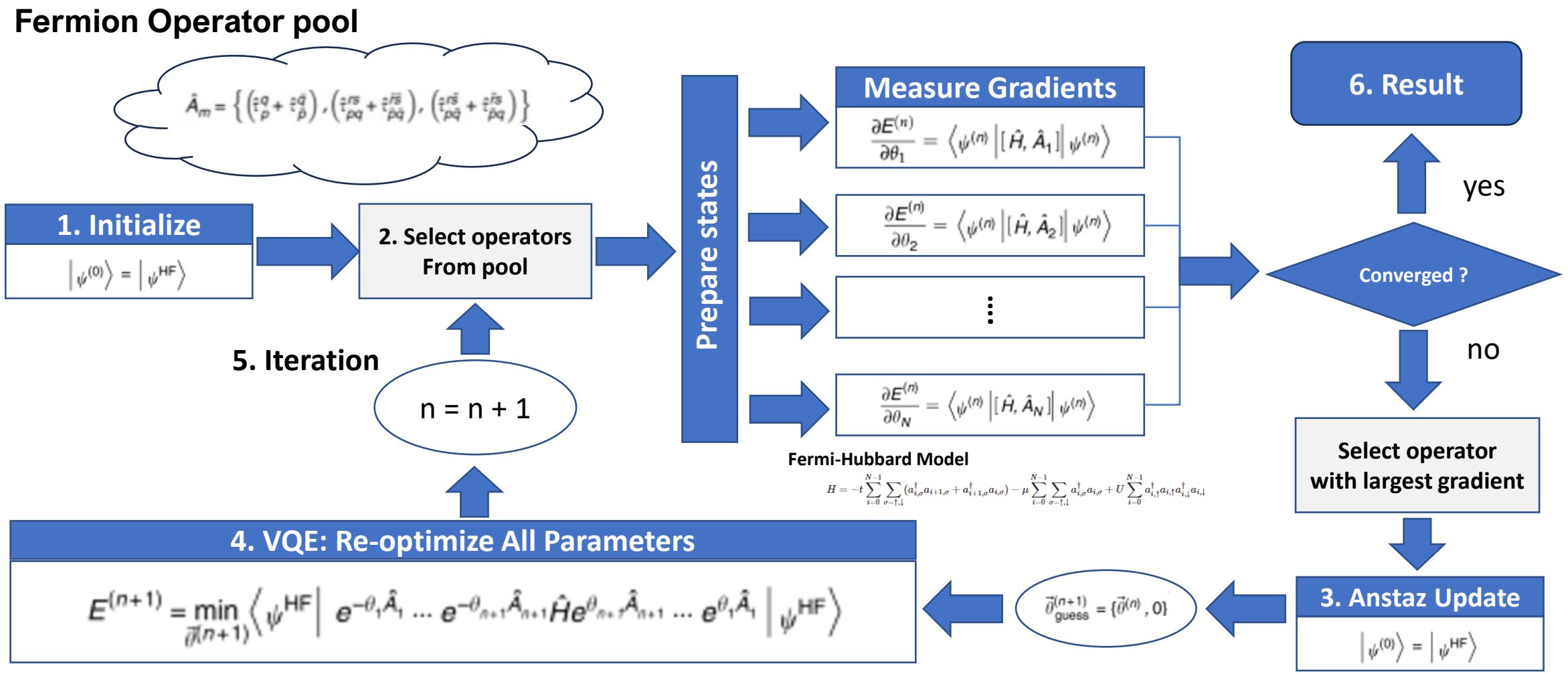


Grimsley, Harper R., et al. "An adaptive variational algorithm for exact molecular simulations on a quantum computer." *Nature communications* 10.1 (2019): 3007.

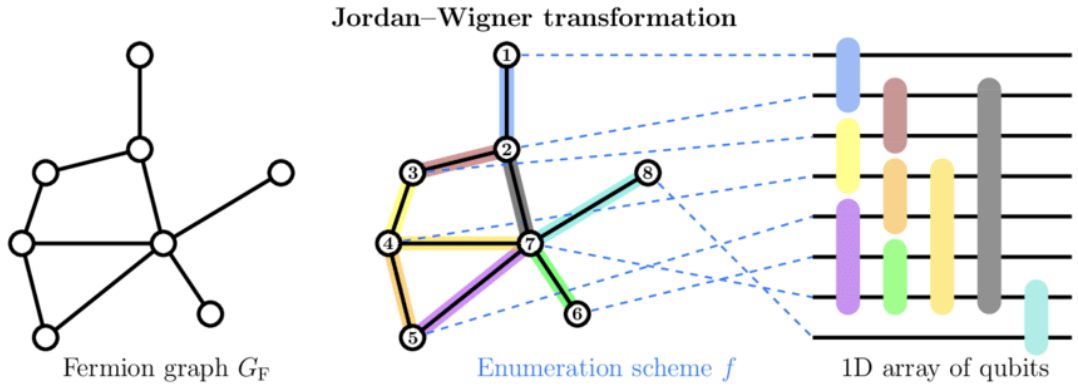
Process Flow of Adapt-VQE For Fermi-Hubbard Model

Team: QuanInt

Quantum Algorithm Grand Challenege 23'

Step 1: Initialization:

- The algorithm starts by initializing the Hamiltonian and the number of qubits.
- The fermion pool is initialized based on the number of orbitals (which is half the number of qubits). The fermion pool consists of single and double excitation operators.
- The fermion operators are then transformed into qubit operators using the Jordan-Wigner transformation. This forms the qubit pool.
- The initial state is set to a computational basis state, and the initial ansatz circuit is constructed from the Hartree-Fock state.



Chiew, Mitchell, and Sergii Strelchuk. "Optimal fermion-qubit mappings." *arXiv preprint arXiv:2110.12792* (2021).

Step 2: Operator Selection:

- For each operator in the qubit pool, the algorithm calculates the gradient of the operator with respect to the current state.
- The operator with the largest absolute gradient is selected and added to the ansatz.

Step 3: Ansatz Update:

- The ansatz circuit is updated by appending the selected operator.
- The new parameter associated with the selected operator is initialized to zero.

Step 4: Parameter Optimization:

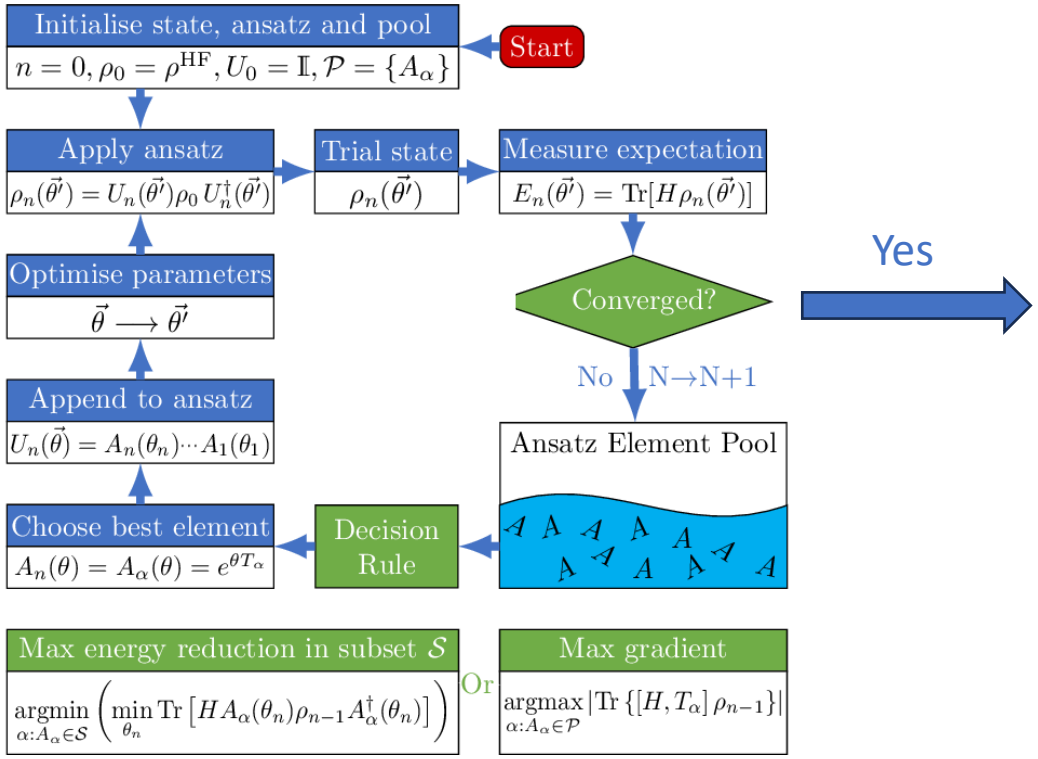
- The parameters of the ansatz circuit are optimized using the **Adam optimizer**.
- The cost function is the expectation value of the Hamiltonian, and the gradient is calculated using the parameter-shift rule.
- The optimization process updates the parameters to minimize the cost function.

Step 5: Iteration:

- Steps 2-4 are repeated until a stopping condition is met. In this case, the stopping condition is when the total quantum circuit time exceeds a certain limit.

Result:

- The final result is the minimum expectation value of the Hamiltonian, which represents the estimated ground state energy of the system.



END

```
Running algorithm(1)..
iteration 1
-7.817853896126992
iteration 2
-7.42228258172591
iteration 3
-7.456232891619905
iteration 4
-7.939863832387813
iteration 5
-7.643200256038577
iteration 6
-7.959757180457868

############## Result ##############
Resulting energy = -7.959757180457868
Circuit time = 1004.1084
####################################
```