

Quantum Simulation to Optimize AI 2: Drug Discovery

Quantum computing promises to solve complex tasks exponentially faster than classical computers, at least in some fields such as drug discovery, which has complicated molecular interaction processes.

In my case of this simulation, I produced a basic Bell State with IBM Quantum Experience and Qiskit. This quantum circuit combines two qubits via the Hadamard gate and the CNOT operator. This is the groundwork of quantum parallelism, as such an entangled qubit may simultaneously model many molecular states.

AI models can be used in drug discovery by searching large databases of molecules to find possible compounds. This may be sped up by Quantum AI, which is described and processed in the superposition of all possible states (molecular structures) and by collapsing that to the best using a quantum algorithm (e.g., Quantum Approximate Optimization Algorithm or Variational Quantum Eigensolver).

Although the current quantum-based hardware devices are underdeveloped (NISQ era), even smaller q-based networks such as this can reveal how AI-based healthcare and pharmacology will be accelerated.