

Quantum Simulation

at Pawsey Supercomputing Research Centre
(Perth, Western AUSTRALIA). v5

eResearch, Christchurch, NZ – Feb 2025

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Who XENON Systems



- **About XENON Systems**

XENON Systems is an Australian-based systems integrator and reseller, headquartered in Melbourne. www.xenon.com.au

- **Established Expertise**

Founded in 1996, XENON now largest and most experienced high-performance computing (HPC) team in the APAC region.

- **Geographic Reach**

Initially operating across Australia, XENON is now expanding its services throughout the APAC region.

- **Core Focus**

The company specialises in HPC, research, and serving the technical and scientific user community.

- **Solutions and Services**

XENON offers Compute, Storage, and Networking solutions, along with tailored services.

- **Customer Base**

Its primary customers include universities, research organisations, and government agencies.

- **Unbiased Approach**

XENON is hardware-, software-, and solution-agnostic, ensuring unbiased recommendations and proposed solutions.

- **Commitment to Customers**

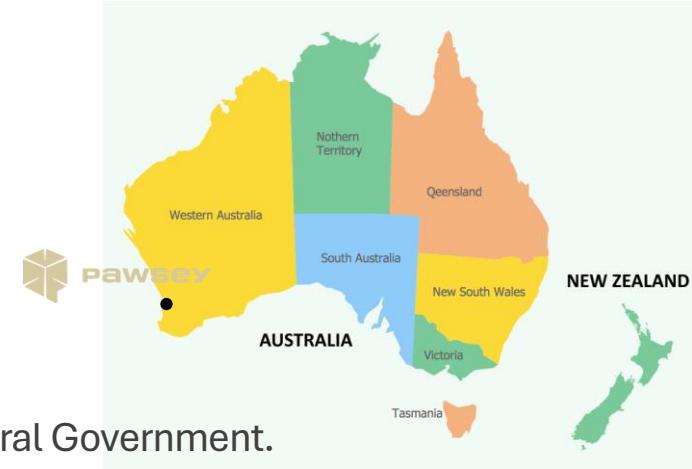
The company delivers first-class, innovative, and price-competitive solutions.

Have supplied and deployed solutions; and provide on-going support to customers in NZ; e.g. NiWA, NeSI and Todd Energy

Who is Pawsey?

- **Pawsey ?**

A supercomputing centre based in Perth (Kensington), Western Australia. <https://pawsey.org.au/>
One of two “Tier-1” national high-performance computing (HPC) facilities in Australia.



- **Funding and Support**

Funded and supported by both the Western Australian State Government and the Australian Federal Government.

- **Setonix Supercomputer**

Home to the most powerful research computer in the Southern Hemisphere, the HPE Cray EX Supercomputer (~1800 nodes).

- **Massive Data Storage**

Hosting some of the largest data storage repositories in the Southern Hemisphere:

- **Acacia:** ~90 PB of Ceph object storage, serving as a warm storage tier. [Expanded by XENON.](#)
- **Banksia:** 130+ PB archive storage (2x 70+ PB tape libraries) for long-term cold storage. [Supplied by XENON.](#)

- **Quantum Computing Pioneer**

Home to the world’s first room-temperature Quantum Computer at a HPC facility.
In partnership with Quantum Brilliance.

- **Grace-Hopper Innovation**

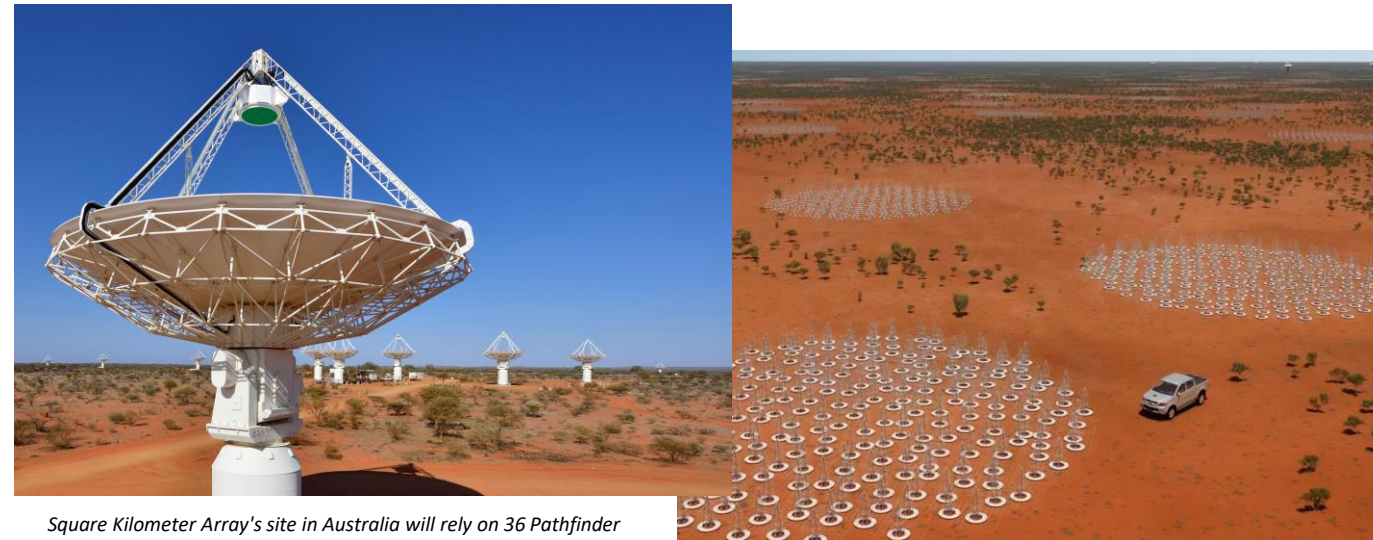
Hosts Australia’s first Grace-Hopper-based HPC cluster.

- **Ella:** Pawsey’s small Grace-Hopper HPC cluster, [supplied by XENON](#), with ½ PB of usable WEKA storage capacity, [also supplied by XENON.](#) Primarily used for running quantum simulations.



What does Pawsey do ?

- **Used by**
Supports over 4,000 researchers.
- **Capabilities**
Provides large scale, high speed computational and data storage resources, and advanced software tools. Used to tackle complex problems across diverse array of scientific fields:
 - **Astronomy:** Supporting projects like the Square Kilometre Array (SKA), the world's largest radio telescope.
 - **Climate Science:** Simulating and analysing climate models to enhance understanding of environmental changes.
 - **Biosciences:** Enabling research in genomics, drug discovery, and bioinformatics.
 - **Engineering:** Facilitating simulations in areas such as fluid dynamics and material sciences.
 - **Energy and Resources:** Assisting geoscience and mineral exploration efforts.
- **Managed by**
Operated by a team of 50+ staff employed through CSIRO (Australia's national science agency).

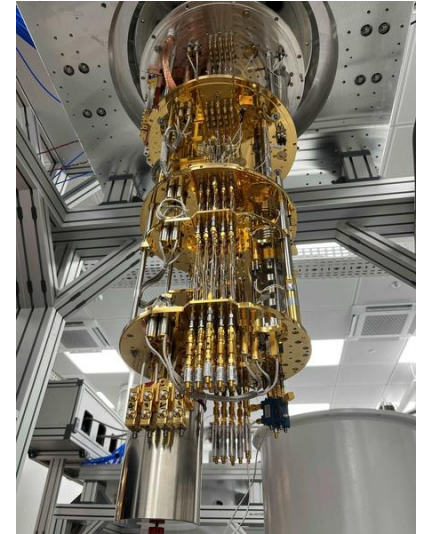


Square Kilometer Array's site in Australia will rely on 36 Pathfinder Survey Telescopes (image : CSIRO, <https://commons.wikimedia.org/w/index.php?curid=35460691>)

An artist's impression of the future Square Kilometre Array (SKA) in Australia, with up to 132,000 low frequency antennas (resembling metal Christmas trees) will be built. (Image: CSIRO)

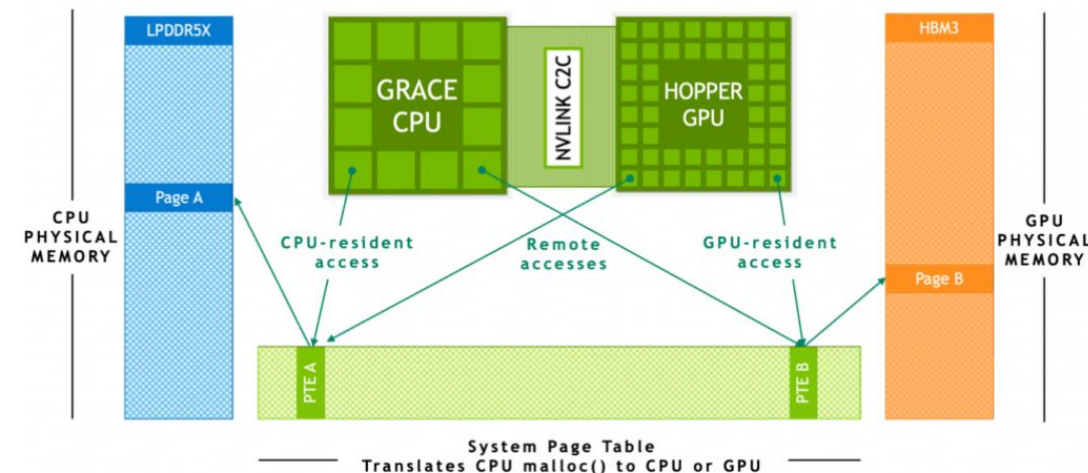
Why run Quantum Simulations on Classical Compute Hardware

- **Quantum Hardware Limitations**
 - Limited qubits (tens to hundreds) restrict problem size and complexity.
 - High sensitivity to noise and errors makes early-stage Quantum Computers unstable
- **Quantum Simulations on Classical Hardware**
 - Allow exploration of Quantum systems without hardware limitations.
 - Provides a practical step for advancing Quantum Computing understanding.
- **Algorithm Development**
 - Enables design, refinement, and debugging of Quantum algorithms
 - Classical simulations makes easier to debug and validate Quantum algorithms - provides deterministic results, computations
 - Allow them to prepare for future – when Quantum Computing becomes more viable to use.
- **Understanding Quantum Phenomena**
 - Providing insights into the key principles of superposition, entanglement, and interference.
- **Use Case Identification**
 - Highlights problems where Quantum Computers may outperform classical ones (e.g., optimisation, cryptography).



Pawsey, the Grace-Hopper SuperChip and Quantum Simulations

- Pawsey leverages Ella, a small Grace-Hopper-based HPC cluster with WEKA storage, for quantum simulations.
- Most of the quantum simulation code was initially developed on x86-based architecture, and Pawsey is migrating to the ARM-based Grace CPU. Porting wasn't "too painful".
- **Why Grace-Hopper, whats makes this interesting ?**
 - The Grace-Hopper SuperChip (Grace CPU + Hopper GPU) architecture offers unified memory
 - Pawsey is exploring how they can streamline Quantum Simulations; and take advantage of the SuperChip's unified memory architecture
 - NVLink-C2C enables memory coherency between CPU and GPU
 - CPU and GPU threads can access the same shared memory pool, that is, no need to move data between CPU and GPU
 - And the OS treats the CPU and GPU as separate NUMA nodes.



more... Pawsey and Quantum Simulations

- **Quantum Simulation Challenges**

Pawsey is tackling hybrid workflow challenges, combining CPUs, GPUs, and QPUs (Quantum Processing Unit).

They use virtual QPUs with noise models to mimic real Quantum hardware, alongside developing orchestration tools and testing system integration.

- **Scalable Quantum Tools**

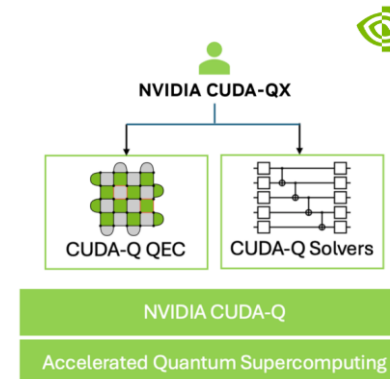
Developing tools for scalable Quantum simulations, addressing inefficiencies in current GPU usage and scaling limitations of existing packages.

- **Quantum Algorithm Focus**

Concentrating on optimisation problems, chemistry applications, and Quantum machine learning techniques.

- **Progress Highlights**

- Advancing several research projects (details forthcoming).
- Benchmarking QC simulation frameworks (e.g., CUDAQ) to identify what works well, and what doesn't.
- Creating in-house, efficient QC simulation codes; optimised for the Grace Hopper Superchip architecture.



NVIDIA CUDA-Q

NVIDIA CUDA-Q is an open-source quantum development platform orchestrating the hardware and software needed to run useful, large-scale quantum computing applications. The platform's hybrid programming model allows computation on GPU, CPU, and QPU resources in tandem from within a single quantum program.

more... Pawsey and Quantum Simulations

- **Intern Contributions**

Three interns are actively testing the system and exploring the scale of QC simulations that can be feasibly achieved.

They are using a variety of QC frameworks and benchmarking them in ways that would be challenging without Ella.

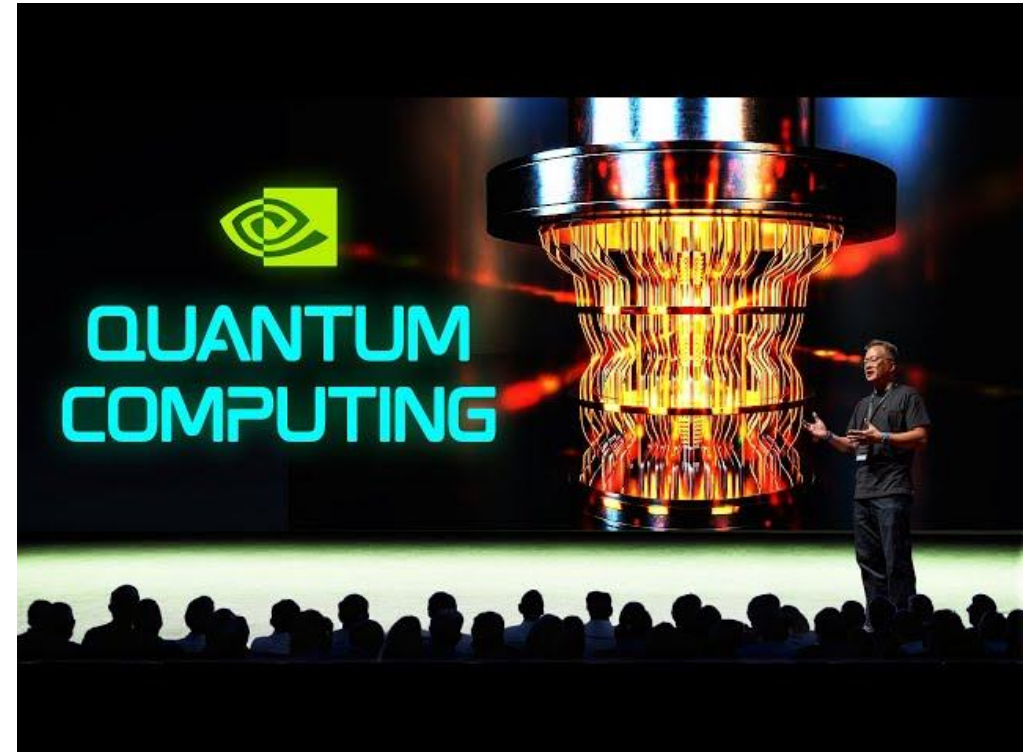
- **In-House Quantum Simulation Development**

Pawsey is also developing in-house quantum simulation codes.

Ella serves as an excellent test-bed to evaluate their scalability.

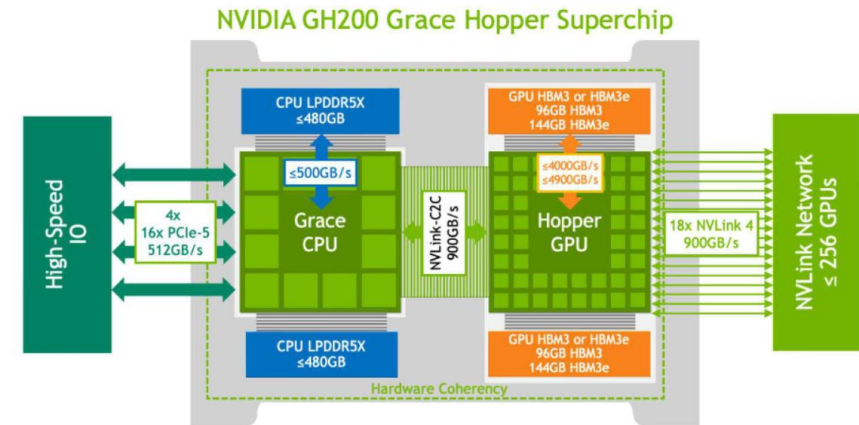
- **Pawsey has stated:**

“Ella has been highly valuable as a non-production system for our team and experienced early adopters...”



In Summary

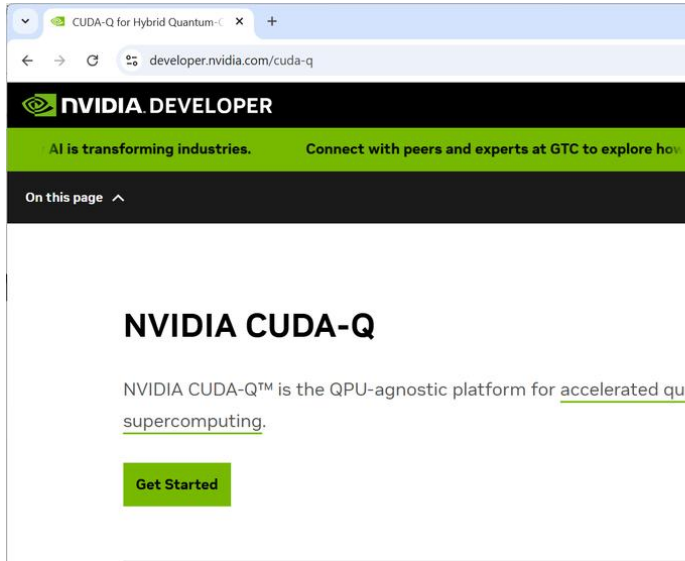
- Pawsey’s Quantum Computing (QC) research, including Quantum simulations on the “Ella” system, is progressing well.
- Pawsey is exploring how Quantum simulations can leverage the unified memory architecture of the NVIDIA Grace Hopper Superchip.
- Pawsey is developing and testing QC algorithms and tools, identifying what works effectively and what does not.
- The team is actively engaged in several QC-based research projects.
- **Pawsey views the Quantum simulation project as a practical and essential first step towards gaining a deeper understanding of QC.**



Would like to thank:

- Dr Pascal Elahi (Supercomputing and Quantum Specialist) and the team from Pawsey

Quantum Simulations @ Pawsey



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AI is transforming industries. Connect with peers and experts at GTC to explore how.

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NVIDIA CUDA-Q

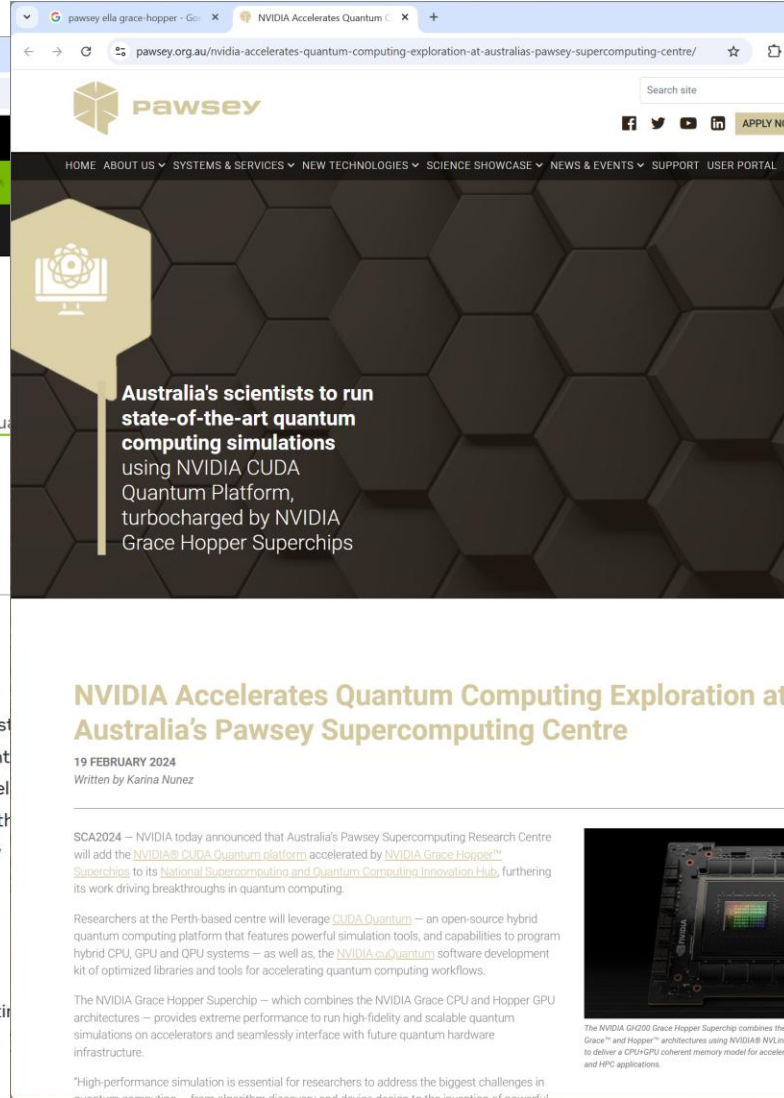
NVIDIA CUDA-Q™ is the QPU-agnostic platform for accelerated quantum computing.

[Get Started](#)

Product Overview

CUDA-Q is an open-source quantum development platform orchestrating the hardware and software needed to run useful, large-scale quantum computing applications. The platform's hybrid programming model combines computation on GPU, CPU, and QPU resources in tandem with a single quantum program. CUDA-Q is "qubit-agnostic"—seamlessly integrating with all QPUs and qubit modalities and offering GPU-accelerated simulations when adequate quantum hardware is not available.

CUDA-Q extends simulation tools far beyond the NISQ-era—charting a course to large-scale, error-corrected quantum supercomputing.



pawsey.org.au/nvidia-accelerates-quantum-computing-exploration-at-australia-pawsey-supercomputing-centre/

NVIDIA Accelerates Quantum Computing Exploration at Australia's Pawsey Supercomputing Centre

19 FEBRUARY 2024
Written by Karina Nunez

Australia's scientists to run state-of-the-art quantum computing simulations using NVIDIA CUDA Quantum Platform, turbocharged by NVIDIA Grace Hopper Superchips

SCA2024 — NVIDIA today announced that Australia's Pawsey Supercomputing Research Centre will add the NVIDIA CUDA Quantum platform accelerated by NVIDIA Grace Hopper Superchips to its National Supercomputing and Quantum Computing Innovation Hub, furthering its work driving breakthroughs in quantum computing.

Researchers at the Perth-based centre will leverage CUDA Quantum — an open-source hybrid quantum computing platform that features powerful simulation tools, and capabilities to program hybrid CPU, GPU and QPU systems — as well as, the NVIDIA cuQuantum software development kit of optimized libraries and tools for accelerating quantum computing workflows.

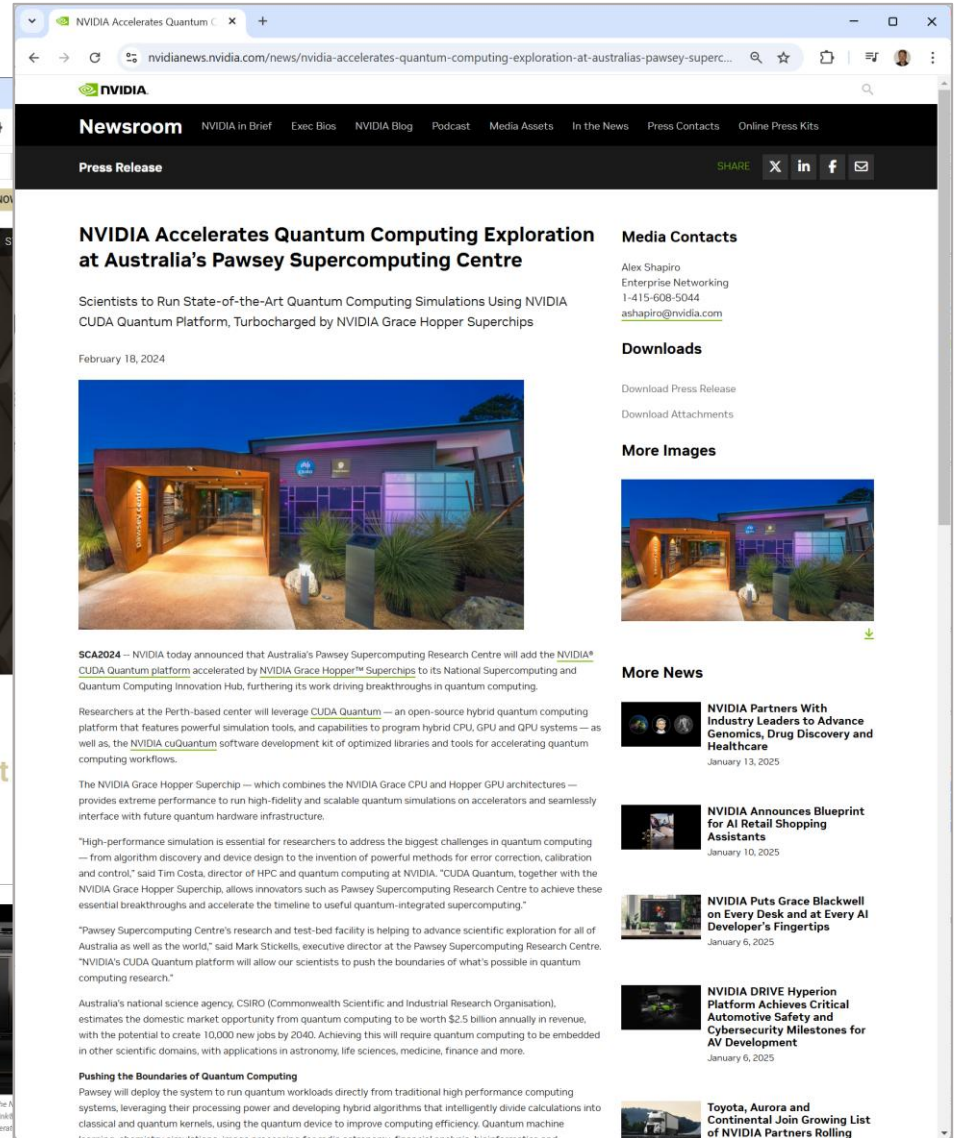
The NVIDIA Grace Hopper Superchip — which combines the NVIDIA Grace CPU and Hopper GPU architectures — provides extreme performance to run high-fidelity and scalable quantum simulations on accelerators and seamlessly interface with future quantum hardware infrastructure.

"High-performance simulation is essential for researchers to address the biggest challenges in quantum computing — from algorithm discovery and device design to the invention of powerful methods for error correction, calibration and control," said Tim Costa, director of HPC and quantum computing at NVIDIA. "CUDA Quantum, together with the NVIDIA Grace Hopper Superchip, allows innovators such as Pawsey Supercomputing Research Centre to achieve these essential breakthroughs and accelerate the timeline to useful quantum-integrated supercomputing."

"Pawsey Supercomputing Centre's research and test-bed facility is helping to advance scientific exploration for all of Australia as well as the world," said Mark Stickle, executive director at the Pawsey Supercomputing Research Centre. "NVIDIA's CUDA Quantum platform will allow our scientists to push the boundaries of what's possible in quantum computing research."

Australia's national science agency, CSIRO (Commonwealth Scientific and Industrial Research Organisation), estimates the domestic market opportunity from quantum computing to be worth \$2.5 billion annually in revenue, with the potential to create 10,000 new jobs by 2040. Achieving this will require quantum computing to be embedded in other scientific domains, with applications in astronomy, life sciences, medicine, finance and more.


Pushing the Boundaries of Quantum Computing
Pawsey will deploy the system to run quantum workloads directly from traditional high performance computing systems, leveraging their processing power and developing hybrid algorithms that intelligently divide calculations into classical and quantum kernels, using the quantum device to improve computing efficiency. Quantum machine learning simulations, image recognition for radio astronomy, financial analysis, climate forecasting and more.



NVIDIA Accelerates Quantum Computing Exploration at Australia's Pawsey Supercomputing Centre

Scientists to Run State-of-the-Art Quantum Computing Simulations Using NVIDIA CUDA Quantum Platform, Turbocharged by NVIDIA Grace Hopper Superchips

February 18, 2024



SCA2024 — NVIDIA today announced that Australia's Pawsey Supercomputing Research Centre will add the NVIDIA CUDA Quantum platform accelerated by NVIDIA Grace Hopper Superchips to its National Supercomputing and Quantum Computing Innovation Hub, furthering its work driving breakthroughs in quantum computing.

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Thank-you !



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High Performance Computing

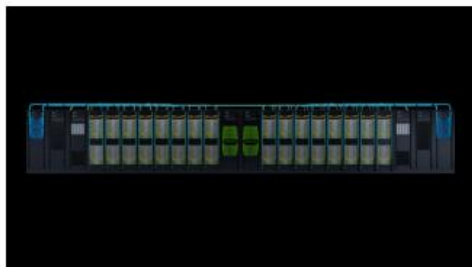
Backup slides

Quantum-Accelerated Supercomputing

Supercomputers are the foundation of Quantum R&D

Simulation

- Quantum computers are small and error-prone -> simulation is an essential tool
- **Today:** Powerful simulators enable algorithm and application R&D - new approaches (e.g. tensor networks)
- **Future:** Digital twins of quantum computers for design and architecture optimization



HPC Quantum Integration

- Useful quantum computing will be hybrid
- **Today:** Enable domain scientists to start developing for QPUs, enable quantum researchers to use accelerated computing
- **Future:** quantum computers will integrate tightly with supercomputers as accelerators and be co-programmed



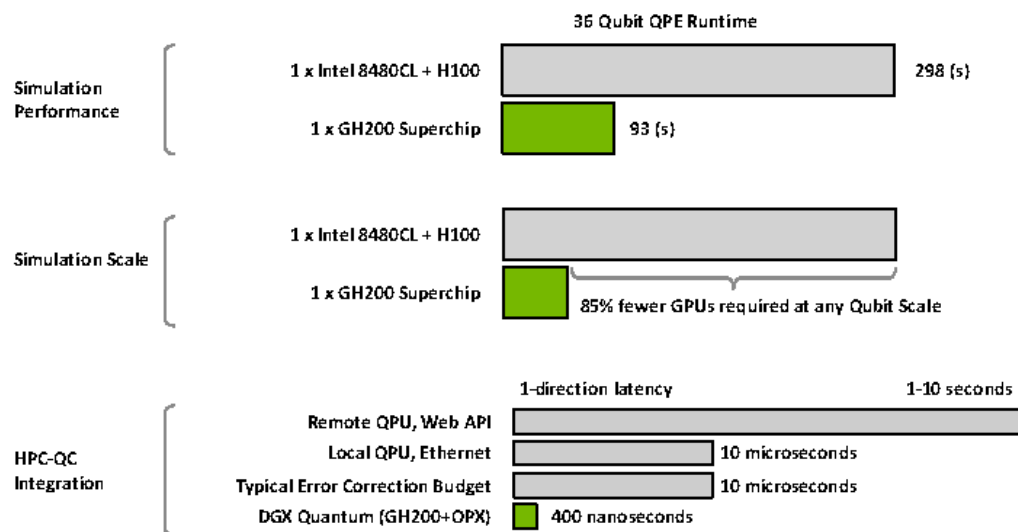
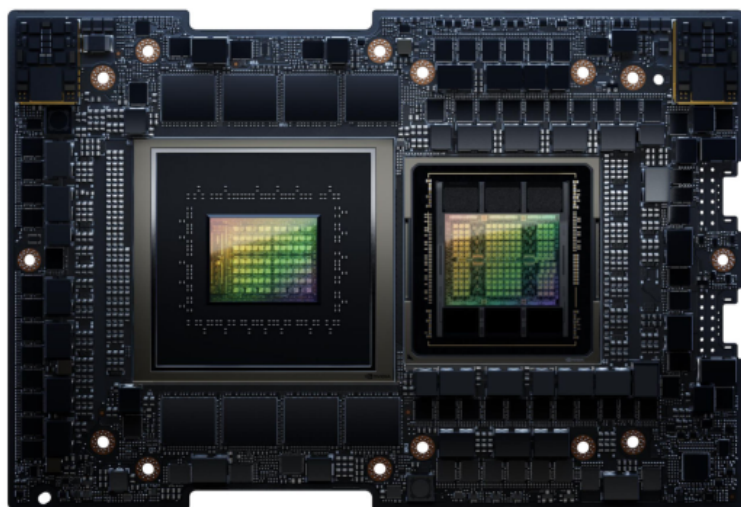
AI for Quantum

- Error correction, calibration, control, compilation are challenging computationally, real-time compute often needed
- Accelerated computing and AI can solve these problems
- **Today:** Enable AI research for all of the above
- **Future:** Hybrid Quantum+AI supercomputer with low-latency link



Coherent CPU+GPU: The Ideal Platform for Quantum

Grace Hopper being deployed worldwide for quantum research



FermionIQ

