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Title: Benchmarking the VQE through HPC-simulation of the ground-state energy of prebiotic molecues

Abstract:

We have used the IBM Qiskit package for the Variational Quantum Eigensolver (VQE) to calculaate the ground state energies of prebiotic molecules - H_2O, H_2O_2, HCN and derivatives. We find that to achieve chemical accuracy requires basis sets that make the number of qubits and circuit depths increase beyond what can be handled by present and near-future high-performance computers (HPC). The great challenge will be to develop adaptive algorithms that efficiently include correlation effects in variational trial functions.