qSimulator: A Novel Method for Rapid Quantum Simulation of Molecules Using Cliques

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When quantum computers were first conceived of by Richard Feynman, the algorithm that motivated it was the simulation of quantum systems. Rapid performance of simulating quantum systems has applications from materials science to drug discovery. Since then, the circuit model theory for simulating a system, broadly known as Hamiltonian simulation, has improved to the optimal scaling. However, this circuit model requires devices with effectively perfect gates–something that is still far away. In the meantime, the current quantum computers can provide proof of concept speedups and may even suffice for outperforming classical algorithms. One method for performing Hamiltonian simulation on a quantum device is to use Trotterization, inspired by the seminal work by Seth Lloyd. Trotterization is the overall measurement of a system from the combination of individual measurements. This project provides an improvement upon this method whereby the individual measurements of the system in the Trotterization are grouped together into commuting cliques, an idea that has yet to be utilized for Hamiltonian simulation. The premise of the use of cliques is that grouping measurements together can provide a speedup for the overall simulation. By using a greedy clique-finding algorithm in pre-processing and feeding these cliques into Trotterization, there are speedups with explicit examples. This project also automates the clique method through the creation of a web app that displays the extreme promise that the clique method can offer.

Awards Won:
Arizona State University: Arizona State University ISEF Scholarship (valued at up to $52,000 each)
University of Arizona: Renewal Tuition Scholarship