QuantFold: Quantum Annealing with Turn Ancilla Encoding and Simulated Protein Folding for Drug Discovery Implications

Liu, Alice (School: Boston Latin School)

The Protein Folding Problem is characterized by the question on how a protein's amino acid sequence can determine its three-dimensional atomic structure. Increased understanding and accurate predicting of a protein's structure-function will allow for the accelerated formation of new protein-based drugs. The computational complexity of this is large, and conventional ways of using classical machine learning techniques are extremely restricted due to computational size limits run on current computers. With the rise of quantum computing relying on quantum mechanical properties such as superposition, entanglement and tunneling, this will allow for speedups in optimization methods. This specific study utilizes quantum annealing in order to simulate 2D lattice protein folding. The process tests the efficiency in the folding of amino acids in the varying lengths of 6, 9, and 12 residues with three different approaches: 1) simulated annealing with the conventional Monte Carlo method as the control variable 2) quantum annealing with turn ancilla encoding on a regular central processing unit (CPU) and 3) quantum annealing with turn ancilla encoding on a quantum processing unit (QPU) using D'Wave's hardware. An annealing algorithm is run where the lowest energy path for each sequence is determined by conducting random walks until the temperature cools to its minimum energy state. The method that leverages quantum annealing with turn ancilla encoding on a regular CPU yielded the highest number of instances that occurred in the lowest energy conformation when folding while quantum annealing with a QPU yielded the lowest runtime when reaching the minimum energy state.

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