Dell Technologies Hybrid Quantum Computing Solution with NVIDIA for the Pharmaceutical Industry

There is a burgeoning interest within the pharmaceutical industry in the potential of Quantum Computing. As quantum computing evolves, it stands to revolutionize the drug discovery process, helping significantly reduce the time and cost required to discover, develop, test, and release new drugs. In traditional drug discovery, once a molecule is identified to treat a disease, millions of compounds must be screened. From this massive pool, only a few hundred are further tested, narrowing the options down to a select group of candidates. These candidates then undergo rigorous clinical trials—a process that is both time-consuming and costly. The screening process is computationally demanding and often yields suboptimal results. However, quantum computing, with its prowess in simulating chemical and biological systems, could revolutionize this process. It strives to provide detailed simulations of drug molecules, providing deeper insights into their interactions with target molecules. While quantum computing technologies are advancing rapidly, fully achieving these capabilities is still several years away. During this period, companies in the pharmaceutical industry are investigating how to best utilize quantum computing.This is the time for learning and experimenting, creating proof of concepts, and understanding how they might adopt quantum-based solutions as the technology matures.

A promising strategy for these companies is adopting a hybrid quantum model. For instance, Dell Technologies' existing quantum architecture, as offered in the Dell Technologies Quantum Computing System (DQCS), when combined with NVIDIA's cuQuantum appliance, provides a robust platform. This hybrid approach integrates classical computing processes before introducing quantum solutions. With NVIDIA enhancing processing speed and capability, this collaborative effort between Dell Technologies and NVIDIA allows steady progress and a smooth transition to a fully quantum-ready state.

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The Need for Hybrid Quantum Computing with Powerful Quantum Simulation

The unparalleled performance anticipated from quantum computing promises to radically change how businesses will solve their most difficult and complex problems. Beyond the financial services industry, quantum computing is expected to be used to address problems in diverse fields such as weather predictions, drug discovery, supply chain optimization, and manufacturing.

To prepare for the emergence of quantum computing, researchers and enterprises need to explore how they might use its capabilities to address these hard problems. To do so, they must develop, test, and validate hypotheses; experiment with new algorithms, and evaluate how quantum operations may be used as they prepare themselves for the coming availability of quantum processing. This means there is a real need for a platform that puts quantum computing's potential within arm's reach, with the hardware and software that provides an environment to empower organizations to explore quantum effectively.

The solution for this platform is Hybrid Quantum Computing, where classical computing handles the heavy processing necessary before and after executing quantum algorithms and provides the virtual Quantum Processing Units (vQPUs) used to simulate quantum computing. The hybrid architecture provides the environment necessary for users to experiment, develop, and test hypotheses today, and be ready to run these on real quantum computers as they mature.

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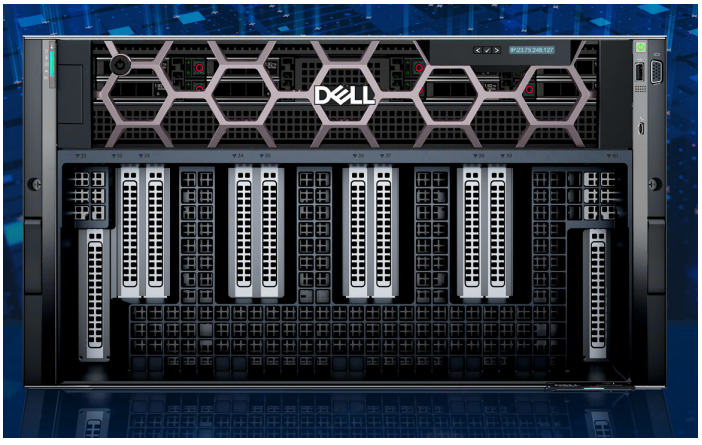
Dell Technologies Hybrid Quantum Solution + NVIDIA cuQuantum Appliance on Dell XE9680

Dell Technologies is taking the lead in hybrid quantum computing, helping its customers to speed time to innovation and discovery.

Previously, Dell Technologies has demonstrated a hybrid solution, joining Dell PowerEdge R740xd with IonQ's simulation engine and quantum processing unit (QPU), to support integrated classical and quantum simulation workloads running on-premises and connect to remote QPUs when needed. This is described in The Importance of On-Premises Hybrid Classical-Quantum Computing.

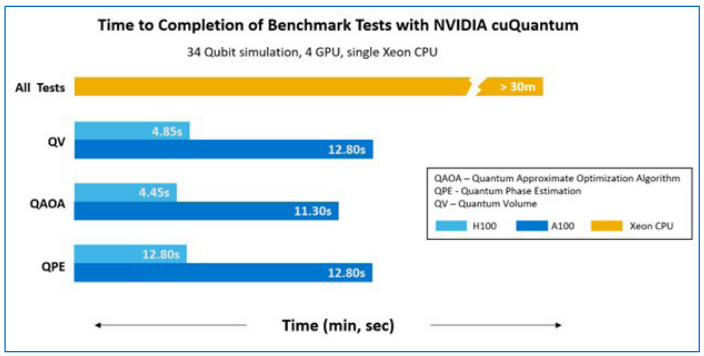
Now Dell Technologies has allied with NVIDIA, creator of the NVIDIA cuQuantum Appliance, to offer a quantum simulation solution that will help academic and business organizations explore the potential of quantum computing as the technology evolves.



Dell XE9680

The NVIDIA cuQuantum Appliance is built on the world's most popular AI accelerator—NVIDIA H100—and powered by NVIDIA's containerized cuQuantum software stack. It is a complete quantum simulation solution in a box, allowing users to get up and running quickly.

Key to any solution's success its ability to deliver results quickly and that means providing the infrastructure necessary to power the workloads. Dell Technologies recently executed benchmark quantum algorithm to check the performance of quantum algorithms on the Dell Technologies + NVIDIA solution; the results are presented here.



Results based on testing by Dell Technologies, May, 2023.
Actual performance may vary.

The benchmark tests executed on systems running cuQuantum: a PowerEdge XE9680 using 4 of its 8 H100 GPU, and a PowerEdge R740xd, using its full complement of 4 A100s. The algorithms included: a QV algorithm, which is a pure quantum benchmark, QAOA, typically used for optimization problems, and QPE, a fundamental subroutine for chemistry and biology problems. Testing demonstrated the dramatic performance of the GPUs, with the A100 configuration running 140x faster than on a single Xeon CPU, the H100 **up to 400x faster.**

Key Benefits of the Dell Technologies + NVIDIA Solution

- **Discover:** Lower the barriers to entry with learning and experimentation.

  The cuQuantum Appliance is a breakthrough solution that makes quantum exploration accessible to developers and researchers around the world.

  Dell Technologies provides the guidance, documentation, and hardware and software infrastructure, integrated with cuQuantum, for a full hybrid quantum solution that accelerates the discovery, test and validation of key concepts needed to deliver optimized solutions based on hybrid quantum computing.

- **Identify:** Reduce adoption risks by exploring uses case and benefits.

  Using Dell Technologies' hybrid quantum solution with NVIDIA cuQuantum, businesses can experiment with how they might best apply quantum computing to its most business-critical use cases, to gain a competitive edge. Dell Technologies can also act as your trusted advisor for the tools, expertise and infrastructure needed for success.

- **Deploy:** Choose the right execution environment and achieve real business benefits.

  By using the Dell Technologies and NVIDIA cuQuantum solution, enterprises will de-risk future application development with a ready-to-run platform that bypasses the constraint of on-boarding quantum infrastructure when transitioning from a vQPU to a real QPU.

Learn more about the
Dell Quantum Advantage