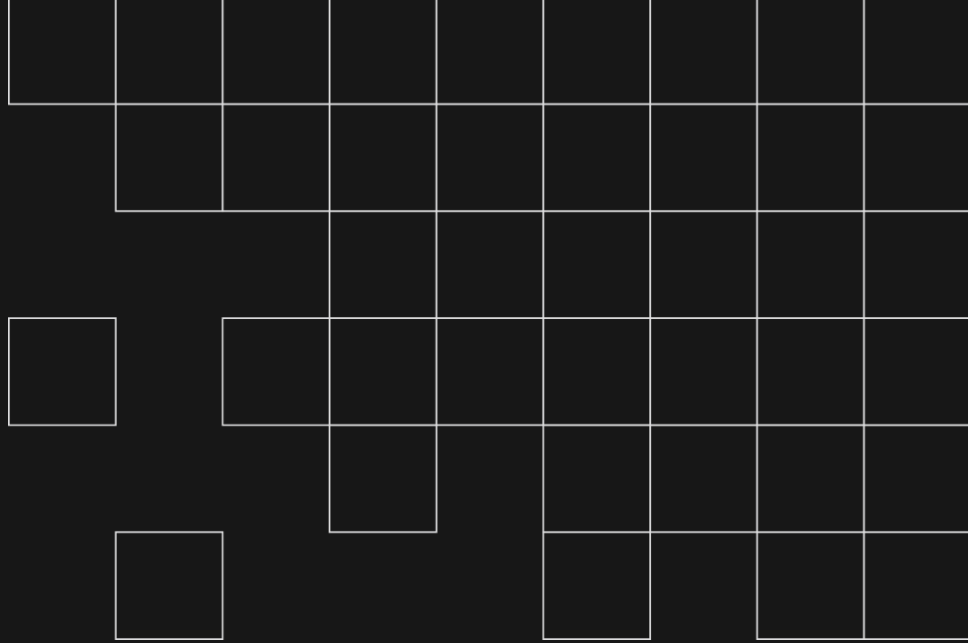# Tools for the Protein Folding Problem in Qiskit Nature

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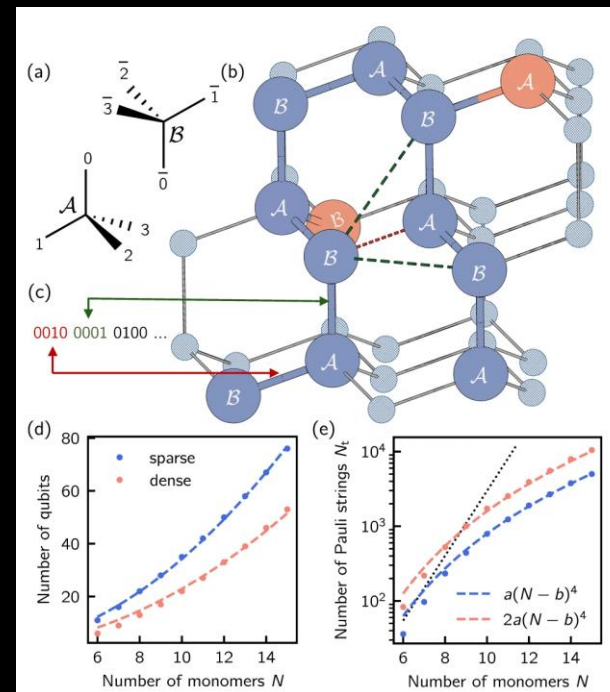Qiskit

What is the Protein Folding Problem?

Qiskit

- The protein folding problem refers to the task of analyzing how a protein chain folds and structures itself.

- Proteins perform a variety of functions such as acting as enzymes or hormones.

- A protein's function depends on its shape.

- The problem has been around for 50 years and is still considered intractable with modern computational methods. It is an NP-hard optimization problem.

- Understanding how proteins fold leads to a better understanding of other molecular processes and structures.

Quantum Computing for Protein Folding

- Recent experimental work in <u>Robert et al., 2021</u> demonstrates a NISQ-era solution.

- Represent the protein structure on a tetrahedral lattice.

- Encode constraints in a polynomial scaling Hamiltonian.

- Leverage variation quantum algorithms to simulate protein folding and compute energy of the conformations.

Proposed Project

- The current output of the protein folding algorithm in Qiskit Nature is a bit string corresponding to the folding sequence of the given protein.

- The resulting shape of the protein is not easily decoded from the bit string by the user.

- This project proposes to develop a system in Qiskit Nature to convert the bit string to a set of spatial coordinates that could easily be visualized or interpreted by the user.

- This entails understanding the protein encoding, modifying old PoC code to transform the output, exploring 3D plotting, and investigating more sophisticated visualization methods, and is concluded by a pull request to Qiskit Nature

Thank you

Matt Wright