

April 26th 2024

## **Senior quantum HPC software engineer (M/F)**

Qubit Pharmaceuticals is French-American deeptech startup, focussing on discovering novel small molecule drug candidates for complex disease targets deemed 'undruggable'. Using our proprietary cutting-edge technologies, we develop our own drug discovery programs that we either co-develop with or license out to pharmaceutical companies. We leverage proprietary molecular simulation and quantum-physics based modeling technology based on over 30 years of research by our academic founders

Qubit Pharma uses a hybrid of classical and quantum computing approach to design more effective and safer drugs, aiming to significantly reduce the time and investment needed to discover new drug candidates. In less than 18 months, Qubit Pharmaceuticals grew its drug discovery portfolio to 6 programs in oncology, inflammation & antivirals leveraging its proprietary platform, Atlas.

Drug discovery through simulation and modeling requires unprecedented computational capabilities beyond the petaflop, or more than one million billion operations per second. Qubit Pharmaceuticals, a deeptech company, has worldwide access to existing and emerging supercomputers with one of the largest private GPU supercomputers for life sciences in France. Our in-house platform Atlas integrates advanced simulation technologies that run on these supercomputers to accelerate calculations by a factor of 100 000, thus performing calculations in a few hours versus over a year's time. These simulations, along with optimized small molecule identification strategies and in-house experts in computational and medicinal chemistry, will allow several chemical series to be explored in parallel.

**Qubit Pharmaceuticals is looking for a Senior quantum HPC software engineer to develop and maintain the Hyperion quantum emulator.**

### **The perfect fit for this job**

At Qubit Pharmaceuticals, we are looking for candidates who are quick at adapting to new challenges and issues. A senior quantum HPC software engineer who is willing to learn, meets the needs of users and works in a collaborative process with other teammates and across multiple teams.

### **Your role**

- As a member of the Quantum team, you will be responsible for the full HPC software development cycle, including coding, testing, optimization, maintenance, debugging, porting.
- Compiling new versions of codes for different HPC clusters and making them available for users.
- Providing technical support to users.
- Writing technical documentations for user support on HPC.

- Taking part in weekly Quantum team meetings.
- Implementing new algorithms in codes as required by users.
- Proactively work on optimization of codes using various profiling tools.
- Reporting monthly activities.
- Taking part in scientific article writings.

### Your Qualifications

- Master degree or equivalent in Applied Maths / Computer Science / Physics / Chemistry.
- PhD in Quantum Chemistry/Physics with HPC code development is strongly preferred.
- Minimum of 5 years work experience (including PhD) is required.
- Knowledge of quantum computing and tensor networks is strongly preferred.
- Proficiency in at least one of the following GPU programming paradigms:
  - OpenMP/OpenACC
  - CUDA/HIP/SYCL
- Advanced hands-on experience in C++ and Python are required.
- Distributed memory (multi-node) programming (MPI).
- Working on HPC clusters (Slurm, HPC software installations etc.).
- Code optimization:
  - Compiler tuning (GCC, NVCC, CCE).
  - Profiler tools (nsight, vtune, gprof, rocprof, valgrind, etc.).
  - Porting code for different GPU architectures (NVIDIA/AMD/Intel).
- Linux code building tools (make, cmake etc. ).
- Good knowledge of Containerization technologies (Docker, Singularity).
- Knowledge of CI/CD & version control Git.
- Open-source code development and maintenance is valuable.

### The proposal benefits & perks

- Duration: Full time – Permanent
- Starting date: September 2024
- Salary according to profile
- Health insurance and provident fund 100% covered
- Lunch vouchers worth €9 covered at 50%.
- Possibility of remote work for 2 days per week.
- Location: Paris 14th arrondissement

To [apply](#)

For more information about Qubit Pharmaceuticals: [www.qubit-pharmaceuticals.com](http://www.qubit-pharmaceuticals.com)

## **Join our journey to push the frontiers of science, technology and your career!**

*“At Qubit Pharma, we don't just dream big—we turn those dreams into real-life innovations in the Drug Discovery world. That's what makes this more than a job - it's a journey where your best ideas can turn into disruptive and game-changing realities.”*

- Yassine, Atlas Team

*“Join Qubit Pharma for a multicultural, multidisciplinary environment that fuels growth. We're a team where diverse perspectives converge, offering scientists and experts like you the opportunity to cultivate expertise and contribute to groundbreaking discoveries.”*

- Daniele, Research Team

## **Qubit mission vision and values**

### **A unique career**

Qubit Pharmaceuticals is looking for talented professionals to join our team – individuals who have a passion for science, drug discovery and molecular modeling.

### **Our Vision**

Unlock the power of quantum at scale to design better treatments for any target and every patient.

### **Our Mission**

We pioneer quantum-aided drug design and leverage cutting-edge science to design novel molecules for complex targets.

### **Workplace and culture**

We're a diverse mix of expertise, experience and perspectives, united around the passion to make a positive impact in drug design and discovery using the best computational technology.

We're proud of our inclusive culture where individuals are encouraged to collaborate, lead and grow.

### **Our Values**

We live and work by our values:

- We care genuinely
- We encourage diversity
- We value scientific excellence
- We foster resilience
- We succeed together