Electronic Energy Calculations using Hybrid Quantum-Classical Algorithms

Utkarsh[1], Shweta Sahoo, Harjinder Singh

Center for Computational Natural Sciences and Bioinformatics,
International Institute of Information Technology, Hyderabad

ABSTRACT

There are many computational problems that scale exponentially with the size and hence cannot be solved in polynomial time using classical computers. Quantum computing can offer an advantage by solving such problems in polynomial time. The computational capabilities of current *Noise Intermediate-Scale Quantum (NISQ)* devices are considerably restricted due to limited connectivity, short coherence time, poor qubit quality, and minimal error-correction. However, they still are very useful in simulating mathematically complex chemical systems that cannot be practically simulated on classical computers. We examine three hybrid quantum-classical algorithms to calculate the electronic energies of molecules: *Variational Quantum Eigensolver[1] (VQE)*, *Quantum Subspace Expansion[1] (QSE),* and *Variational Imaginary Time Evolution (VITE)[2]*. Here, for H_2 and HeH^+ molecular systems, the latter two are used for calculating the excited states, while the former for the ground state, and are implemented in the IBM Qiskit platform.

METHOD

1. The VQE attempts to find the ground state of a given problem Hamiltonian, by classically searching for the optimal parameters $\vec{\theta}$ to minimise: $\langle\Psi(\vec{\theta})|\hat{H}|\Psi(\vec{\theta})\rangle \geq E_0$ where E_0 is the lowest energy eigenvalue of the Hamiltonian *H*.
2. The state preparation and measurement subroutines are performed on the quantum computer: $|\Psi_{ref}\rangle = U_{prep}|0\rangle \qquad |\Psi(\vec{\theta})\rangle = U(\vec{\theta})|\Psi_{ref}\rangle$
3. We refer to $|\Psi(\vec{\theta})\rangle$ as the *ansatz state*, $U(\vec{\theta})$ as the *ansatz circuit*, and the set of all possible states that can be created by the circuit *U* is known as the *ansatz space*.
4. The measured observable $O(\vec{\theta})$ and parameter values are fed into a classical optimisation routine, which outputs new values of the parameters.
5. The QSE attempts to find the excited states by expanding the wavefunction in a subspace around the ground state by solving a generalised eigenvalue problem in fermionic Fock space.
6. The Hamiltonian projected into the subspace is given by $H^{QSE}_{ij,kl} = \langle E_0|a_i a_j^\dagger H a_k^\dagger a_l|E_0\rangle$ and the overlap matrix, required because the subspace states are not orthogonal to each other, is given by: $S^{QSE}_{ij,kl} = \langle E_0|a_i a_j^\dagger a_k^\dagger a_l|E_0\rangle$
7. Energies for excited states can then be calculated by solving the following: $H^{QSE}C = S^{QSE}CE$
8. In VITE, given an initial trial state $|\psi(\vec{\theta})\rangle$ the normalised imaginary time evolution is defined by: $|\psi(\vec{\theta},\tau)\rangle = A(\tau)e^{-H\tau}|\psi(\vec{\theta},0)\rangle$, where $\tau = it$.
9. To simulate the imaginary time evolution of the trial state, we use McLachlan's variational principle $\delta||(\partial/\partial\tau + H - E_\tau)|\psi(\vec{\theta}_\tau,\tau)\rangle|| = 0$ where the term $E_\tau = \langle\psi(\theta\tau)|H|\psi(\theta\tau)\rangle$ and evolution of parameters is obtained from the resulting differential equation:

$$\sum_j \mathscr{R}\left(\frac{\partial\langle\psi(\theta_\tau)|}{\partial\theta_i}\frac{\partial|\psi(\theta_\tau)\rangle}{\partial\theta_j}\right)\dot{\theta}_j = \mathscr{R}\left(\sum_\alpha \lambda_a \frac{\partial\langle\psi(\theta_\tau)|}{\partial\theta_i}h_\alpha|\psi(\theta_\tau)\rangle\right)$$

10. To get the (n+1)[th] excited state via *VITE*, we update our molecular Hamiltonian H using n[th] state previously obtained: $H' = H + \alpha|g\rangle\langle g| + \sum_{j=1}^{n}|e_j\rangle\langle e_j|$

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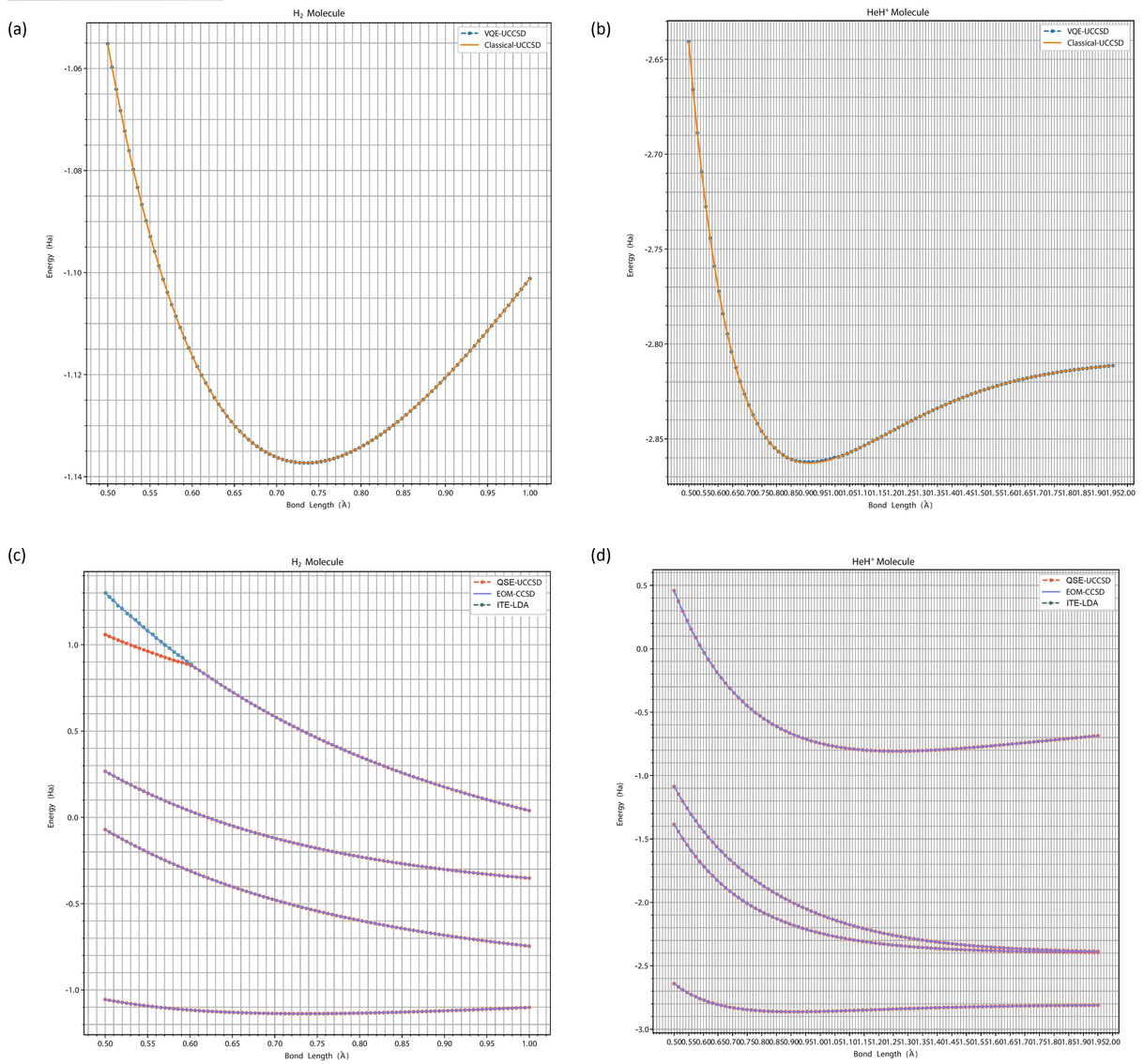
HYDERABAD

RESULTS



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[1] *utkarsh.azad@research.iiit.ac.in*