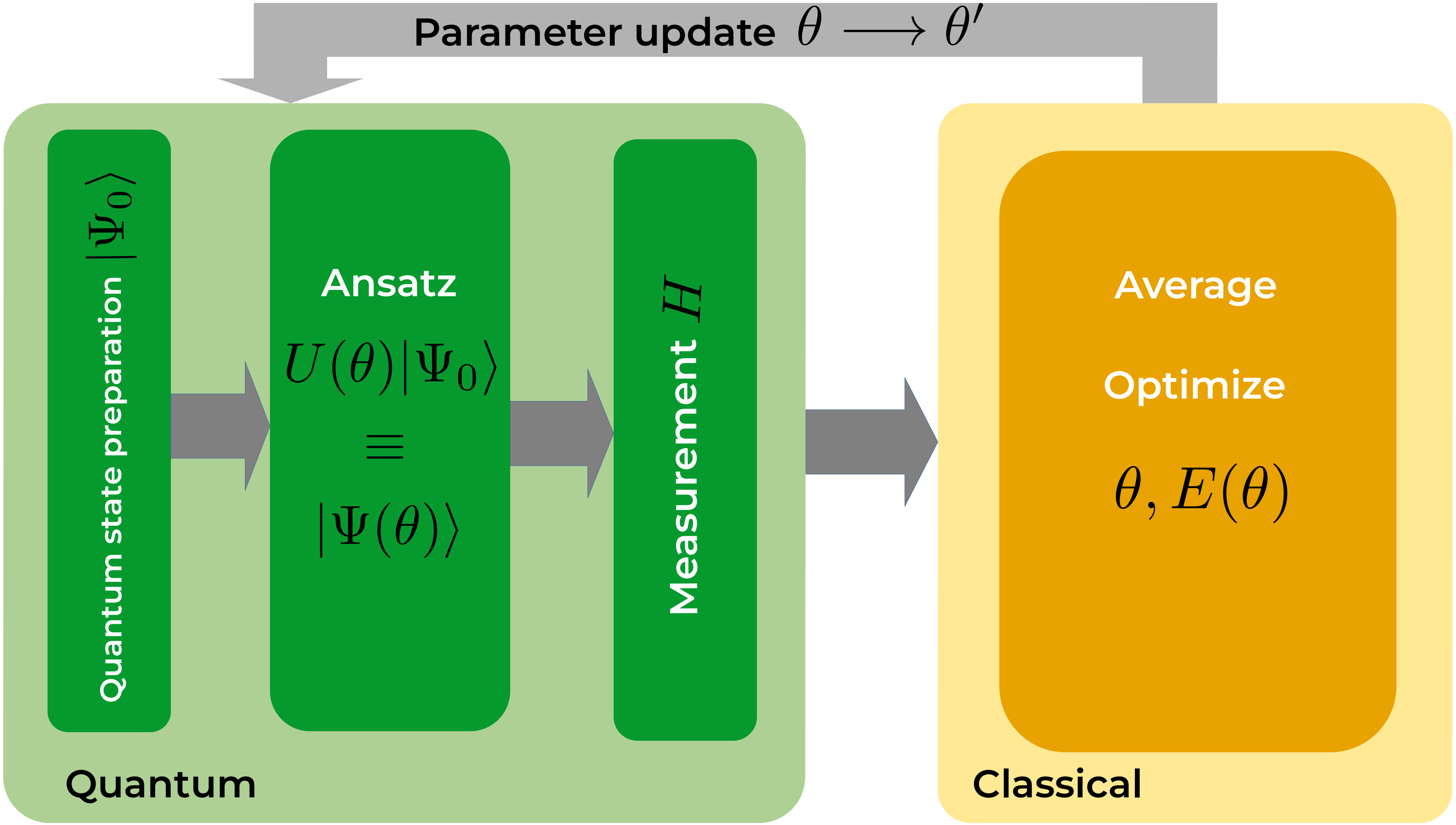
Variational principle

- Hamiltonian H describes the electronic structure of a molecule or solid state system
- Find a trial state $|\Psi(\theta)\rangle$ with parameters θ and compute $\langle H\rangle$
- Vary parameters θ to find the lowest value of $\langle H\rangle$

$$E_0 \leq \langle\Psi(\theta)|H|\Psi(\theta)\rangle \equiv \langle H\rangle$$

Variational principle

- It is extremely powerful and easy to use
- Even if $|\Psi(\theta)\rangle$ has no relation to the actual ground state, one often gets accurate values for the ground state E_0
- Disadvantage: we never know how close we are to the target value — only know that we have upper bound



Parameter update $\theta \longrightarrow \theta'$
Quantum state preparation $|\Psi_0\rangle$
Ansatz
$U(\theta)|\Psi_0\rangle \equiv |\Psi(\theta)\rangle$
Measurement H
Quantum
Average
Optimize
$\theta, E(\theta)$
Classical

Electronic structure

- Molecule characterized by Hamiltonian

$$H_{\mathrm{mol}} = H_{\mathrm{nucl}} + H_e$$

- Only interested in the electronic structure

$$H_e = \underbrace{-\sum_i \frac{\nabla_i^2}{2}}_{\text{electron kinetic}} \underbrace{-\sum_{i,I} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|}}_{\text{electron-nucleus}} + \underbrace{\frac{1}{2}\sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}_{\text{electron-electron}}$$

Electronic structure

- Express in second quantization

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

- $h_{p,q}$ kinetic energy of electrons and Coulomb interaction with nuclei

- $h_{p,q,r,s}$ electron-electron Coulomb repulsion

Map Hamiltonian to quantum computer

- Map fermionic Hamiltonian to qubit Hamiltonian

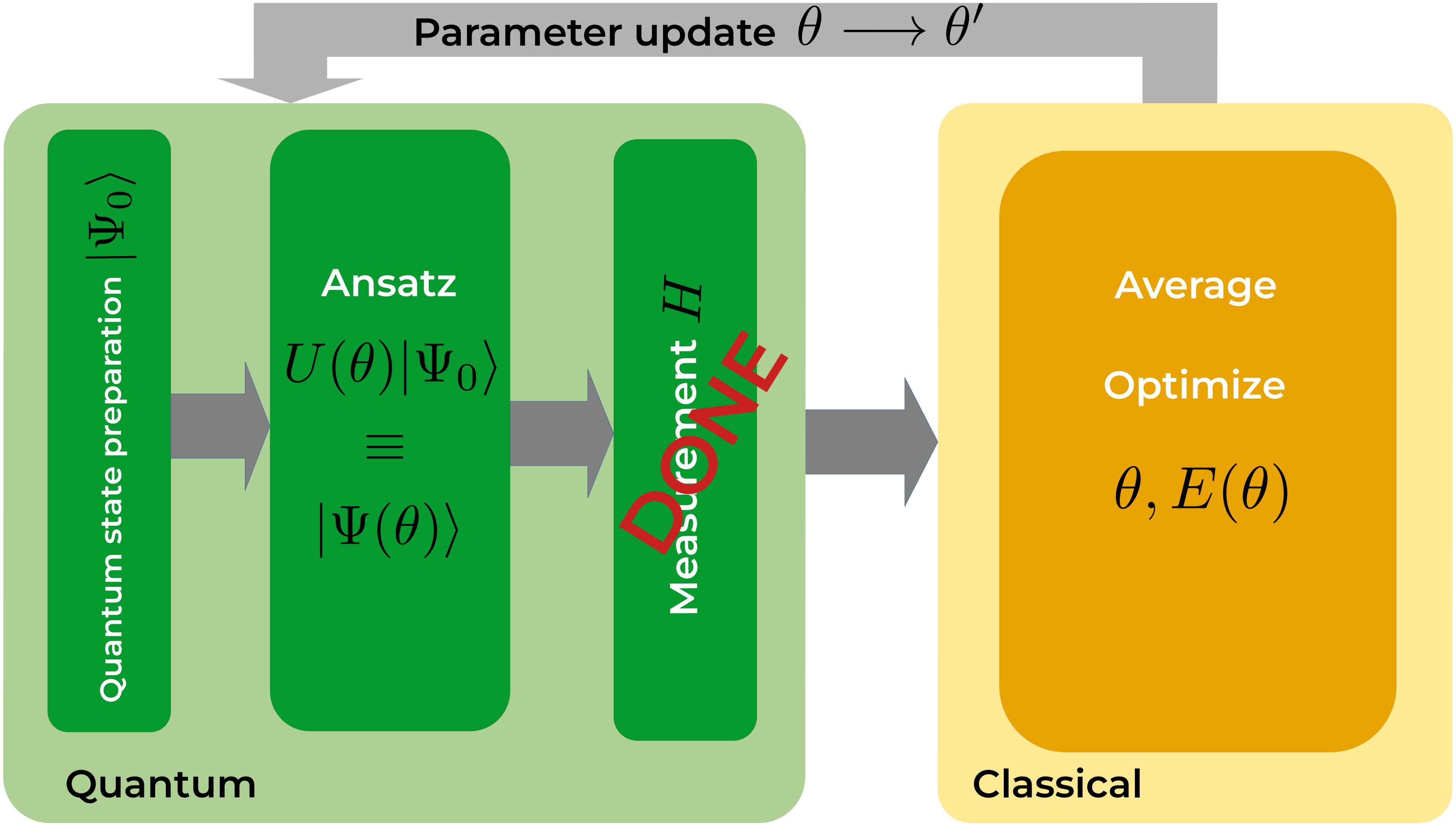
$$H = \sum_{p,q} h_{p,q} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} a_p^\dagger a_q^\dagger a_r a_s$$

$$H = \sum_j h_j \Pi \sigma_i^j$$

Map Hamiltonian to quantum computer

- **Qubit Hamiltonian: sum of Pauli strings**
- **Example: 4 qubit Hamiltonian for** H_2

$$
\begin{aligned}
H = {} & h_0 I + h_1 Z_0 + h_2 Z_1 + h_3 Z_2 + h_4 Z_3 \\
& + h_5 Z_0 Z_1 + h_6 Z_0 Z_2 + h_7 Z_1 Z_2 + h_8 Z_0 Z_3 + h_9 Z_1 Z_3 \\
& + h_{10} Z_2 Z_3 + h_{11} Y_0 Y_1 X_2 X_3 + h_{12} X_0 Y_1 Y_2 X_3 \\
& + h_{13} Y_0 X_1 X_2 Y_3 + h_{14} X_0 X_1 Y_2 Y_3
\end{aligned}
$$



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Ansatz circuit

- Inspiration from computational chemistry: Coupled Cluster (CC) method

$$|\Psi_{CC}\rangle = e^{T}|\Psi_0\rangle$$

$$T = \sum_i T_i \qquad T_1 = \sum_{i,\alpha} t_\alpha^i a_\alpha^\dagger a_i \qquad T_2 = \sum_{i,j,\alpha,\beta} t_{\alpha\beta}^{ij} a_\alpha^\dagger a_\beta^\dagger a_i a_j$$

- Unitary Couple Cluster (UCC) ansatz on quantum computers

Ansatz circuit

- UCC is the unitary version of CC

$$|\Psi_{UCC}\rangle = e^{T-T^\dagger}|\Psi_0\rangle$$

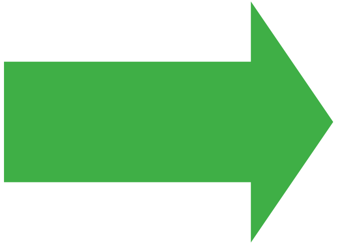
- Unitary $e^{T-T^\dagger}$ can be implemented on a quantum computer

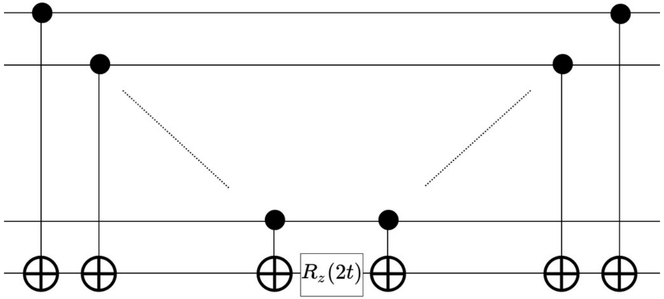
- Usually truncated to Single and Double excitations: UCCSD

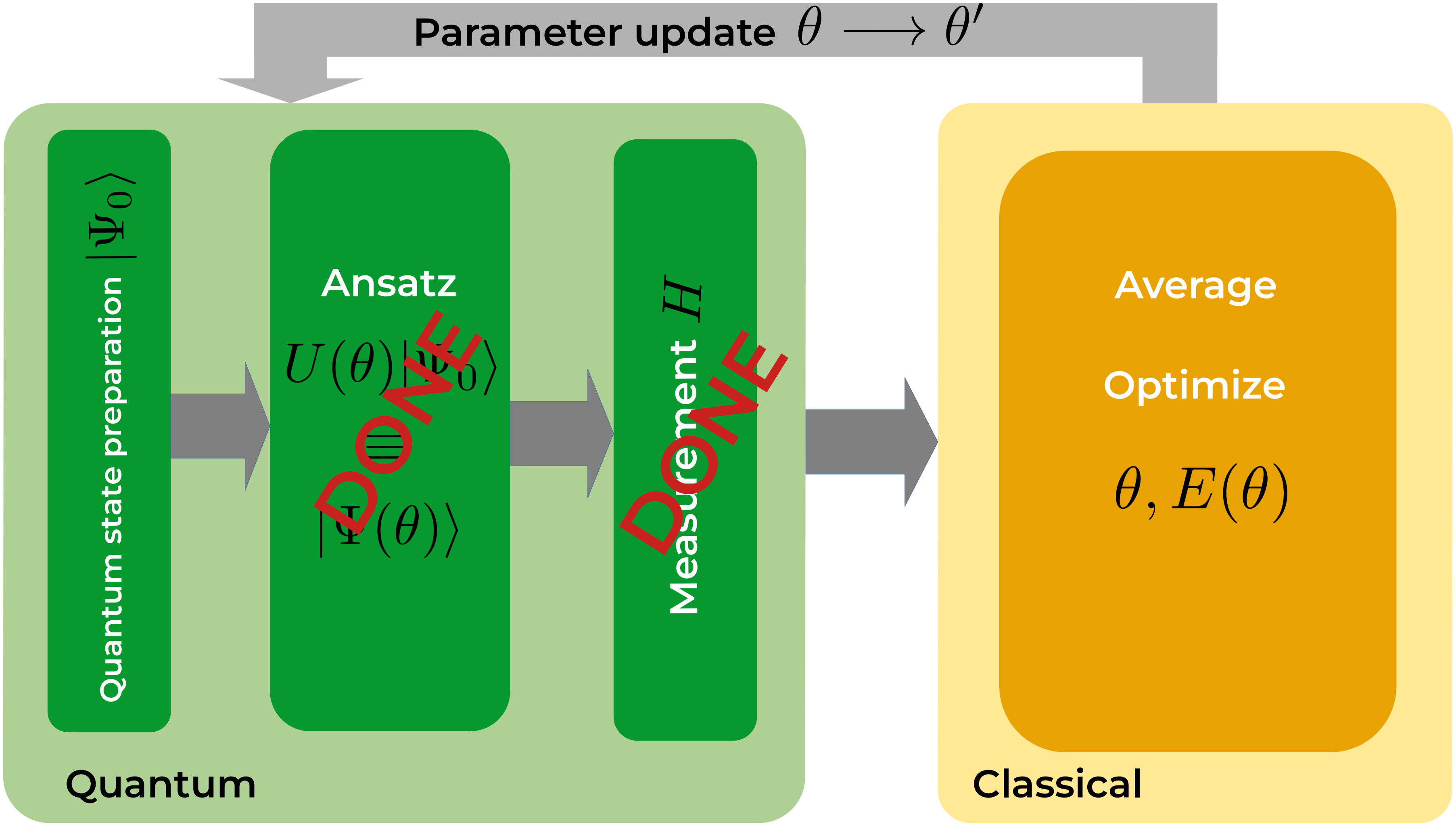
Ansatz circuit

- Implement UCC using Trotter-Suzuki decomposition of cluster operator $e^{T-T^\dagger}$
- Map exponents to qubits
- Qubit exponents realized as circuits

$$e^{-i\theta Z_1 X_2 \ldots Y_n}$$



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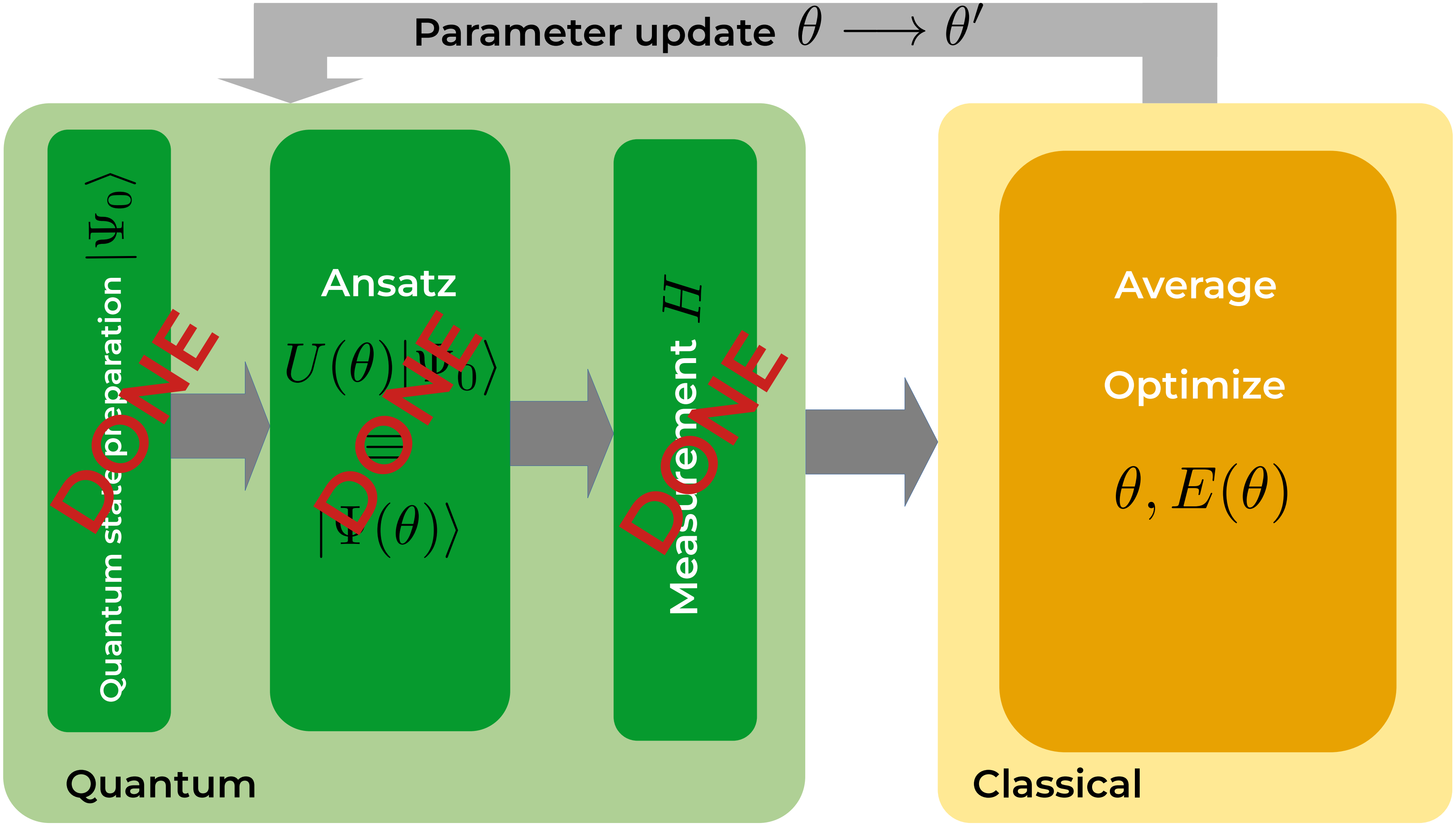
Initial state

- Classically compute the Hartree-Fock (HF) state
- Map to qubit state using Jordan-Wigner mapping, and prepare on the quantum computer
- Example: H_2 with 4 qubits

$$|\Psi_0^{\mathrm{HF}}\rangle = |0011\rangle$$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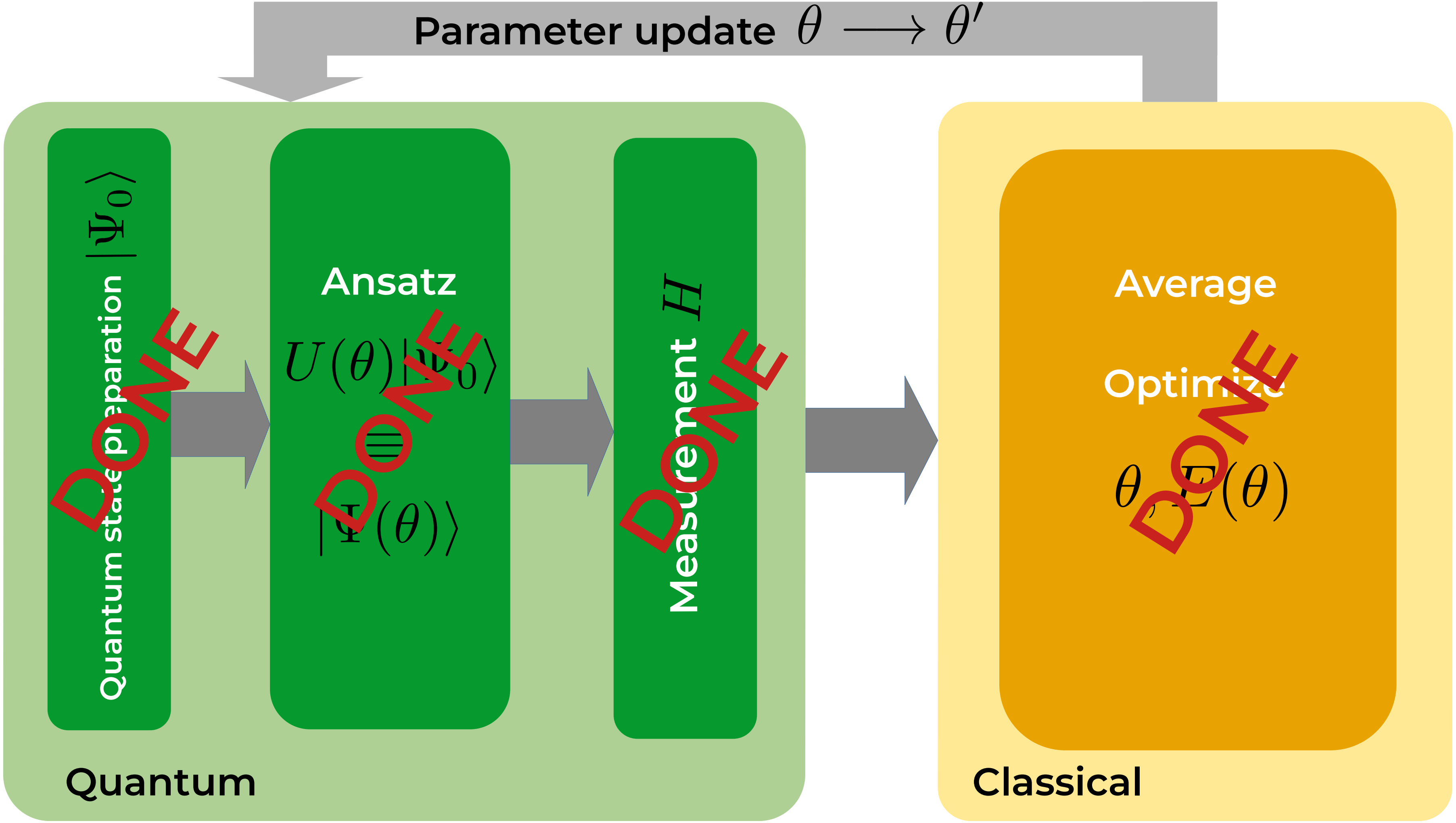
Optimization

- Optimization algorithm (Nelder-Mead, COBYLA, TNC, etc)
- Gradient based algorithms
- Combinations of different approaches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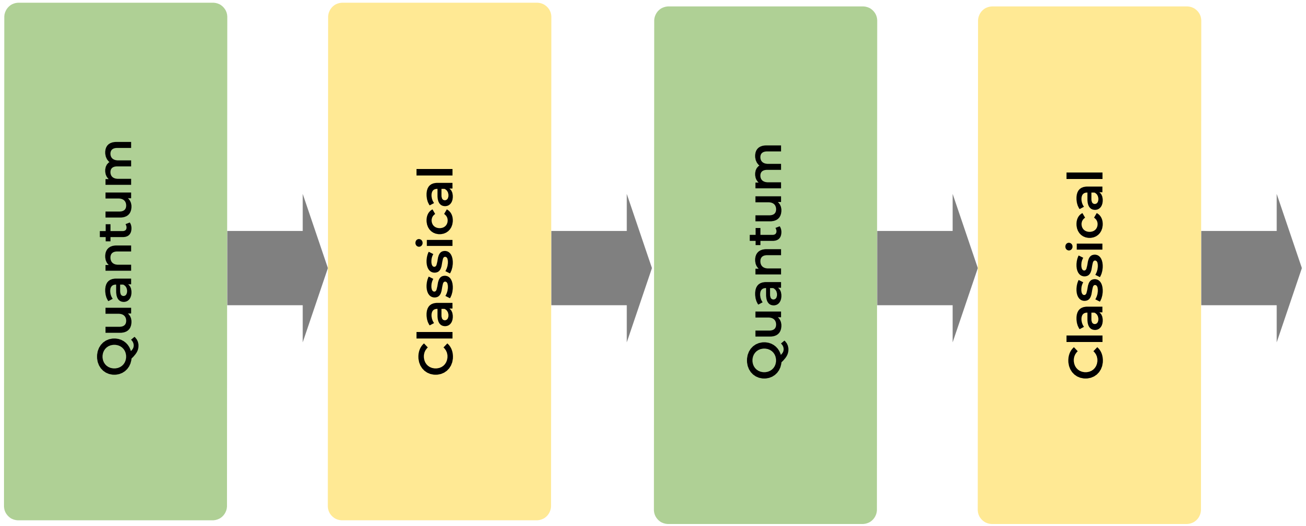
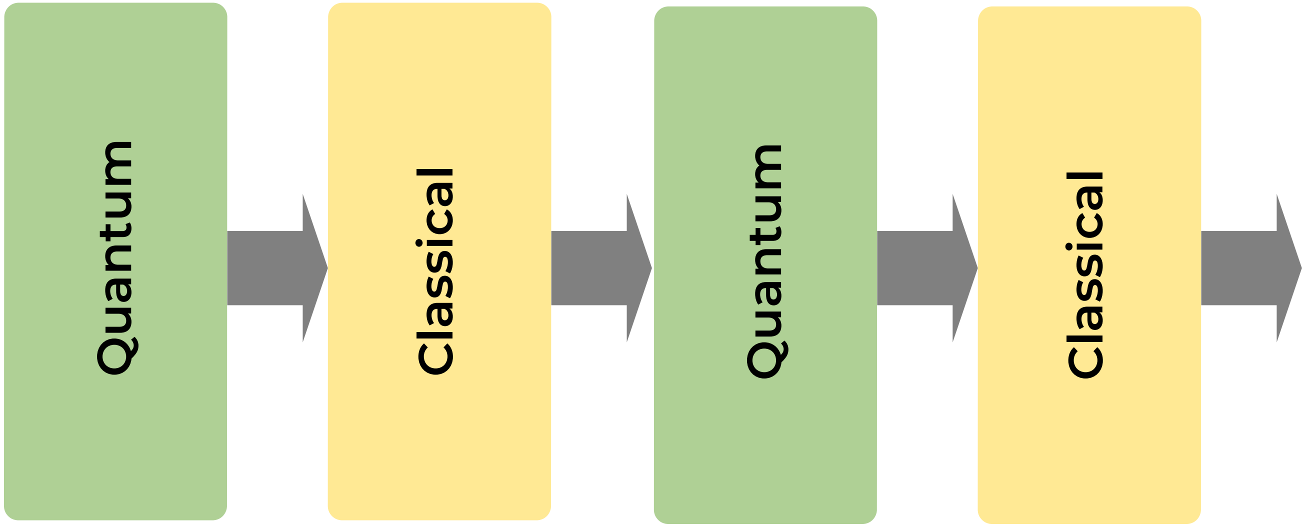
Running VQE



VQE advantage:

after each run the quantum circuit is reset, so "short" coherence time enough

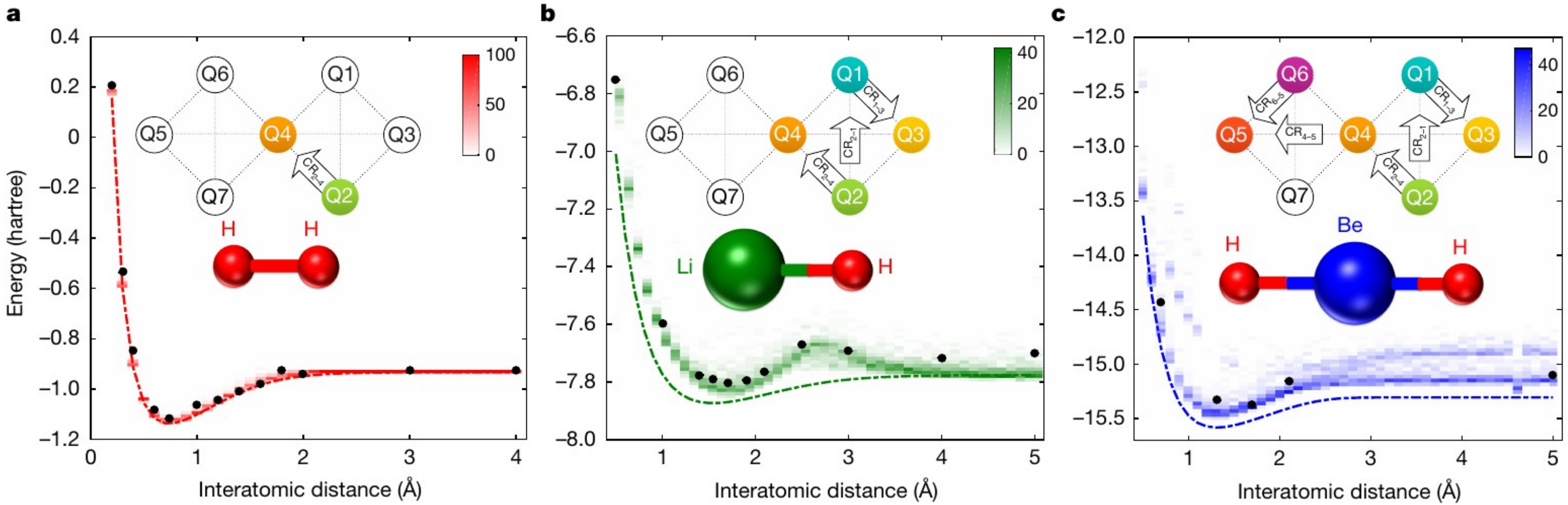
Running VQE



VQE challenge:
is quantum coherence time long enough?

Results: small molecules

- H2, LiH, BeH2 implemented on quantum hardware



Kandala etal 2017, Nature 549, 242-246

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