

2. Use Case: Faster Drug Discovery with Quantum + AI

Problem

Traditional computers struggle to simulate complex molecules or protein folding due to the combinatorial explosion of quantum states.

Quantum Advantage

Quantum computers naturally process quantum phenomena like entanglement and superposition, enabling them to:

Simulate molecular structures more efficiently

Explore massive chemical search spaces in parallel

Speed up optimization tasks like binding energy calculations

AI + Quantum Synergy

AI (e.g., deep learning) can predict molecular properties.

Quantum helps simulate those molecules more accurately and quickly.

Together, they reduce the time and cost of discovering viable drug candidates.

Example:

A Variational Quantum Eigensolver (VQE) could find the lowest energy state of a molecule (most stable), and AI could predict which of those molecules are most likely to succeed in clinical trials.