## Digitized-Counterdiabatic Quantum Algorithm for Protein Folding

June 8, 2023

## Summary

This paper presents a hybrid classical-quantum digitized-counterdiabatic algorithm for solving the protein folding problem. The protein folding problem involves determining the lowest energy configuration for a given amino acid sequence. The algorithm utilizes a parametrized quantum circuit (PQC) inspired by counterdiabatic (CD) protocols, along with a classical optimization routine, to optimize the parameters of the circuit.

The algorithm is tested on proteins with up to 9 amino acids using different quantum hardware platforms such as trapped ions and superconducting circuits from Google and IBM. The results demonstrate that the algorithm achieves high success probabilities and is well-suited for implementation in the Noisy Intermediate-Scale Quantum (NISQ) era, where quantum computers have limited qubits and are subject to noise.

## Open problems

- 1. Selection of Suitable CD Terms: The paper needs more advanced techniques to choose the best CD term from the pool of NC operators, as the current selection is heuristic.
- 2. Difficulty in Finding Ground States for Large Systems: As system sizes increase, finding the exact ground state becomes harder due to the huge Hilbert space, requiring more efficient search methods.
- 3. Circuit Optimization for Real Hardware: Although the proposed ansatz reduces circuit depth, additional optimization strategies are necessary to improve performance on real quantum devices with limitations and constraints.

## Comments

The difficulty of the paper is high. We can work with the challenge of selecting Suitable CD Terms.