Qubit Pharmaceuticals Accelerates Drug Discovery With Hybrid Quantum Computing

Startup adopts NVIDIA QODA to reduce the time and investment needed to identify promising treatments for incurable diseases.

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The promise of quantum computing is to solve unsolvable problems. And companies are already making headway with hybrid approaches — those that combine classical and quantum computing — to tackle challenges like drug discovery for incurable diseases.

By accelerating drug molecule simulation and modeling with hybrid quantum computing, startup Qubit Pharmaceuticals is significantly reducing the time and investment needed to identify promising treatments in oncology, inflammatory diseases and antivirals.

Qubit is building a drug discovery platform using the NVIDIA QODA programming model for hybrid quantum-classical computers and the startup's Atlas software suite. Atlas creates detailed simulations of physical molecules, accelerating calculations by a factor of 100,000 compared to traditional research methods.

Founded in 2020, the Paris and Boston-based company is a member of NVIDIA Inception , a program that offers go-to-market support, expertise and technology for cutting-edge startups.

Qubit has one of France's largest GPU supercomputers for drug discovery, powered by NVIDIA DGX systems . The startup aims for pharmaceutical companies to begin testing their first drug candidates discovered through its GPU-accelerated research next year.

"By combining NVIDIA's computational power and leading-edge software with Qubit's simulation and molecular modeling capabilities, we are confident in our ability to dramatically reduce drug discovery time and cut its cost by a factor of 10," said Robert Marino, president of Qubit Pharmaceuticals. "This unique collaboration should enable us to develop the first quantum physics algorithms applied to drug discovery."

Computational drug discovery involves generating high-resolution simulations of potential drug molecules and predicting how well those molecules might bind to a target protein in the body.

For accurate results, researchers need to perform massive sampling, simulating hundreds of different conformations — possible spatial arrangements of a molecule's atoms. They must also correctly model molecules' force fields, the electric charges that predict affinity, or how a molecule will bind to another.

This simulation and modeling requires high performance computing, so Qubit selected an in-house supercomputer built with NVIDIA DGX systems and other NVIDIA-accelerated servers, totaling 200 NVIDIA Tensor Core GPUs . The supercomputer runs Qubit's Atlas software, performing in just a few hours calculations that would take several years with conventional methods.

Atlas models quantum physics at the microscopic level to achieve maximum accuracy. The Qubit team is adopting NVIDIA QODA to explore the hybrid use of GPU-accelerated supercomputers and quantum computers, where QPUs , or quantum processing units, could one day speed up key software kernels for molecular modeling.

Using the NVIDIA cuQuantum SDK , Qubit's developers can simulate quantum circuits, allowing the team to design algorithms ready to run on future quantum computers.

Qubit estimates that while conventional research methods require pharmaceutical developers to start by synthesizing an average of 5,000 drug compounds before preclinical testing to bring a single drug to

market, a simulation-based drug discovery approach could reduce the figure to about 200 — saving hundreds of millions of dollars and years of development time.

The company's Atlas software includes AI algorithms for every stage of the drug discovery cycle. To support target characterization, where researchers analyze a protein that plays a role in disease, Atlas supports molecular dynamics simulations at microsecond timescales — helping scientists identify new pockets for drug molecules to bind with the protein.

During drug candidate screening and validation, researchers can use AI models that help narrow the field of potential molecules and generate novel compounds. Qubit is also developing additional filters that predict a candidate molecule's druggability, safety and cross-reactivity.

Learn more about Qubit's HPC and quantum-accelerated molecular dynamics software from company co-founders Jean-Philip Piquemal and Louis Lagardère through NVIDIA On-Demand .

Main image courtesy of Qubit Pharmaceuticals.

Original URL: https://blogs.nvidia.com/blog/2022/11/30/qubit-pharmaceuticals-accelerates-drug-discovery-quantum-computing/