



Press release

# Qubit Pharmaceuticals and Sorbonne University achieve a major scientific breakthrough by simulating quantum calculations at more than 40 qubits on conventional computers

- Qubit Pharmaceuticals introduces its Hyperion-1 emulator, developed in close collaboration with Sorbonne University and capable of running accelerated and accurate quantum algorithms at over 40 qubits.
- Leveraging the latest improvements in high-performance computing, Hyperion-1 demonstrates a computational speed unique in the world, placing Qubit Pharmaceuticals among the leaders in accurate quantum computer simulation on classical HPC calculation infrastructure.
- Hyperion-1 will accelerate the development of quantum algorithms for real industry applications.
- A breakthrough that reinforces the company's goal of becoming the leader in molecular modeling-based drug discovery.

**Paris, December 6<sup>th</sup>, 2023** - Qubit Pharmaceuticals, a deeptech company specializing in the discovery of new drug candidates through molecular simulation and modeling accelerated by hybrid HPC and quantum computing, announces a major scientific breakthrough after achieving quantum computations simulating 40 qubits with its new Hyperion-1 emulator.

« This is an exact simulation of 40 logic qubits carried out at very high velocity, which is an unprecedented achievement in the application of quantum computation, in particular to quantum chemistry », confirms Jean-Philip Piquemal, Professor at Sorbonne University and Director of the Theoretical Chemistry Laboratory (Sorbonne University/CNRS), co-founder and Scientific Director of Qubit Pharmaceuticals, and head of the team that developed Hyperion-1.

Such a level of performance places Qubit Pharmaceuticals among the world's leading actors in quantum computing, all the more so as it was achieved without approximation and with the highest level of fidelity, i.e. without error (or "noise", to use the prevailing expression in quantum physics) and in a very short time, close to what one would expect from a true quantum computer. This performance was achieved in partnership with Sorbonne University's Theoretical Chemistry Laboratory, and the calculations were carried out in just a few hours on GENCI's Jean Zay HPC/IA converged supercomputer on 16 computing nodes (128 GPUs<sup>(1)</sup> A100 NVIDIA) hosted and operated by IDRIS computing center (CNRS), on which the Hyperion-1 emulator was developed.

# The ultimate objective: select a drug candidate in half the time

This achievement reinforces Qubit Pharmaceuticals' ambition to become the industry reference in molecular modeling-based drug discovery. The result of academic research carried out by internationally renowned scientists<sup>2</sup> in France and the United States, Qubit Pharmaceuticals models molecules and simulates their interactions to identify more effective and safer drug candidates. The aim is to halve the time needed to select and optimize a candidate of interest, and more than 10-fold





the investment required. This process requires immense computing capacities, available today with supercomputers and multiplied tomorrow with quantum computers.

## Key benefits of Hyperion-1, the new emulator from Qubit Pharmaceuticals

Revolutionary simulations: Hyperion-1 is capable of achieving 40 qubit (and more) converged simulations in production without error or noise, setting new standards of precision in quantum research.

Massively parallel processing capability: thanks to its emulation of a quantum computer on a classical architecture accelerated by GPUs<sup>(1)</sup>, Hyperion-1 offers exceptional precision and massively parallel processing capability capable of concentrating classical computing power.

Exceptional performance: Hyperion-1 has demonstrated outstanding performance in high-speed simulations of complex quantum circuits of up to 40 qubits, using moderate computing resources, i.e. 16 Jean Zay nodes each accelerated by 8 NVIDIA A100 80GB GPUs. This increased speed makes it possible to converge quantum chemistry simulations requiring hundreds of algorithm iterations.

Advanced technology: Featuring optimized internal code based on a mathematical library that is proprietary and agnostic, i.e. able to use any type of supercomputer, Hyperion-1 uses parallel acceleration via MPI and takes full advantage of the new generation of NVIDIA DGX-A100 accelerated nodes for enhanced performance.

## The Hyperion-1 quantum emulation opens up new perspectives on the technology of tomorrow

In the ever-evolving landscape of quantum computing, a critical gap persists between machines with a limited number of perfect qubits and those with a large number of qubits but laden with error (noise and instability). Hyperion-1, with the velocity and accuracy of its calculations, is a testament to the immense possibilities that lie ahead. Its capabilities demonstrate what will be possible in the wider landscape of quantum emulation and quantum computing. Qubit Pharmaceuticals is proud of Hyperion-1's potential, not only as a proprietary tool, but also as a symbol of perfect emulation, fostering a new era of technological innovation with far-reaching implications for sectors such as pharmaceuticals, finance, encryption, and many others.

**Robert Marino, CEO Qubit Pharmaceuticals**, states: "These quantum chemistry calculations on 40 exact qubits far exceed the performance achieved to date in Europe, and place Qubit Pharmaceuticals on the same footing as some of the top American tech giants. This breakthrough enables us to carry out in a few hours calculations that traditionally take several months."

Jean-Philip Piquemal, Professor at Sorbonne University and Director of the Theoretical Chemistry Laboratory (Sorbonne University/CNRS), co-founder and Chief Scientific Officer at Qubit Pharmaceuticals, states: "Hyperion-1 allows quantum state simulation while benefiting from the stability of classical computers, thus avoiding the errors inherent in today's quantum computers. Thanks to the GPUs in our machines and GENCI's infrastructure, we are able to develop and validate new quantum algorithms applied to drug discovery - a field of research with real public utility."





**Élisabeth Angel-Perez, Vice President of Research and Innovation at Sorbonne University**: "Sorbonne University is a community of talent, and it's also a commitment: a commitment to supporting innovation stemming from French research. And it's because we've given ourselves the necessary resources to develop an ecosystem for the transfer of expertise and innovation that we've been able to accompany and support genuine nuggets such as Qubit Pharmaceuticals. Science must be at the service of society and its well-being. That's the dynamic we're supporting alongside the researchers who make Sorbonne University so rich."

<sup>(1)</sup> GPU= Graphics Processing Unit

<sup>(2)</sup> Louis Lagardère (Sorbonne University and CNRS), Matthieu Montes (CNAM), Jean-Philip Piquemal (Sorbonne University and CNRS), Jay Ponder (Washington University in St Louis), Pengyu Ren (University of Texas at Austin).

#### **About Qubit Pharmaceuticals**

Qubit Pharmaceuticals was founded in 2020 with the vision of co-developing novel, more effective and safer drugs in partnership with pharmaceutical and biotech companies. A spin-off from the research work of five internationally renowned scientists - Louis Lagardère (Sorbonne University and CNRS), Matthieu Montes (CNAM), Jean-Philip Piquemal (Sorbonne University and CNRS), Jay Ponder (Washington University in St Louis), Pengyu Ren (University of Texas at Austin) - Qubit Pharmaceuticals leverages its Atlas platform to discover new small molecule drugs through simulation and molecular modeling accelerated by hybrid HPC and quantum computing. The multidisciplinary team, led by CEO Robert Marino, and the founders are based in France at the Paris Santé Cochin incubator and in the USA in Boston.

For more information, or to join an ambitious team, visit www.qubit-pharmaceuticals.com

#### **About Sorbonne University**

Sorbonne University is a multidisciplinary, research-intensive university covering the humanities, health, science and engineering. Anchored in the heart of Paris and with a regional presence, Sorbonne University has 55,000 students, 3,300 teaching and research staff, 4,000 national researchers and over a hundred laboratories. Alongside its partners in the Sorbonne University Alliance, and via its institutes and multidisciplinary initiatives, it conducts research and educational activities to strengthen its contribution to the challenges of three major transitions: a global approach to health (One Health), resources for a sustainable planet (One Earth), and changing societies, languages and cultures (One Humanity). Sorbonne University is also a member of Alliance 4EU+, an innovative model for European universities that develops strategic international partnerships and promotes the openness of its community to the rest of the world. https://www.sorbonne-universite.fr

#### About GENCI

Created by the public authorities in 2007, GENCI is a major research infrastructure. This public operator aims to democratize the use of digital simulation through high performance computing associated with the use of artificial intelligence, and now quantum computing, to support French scientific and industrial competitiveness.

GENCI is in charge of three missions:

- To implement the national strategy for the provision of high-performance computing resources, storage and processing of massive data associated with AI technologies for the benefit of French open scientific research in conjunction with the three national computing centers.
- Support the creation of an integrated HPC ecosystem at the national and European levels.





• Promote digital simulation through HPC to academic research and industry scale.

GENCI is a civil company, of which is owned 49% by the French government, represented by the Ministry of Higher Education and Research, 20% by the CEA, 20% by the CNRS, 10% by Universities represented by France Université and 1% by Inria.

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