Variational Quantum Eigensolver for H_2: Serial Implementation and Parallelization Strategy

MA453 - High Performance Computing

Fall 2025

1 Introduction

The Variational Quantum Eigensolver (VQE) is a hybrid quantum-classical algorithm designed to compute ground state energies of quantum systems. This report describes a serial implementation of VQE for the hydrogen molecule (H_2) and outlines a strategy for high-performance computing optimization.

2 Mathematical Model

2.1 The Variational Principle

VQE exploits the variational principle of quantum mechanics: for any trial wavefunction $|\psi(\theta)\rangle$ parameterized by θ, the expectation value of the Hamiltonian provides an upper bound on the ground state energy:

$$E(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle \geq E_0 \tag{1}$$

where E_0 is the true ground state energy and H is the molecular Hamiltonian.

2.2 Molecular Hamiltonian

For the H_2 molecule, the electronic Hamiltonian in second quantization is:

$$H = \sum_{i,j} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,\ell} h_{ijk\ell} a_i^\dagger a_j^\dagger a_k a_\ell \tag{2}$$

where h_{ij} are one-electron integrals and $h_{ijk\ell}$ are two-electron integrals computed using the Hartree-Fock method with the STO-3G basis set. This Hamiltonian is mapped to qubit operators via the Jordan-Wigner transformation.

2.3 Quantum Circuit Ansatz

The trial wavefunction is prepared using a parameterized quantum circuit:

$$|\psi(\theta)\rangle = U(\theta)|\text{HF}\rangle \tag{3}$$

where $|\text{HF}\rangle$ is the Hartree-Fock reference state and $U(\theta)$ is a unitary operator implemented as a double excitation gate:

$$U(\theta) = \exp\left(-i\frac{\theta}{2}(a_0^\dagger a_1^\dagger a_2 a_3 - a_3^\dagger a_2^\dagger a_1 a_0)\right) \tag{4}$$

This ansatz captures the dominant electron correlation effects in H_2 while requiring only a single variational parameter.

2.4 Optimization Problem

The VQE algorithm solves:

$$\theta^* = \arg\min_\theta E(\theta) = \arg\min_\theta \langle\psi(\theta)|H|\psi(\theta)\rangle \tag{5}$$

using the Adam optimizer with learning rate $\alpha = 0.01$ for 200 iterations per bond configuration.

3 Computational Approach

3.1 Problem Structure

The computational task consists of computing the potential energy surface by evaluating $E(\theta^*)$ for $N_b = 40$ bond lengths in the range $[0.1, 3.0]$ Å. For each bond length d_i:

1. Generate molecular Hamiltonian $H(d_i)$ using Hartree-Fock
2. Initialize variational parameters $\theta_0 = 0$
3. Optimize: $\theta_i^* = \text{Adam}(E(\theta), \theta_0, N_{\text{iter}} = 200)$
4. Store ground state energy $E_i = E(\theta_i^*)$

3.2 Serial Algorithm

Algorithm 1 Serial VQE for H_2 Potential Energy Surface

Input: Bond lengths $\{d_1, \ldots, d_{40}\}$
Output: Energies $\{E_1, \ldots, E_{40}\}$

for $i = 1$ to 40 **do**
    Generate $H(d_i)$ using Hartree-Fock
    $\theta \leftarrow 0$
    for $j = 1$ to 200 **do**
        $E \leftarrow \langle\psi(\theta)|H(d_i)|\psi(\theta)\rangle$ ▷ Quantum circuit
        $\theta \leftarrow \text{Adam\_step}(\theta, \nabla_\theta E)$
    end for
    $E_i \leftarrow E(\theta)$
end for
return $\{E_1, \ldots, E_{40}\}$

3.3 Computational Complexity

Each quantum circuit evaluation requires $O(4^n)$ operations for an n-qubit system using classical simulation. For our 4-qubit system:

- Circuit evaluations per bond length: 200
- Total circuit evaluations: $40 \times 200 = 8{,}000$
- State vector dimension: $2^4 = 16$

4 Performance Baseline

The serial implementation was benchmarked on a desktop CPU:

Metric	**Value**
Total Runtime	50.64 seconds
Time per Bond Length	1.27 seconds
Time per VQE Iteration	6.3 ms
Circuit Evaluations/sec	157.98

Table 1: Serial implementation performance metrics.

5 Parallelization Strategy

5.1 Embarrassingly Parallel Structure

The outer loop over bond lengths exhibits embarrassing parallelism: each bond length calculation is independent with no data dependencies. Mathematically:

$$E_i = f(d_i) \quad \text{for } i = 1, \ldots, 40 \tag{6}$$

where f is the VQE optimization procedure. This enables straightforward parallelization.

5.2 Proposed Optimization Phases

Phase 1: JIT Compilation

- Apply JAX just-in-time compilation to cost function
- Expected speedup: 2–5× from optimized circuit execution

Phase 2: Shared-Memory Parallelism

- Parallelize outer loop using Python multiprocessing
- Distribute $N_b = 40$ bond lengths across p cores
- Expected speedup: $S_p = p$ (ideal), $0.8p$ (realistic) for $p \leq 8$

Phase 3: Distributed-Memory Parallelism

- Use Ray for task-based distribution across cluster nodes
- Each node computes subset of bond lengths
- Expected speedup: Linear up to $p = 40$ nodes

5.3 Performance Model

For strong scaling with p processors and Amdahl's law:

$$S_p = \frac{1}{f_s + \frac{f_p}{p}} \tag{7}$$

where $f_s \approx 0.05$ (setup overhead) and $f_p \approx 0.95$ (parallel fraction). Predicted speedup:

Processors	**Ideal Speedup**	**Predicted Speedup**
4	4.0×	3.48×
8	8.0×	6.15×
16	16.0×	10.39×
40	40.0×	18.87×

Table 2: Predicted parallel speedup using Amdahl's law.

5.4 Efficiency Metrics

We will measure:

- **Speedup**: $S_p = T_1/T_p$ where T_p is runtime with p processors
- **Efficiency**: $E_p = S_p/p$
- **Strong scaling**: Fixed problem size, varying p
- **Weak scaling**: Problem size scales with p

6 Conclusion

The serial VQE implementation successfully computes the H_2 potential energy surface with well-characterized performance (0.84 minutes for 40 bond lengths). The embarrassingly parallel structure of the outer loop provides clear opportunities for HPC optimization with expected near-linear scaling up to 40 processors. Future work will implement the three-phase parallelization strategy and validate the performance predictions.