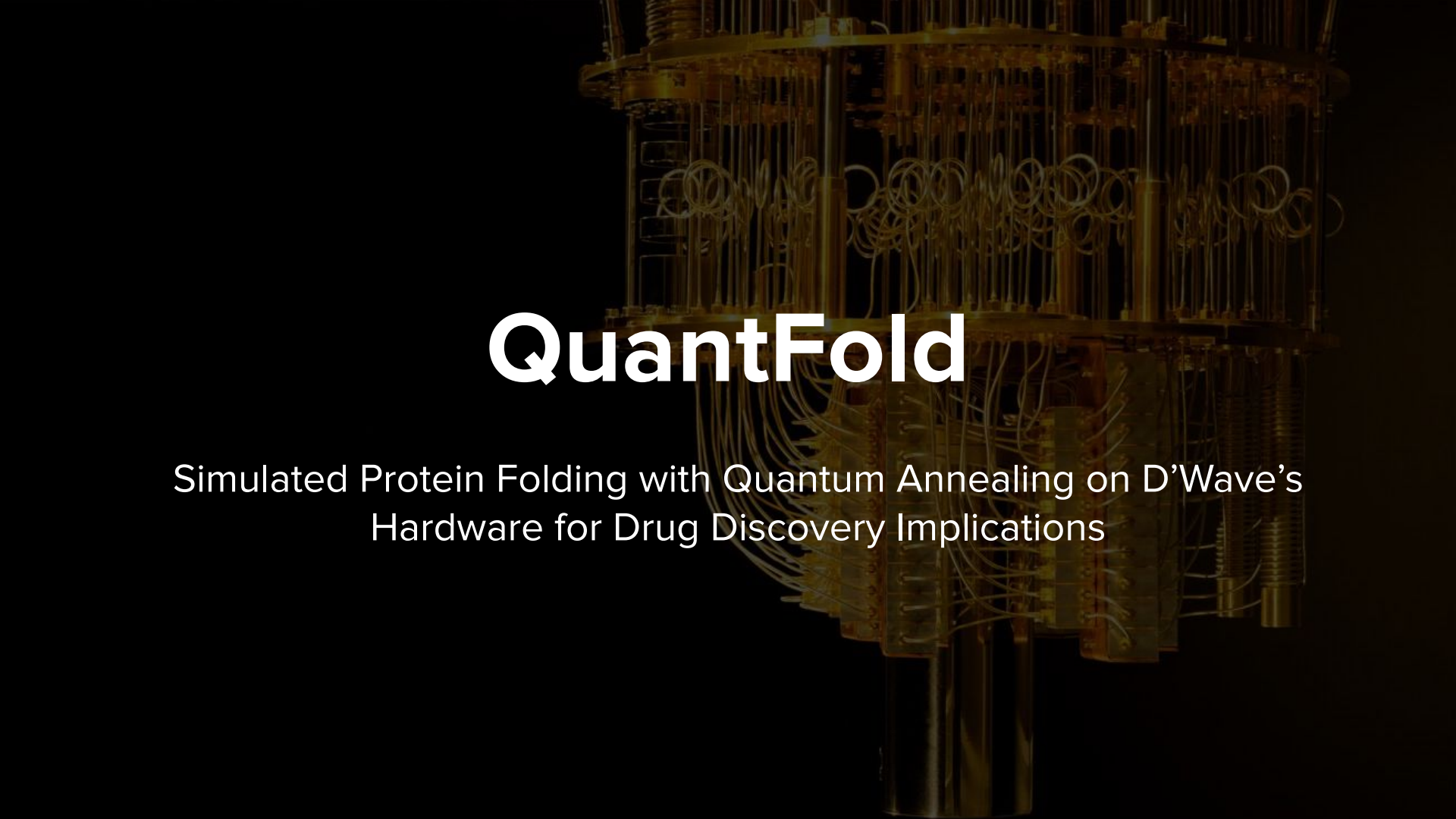
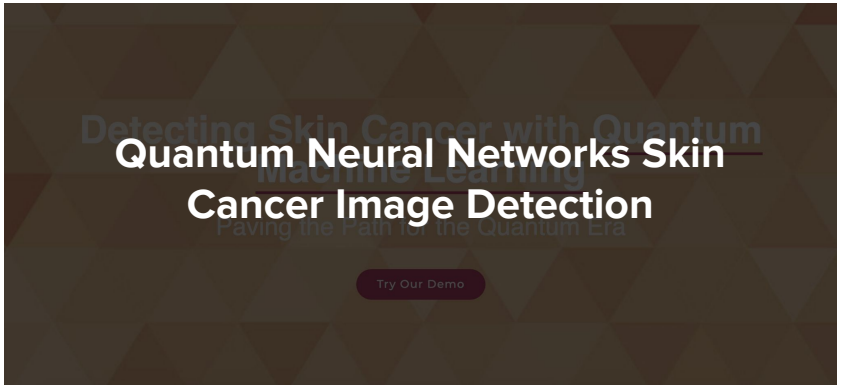


QuantFold

Simulated Protein Folding with Quantum Annealing on D’Wave’s Hardware for Drug Discovery Implications

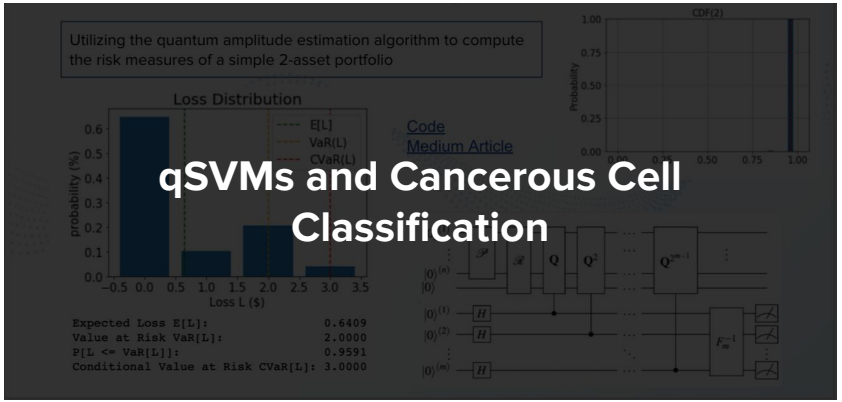
Quantum Neural Networks Skin Cancer Image Detection



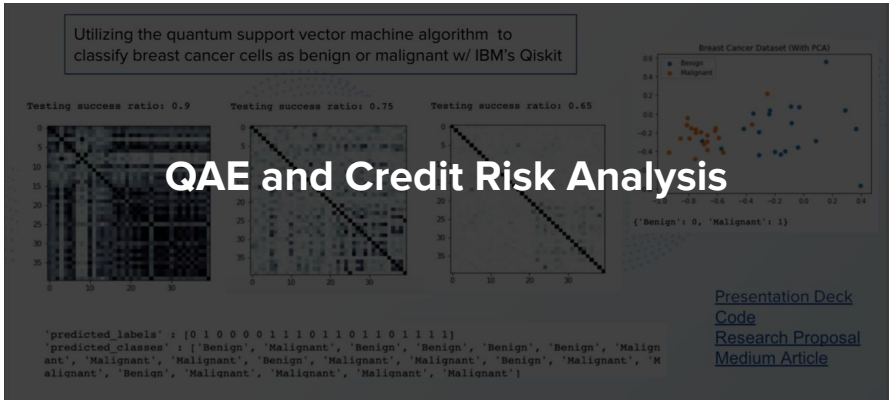
Anaxa - securing the storage & transmission process of health data

https://anaxa.tech/

qSVMs and Cancerous Cell Classification



QAE and Credit Risk Analysis



Over 6 million deaths per year due to neurodegenerative disorders

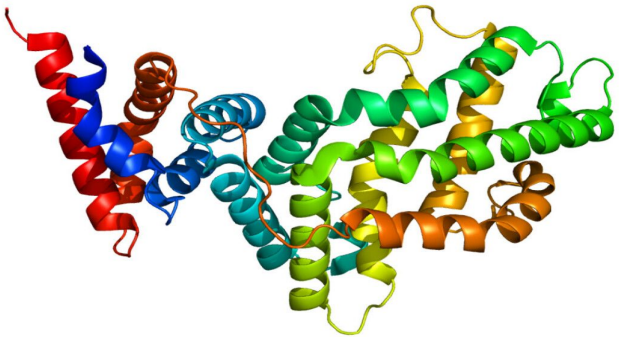
The Protein Folding Problem

> How can a protein's amino acid sequence dictate its three-dimensional atomic structure?

Sequence

GIAISVGFAYIMINTYFEVLVAF
WCCACWWFPKQNPKIHKHT
MIQTAEGQIMNPAGWHWR
GNIEKVGFACFNSTCLDICTW
WIDPETSEYAYNWMVHMDN

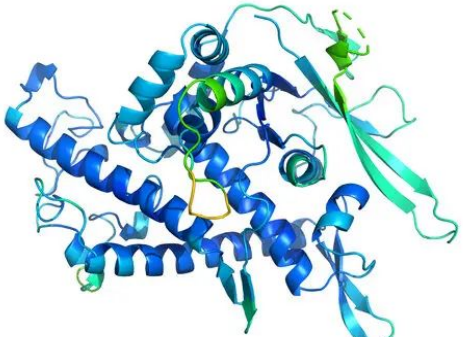
Structure



The Protein Folding Problem

> How can a protein's amino acid sequence dictate its three-dimensional atomic structure?

3D-Structure Relationship



Computational Drug Design

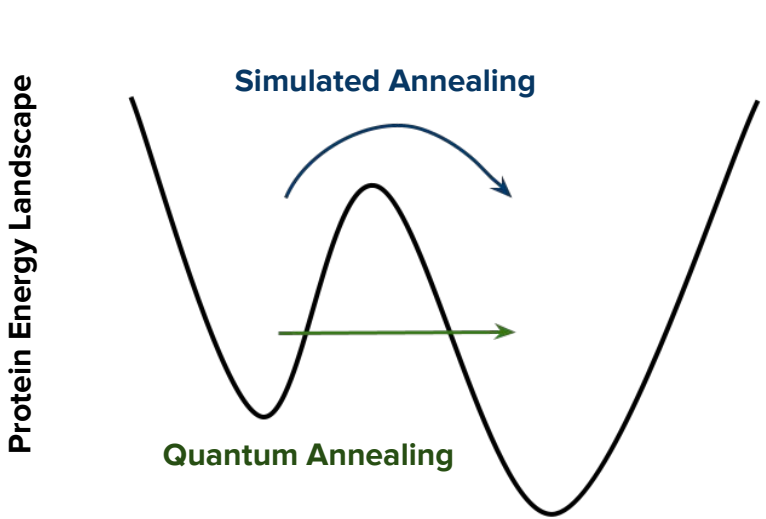
Our current computational methods are not efficient enough.

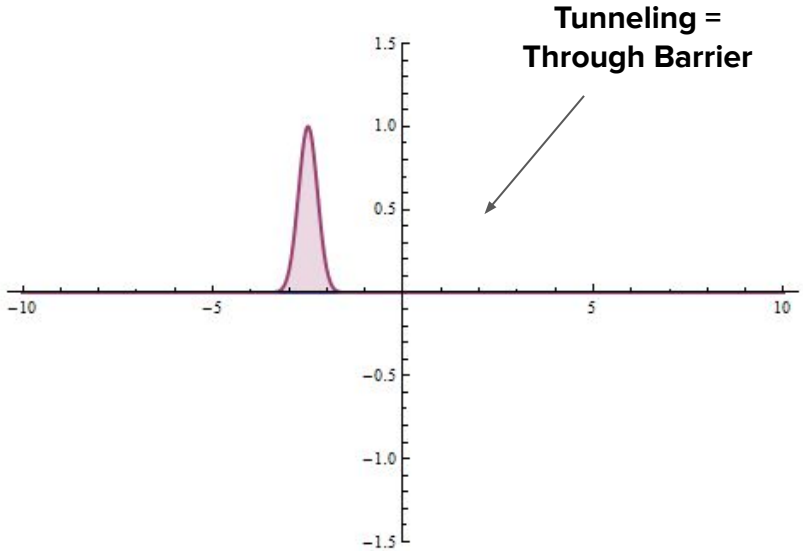
>150 residues proteins unable to be computed

No classical algorithm exists that is able to find a protein's minimum energy in polynomial time

Quantum Tunneling Effect

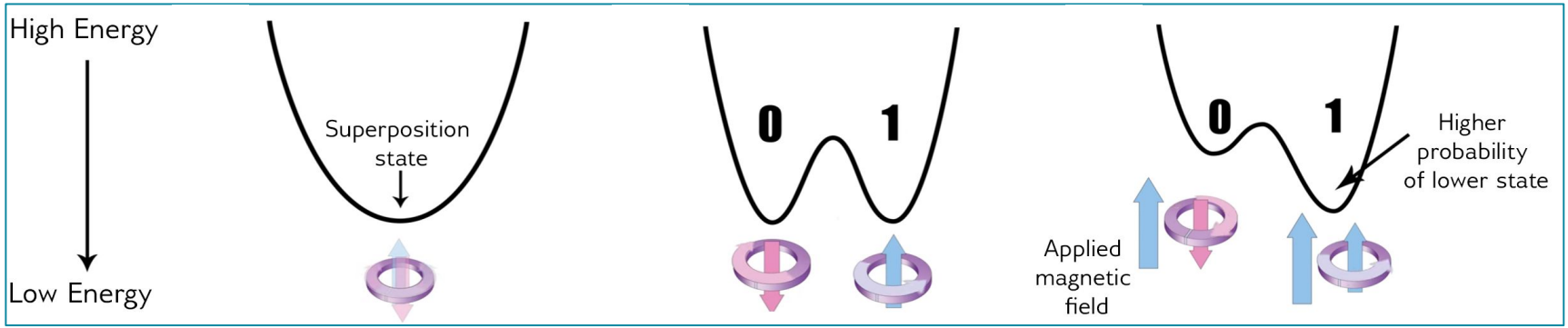
Simulated Annealing = Over Energy Barrier = ↑ Expensive
Quantum Annealing = Through Energy Barrier = ↓ Expensive





Quantum Annealing

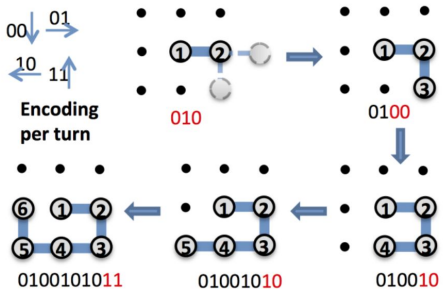
Finds protein's minimum energy with **speedup** from quantum tunneling



1. Apply biases and couplers to superpositions of qubits to optimize for annealing
2. Energy change computed, step is accepted for each residue
3. Energy landscape is defined and energy is minimized to reach native structure

n qubits = 2^n solutions able to be run at the same time

QuantFold



$$E(q) = E_{back}(q) + E_{overlap}(q) + E_{pair}(q)$$

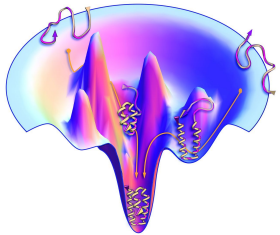
Turn Ancilla Encoding

1. Define a schedule for annealing temperature **T**
2. Randomly choose **ith qubit** q_i
3. Perform a qubit flip
4. Compute energy change in energy **ΔE** = E - E′
5. Accept step if **exp(-ΔE/T)** expresses the probability a state of energy E relative to the probability of a state of zero energy > **random.uniform(0,1)**.
   If $\Delta E <= 0$, always accept

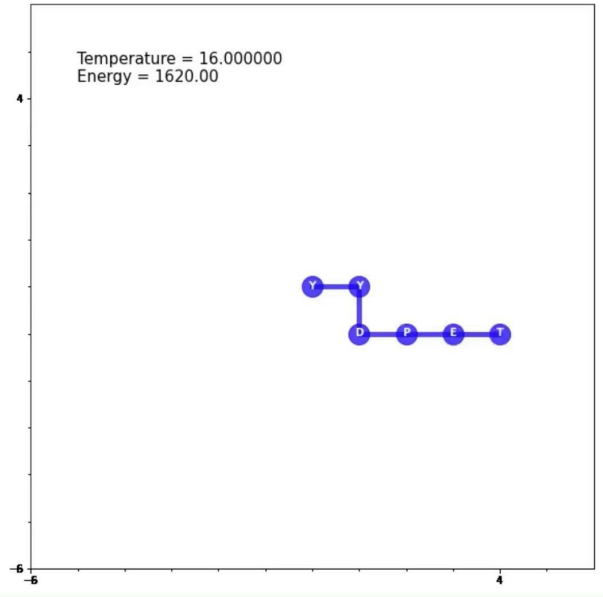
   Probability = $\frac{1}{1+e^{\frac{-\Delta E}{T}}}$
6. Process repeats as T → 0

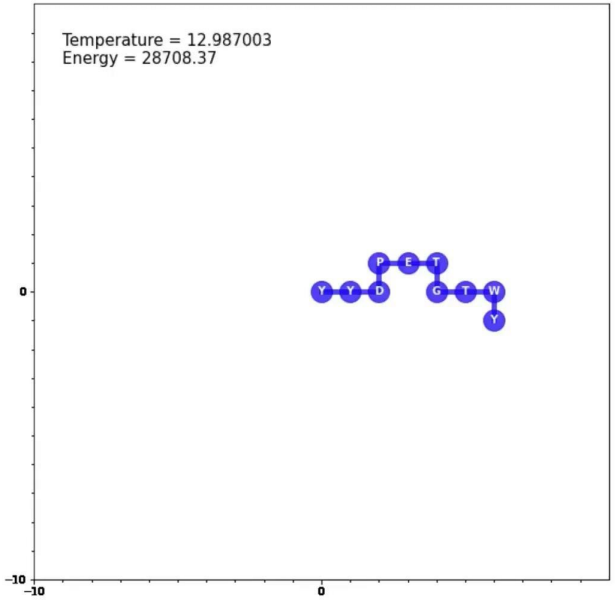
Quantum Annealing

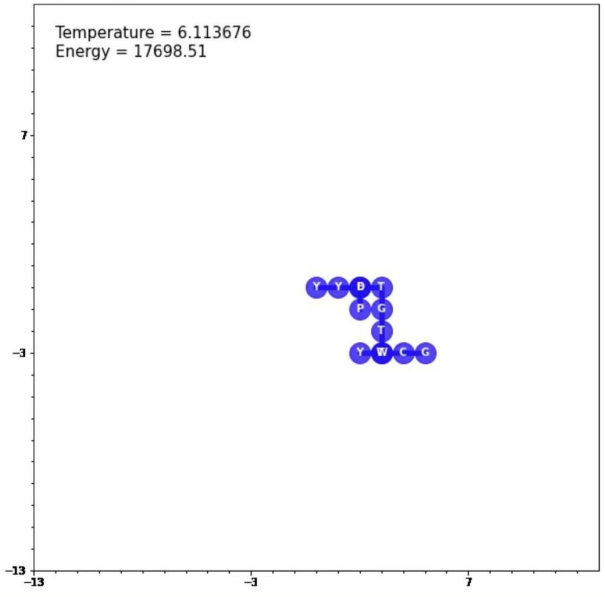
D-Wave
The Quantum Computing Company™



Run on D'Wave Annealer







6 Residues **9 Residues** **12 Residues**

	6 Residues	9 Residues	12 Residues
Conventional Simulated Annealing	**18.6%** **12.2 s**	**13.3%** **25 s**	**6.1%** **38.0 s**
Quantum Annealing, D'Wave's Annealer	**86.6%** **2.6 s**	**70.8%** **8.0 s**	**61.0%** **12.0 s**

QuantFold

Stage 1 **Stage 2** **Stage 3**

Let’s Connect!

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