

Folding lattice proteins with quantum annealing

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Summary

Quantum annealing aims to find the ground state of a Hamiltonian for optimization, and this method is applied to the challenging problem of protein folding using lattice models. The HP model, representing proteins as linear chains of hydrophobic and polar beads on a lattice, is used as a testbed. The authors propose a novel binary encoding approach for lattice proteins, inspired by D-Wave applications and a QUBO formulation. This method outperforms classical simulated annealing, achieving a 100% success rate against exact results for HP chains with up to 30 beads. It also accurately recovers known lowest energies for $N = 48$ and $N = 64$ HP chains. The approach combines quantum and classical techniques, and demonstrate successful folding of an $N = 14$ HP chain using a D-Wave Advantage quantum annealer.