

Learning Quantum-accelerated Scientific Computing with LibKet

IEEE Quantum Week 2021

October 17-22, 2021

Matthias Möller¹ and Carmen G. Almudever²

¹Delft University of Technical (m.moller@tudelft.nl)

²Technical University of Valencia (cargara2@disca.upv.es)

Who we are

Matthias Möller



Associate Professor of Numerical Analysis,
Department of Applied Mathematics, TU Delft

- Numerical methods for PDE problems (FEM, IGA, MPM, ...)
- High-performance/accelerated computing
- Quantum-accelerated scientific computing



Nauman Ahmed



Giorgio Balducci



Merel Schalkers



Smaran Adarsh

Who we are

Carmen G. Almudever

Distinguished Researcher – Quantum Computing Architectures
Computer Engineering Department, Technical University of Valencia (UPV)



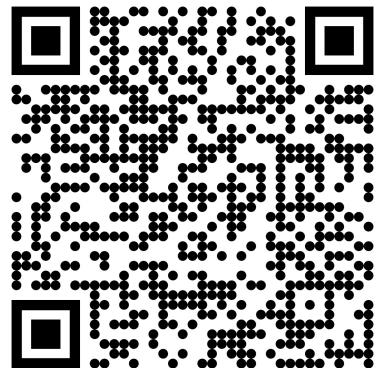
- Quantum software, mapping of quantum algorithms
- QEC and FT quantum computation
- Architecting and benchmarking of quantum computers
- Scalability of quantum computing systems

Funding and support





<https://tinyurl.com/yru4f4yv>



IEEE International Conference
on Quantum Computing
and Engineering — QCE21



Tutorial at IEEE QCE21, October 17-22, 2021

Learning Quantum-accelerated Scientific Computing with LibKet

Organizers: Carmen G. Almudever, Matthias Möller

Session 1: Monday, October 18, 10:45 AM – 12:15 AM MDT (UTC-6)

Time	Content	Lecturer	Slides	Binder
10:45-10:55	Quantum-accelerated scientific computing	Matthias	slides	
10:55-12:15	Hands-on introduction to quantum computing with LibKet	Carmen/Matthias	slides	tutorial 01

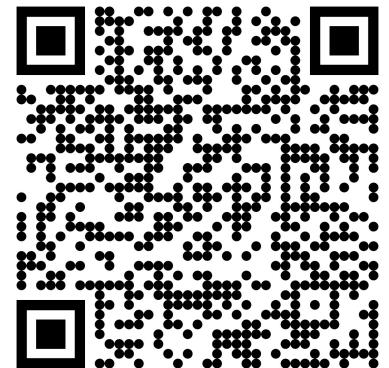
Session 2: Monday, October 18, 1:00 PM – 2:30 PM MDT (UTC-6)

Time	Content	Lecturer	Slides	Binder
1:00-2:10	Hands-on scientific computing with LibKet	Matthias	slides	tutorial 02 tutorial 03
2:10-3:30	Quantum computing today and future perspective	Carmen	slides	

Click now since
first launch can
take some time



<https://tinyurl.com/yru4f4yv>



Starting repository: mmoelle1/LibKet/master

Your session is taking longer than usual to start!
Check the log messages below to see what is happening.

Build logs

hide

```
---> 29bf3cb5b44f
Step 48/51 : RUN ./postBuild
---> Running in 9345aed0e8bf
Cloning into '/home/jovyan/LibKet'...
warning: redirecting to https://gitlab.com/mmoelle1/LibKet.git/
Submodule 'external/OpenQL' (https://github.com/QE-Lab/OpenQL.git) registered for path 'external/OpenQL'
Submodule 'external/QuEST' (https://github.com/QuEST-Kit/QuEST.git) registered for path 'external/QuEST'
Submodule 'external/armadillo' (https://gitlab.com/conradsnicta/armadillo-code.git) registered for path 'external/armadillo'
Submodule 'external/optim' (https://github.com/kthohr/optim.git) registered for path 'external/optim'
Submodule 'external/pegtl' (https://github.com/taocpp/PEGTL.git) registered for path 'external/pegtl'
```



<https://tinyurl.com/yru4f4yv>



jupyter cse21_tutorial01 (autosaved)

File Edit View Insert Cell Kernel Widgets Help

Visit repo Copy Binder link

Not Trusted C++14

Memory: 209.8 MB / 2 GB

ILib

LibKet - The Quantum Expression Template Library.

- Repository: <https://gitlab.com/mmoelle1/LibKet/>
- Documentation: <https://libket.readthedocs.io/>
- API docs: <https://mmoelle1.gitlab.io/LibKet/>

Tutorial #1: Hands-on Introduction to Quantum Computing with LibKet

In this tutorial you will learn how to

1. include the LibKet library in your application
2. write quantum expressions for single- and multi-qubit circuits
3. evaluate quantum expressions on the QuEST quantum simulator

Learning Quantum-accelerated Scientific Computing with LibKet

Quantum-Accelerated Scientific Computing

IEEE Quantum Week 2021

October 17-22, 2021

Matthias Möller¹ and Carmen G. Almudever²

¹Delft University of Technology (m.moller@tudelft.nl)

²Technical University of Valencia (cargara2@disca.upv.es)

Quantum Computing ... why?

Quantum computers can solve problems that are intractable for even the most powerful classical supercomputers (e.g., simulation, search and optimization)



New materials (aerospace, automotive, energy)

New drugs (chemistry and pharma)

Better products and services (logistics, healthcare, finance)

Quantum Computing ... first applications

PRL 103, 150502 (2009)

PHYSICAL REVIEW LETTERS

week ending
9 OCTOBER 2009



Quantum Algorithm for Linear Systems of Equations

Aram W. Harrow,¹ Avinatan Hassidim,² and Seth Lloyd³

¹Department of Mathematics, University of Bristol, Bristol, BS8 1TW, United Kingdom

²Research Laboratory for Electronics, MIT, Cambridge, Massachusetts 02139, USA

³Research Laboratory for Electronics and Department of Mechanical Engineering, MIT, Cambridge, Massachusetts 02139, USA

(Received 5 July 2009; published 7 October 2009)

Solving linear systems of equations is a common problem that arises both on its own and as a subroutine in more complex problems: given a matrix A and a vector \vec{b} , find a vector \vec{x} such that $A\vec{x} = \vec{b}$. We consider the case where one does not need to know the solution \vec{x} itself, but rather an approximation of the expectation value of some operator associated with \vec{x} , e.g., $\vec{x}^\dagger M \vec{x}$ for some matrix M . In this case, when A is sparse, $N \times N$ and has condition number κ , the fastest known classical algorithms can find \vec{x} and estimate $\vec{x}^\dagger M \vec{x}$ in time scaling roughly as $N\sqrt{\kappa}$. Here, we exhibit a quantum algorithm for estimating $\vec{x}^\dagger M \vec{x}$ whose runtime is a polynomial of $\log(N)$ and κ . Indeed, for small values of κ [i.e., poly $\log(N)$], we prove (using some common complexity-theoretic assumptions) that any classical algorithm for this problem generically requires exponentially more time than our quantum algorithm.

DOI: 10.1103/PhysRevLett.103.150502

PACS numbers: 03.67.Ac, 02.10.Ud, 89.70.Eg

Variational Quantum Linear Solver

Carlos Bravo-Prieto,^{1, 2, 3} Ryan LaRose,⁴ M. Cerezo,^{1, 5} Yiğit Subaşı,⁶ Lukasz Cincio,¹ and Patrick J. Coles¹

¹Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA.

²Barcelona Supercomputing Center, Barcelona, Spain.

³Institut de Ciències del Cosmos, Universitat de Barcelona, Barcelona, Spain.

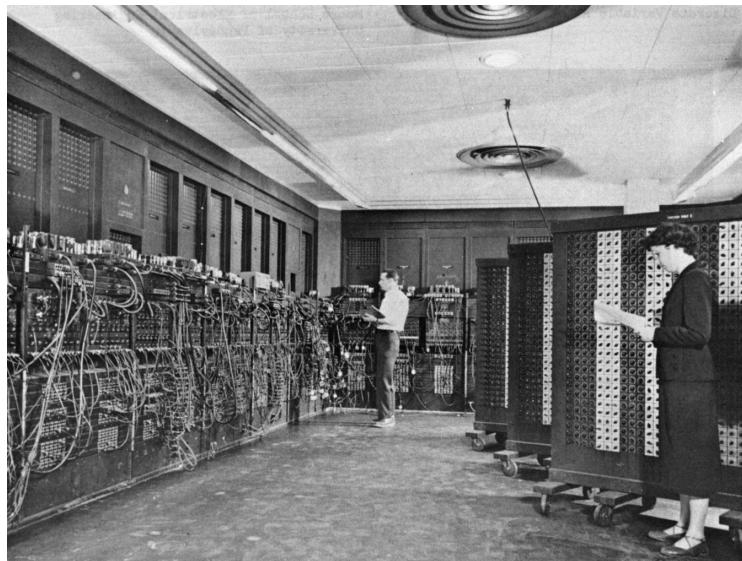
⁴Department of Computational Mathematics, Science, and Engineering & Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48823, USA.

⁵Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM, USA

⁶Computer, Computational and Statistical Sciences Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Previously proposed quantum algorithms for solving linear systems of equations cannot be implemented in the near term due to the required circuit depth. Here, we propose a hybrid quantum-classical algorithm, called Variational Quantum Linear Solver (VQLS), for solving linear systems on near-term quantum computers. VQLS seeks to variationally prepare $|x\rangle$ such that $A|x\rangle \propto |b\rangle$. We derive an operationally meaningful termination condition for VQLS that allows one to guarantee that a desired solution precision ϵ is achieved. Specifically, we prove that $C \geq \epsilon^2/\kappa^2$, where C is the VQLS cost function and κ is the condition number of A . We present efficient quantum circuits to estimate C , while providing evidence for the classical hardness of its estimation. Using Rigetti's quantum computer, we successfully implement VQLS up to a problem size of 1024×1024 . Finally, we numerically solve non-trivial problems of size up to $2^{50} \times 2^{50}$. For the specific examples that we consider, we heuristically find that the time complexity of VQLS scales efficiently in ϵ , κ , and the system size N .

Quantum Computing ... where are we?



ENIAC 1947



Fugaku, #1 in TOP-500 Nov 2020

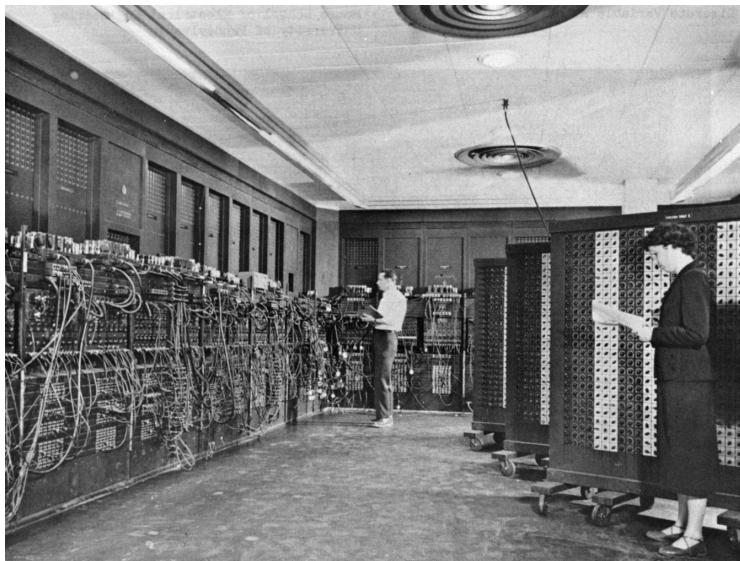
IBM Q 65-qubits, 2020



IBM Q 1000-qubits, 2023



Quantum Computing ... in its infancy!

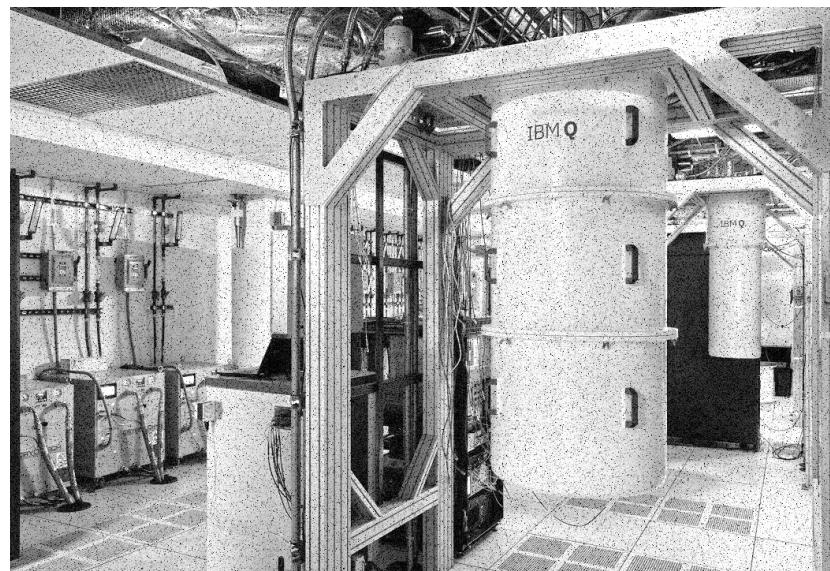


ENIAC 1947

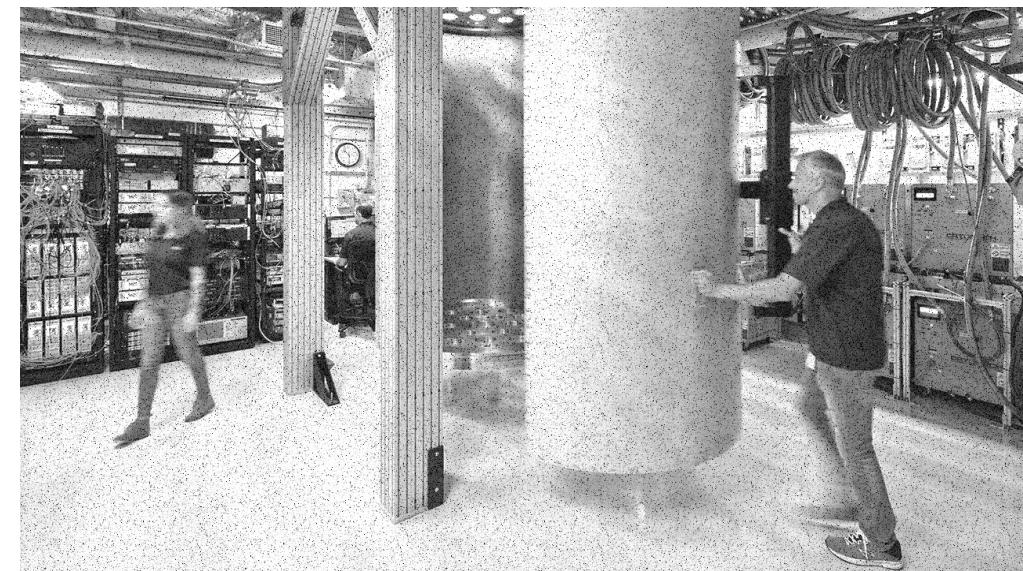


Fugaku, #1 in TOP-500 Jun 2021

IBM Q 65-qubits, 2020



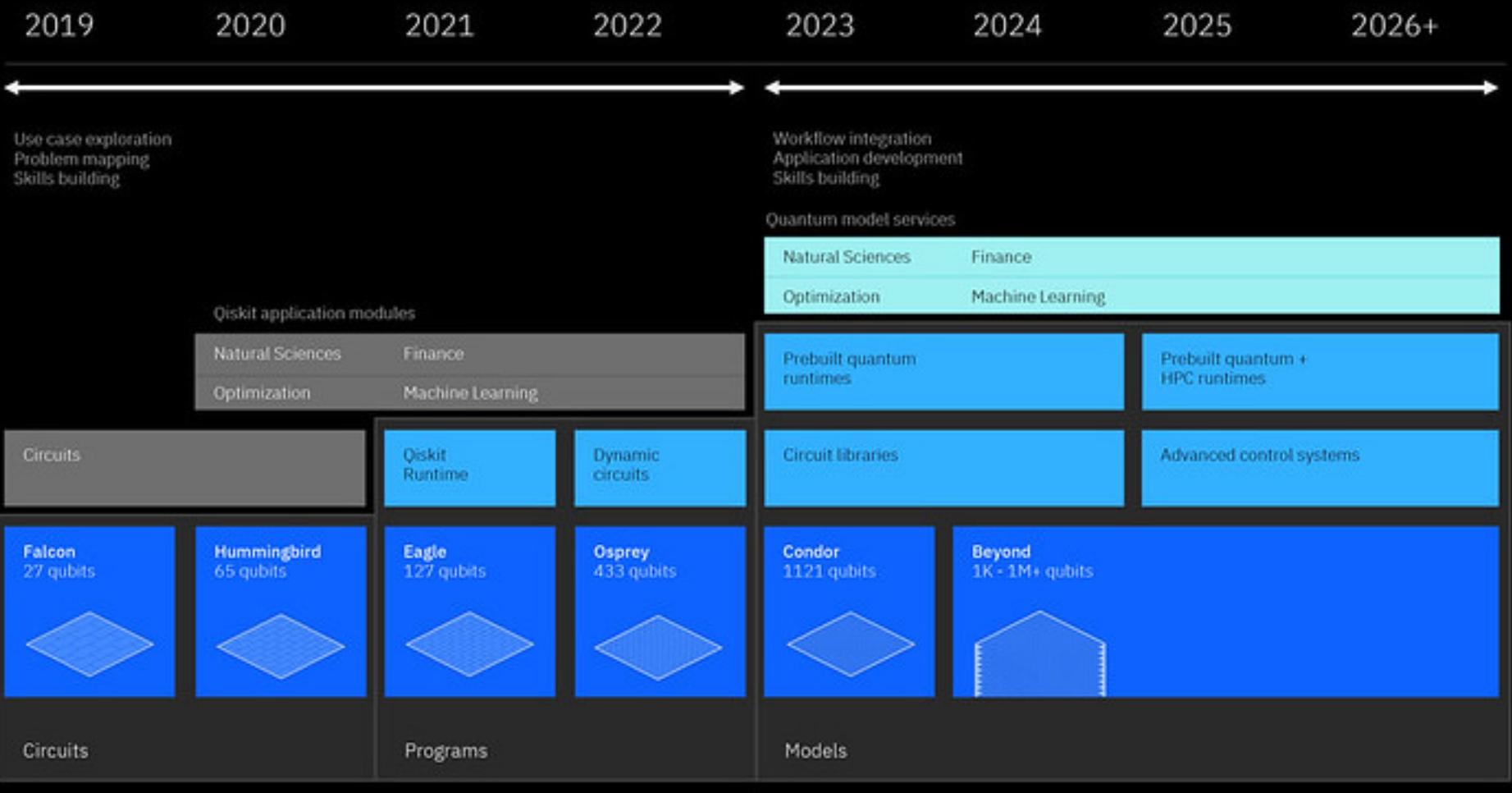
IBM Q 1000-qubits, 2023



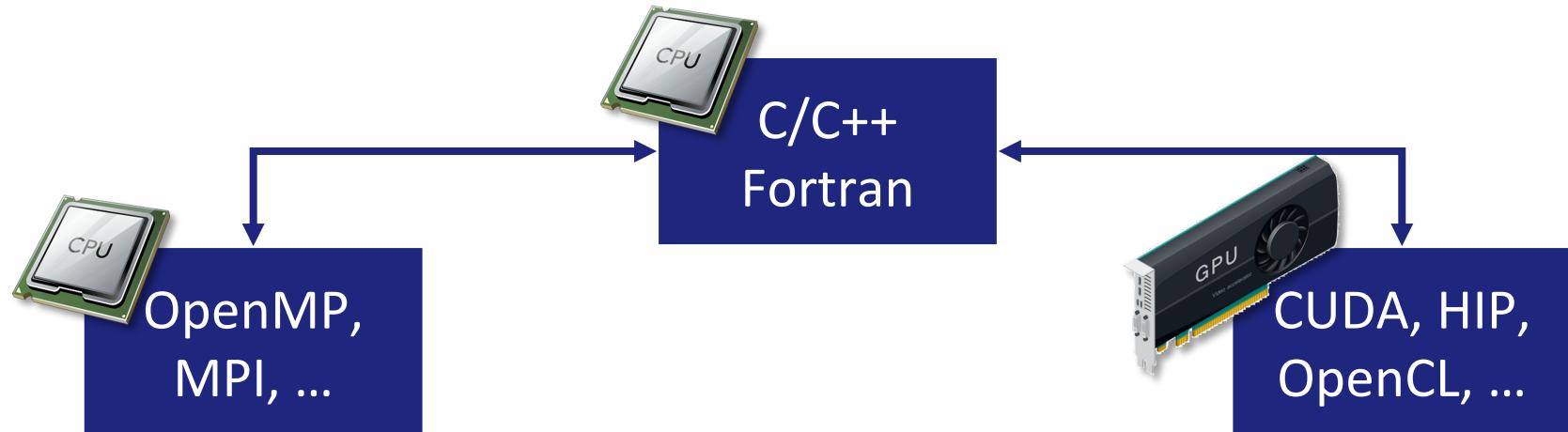
Quantum Computing ... industry interest!

Development Roadmap

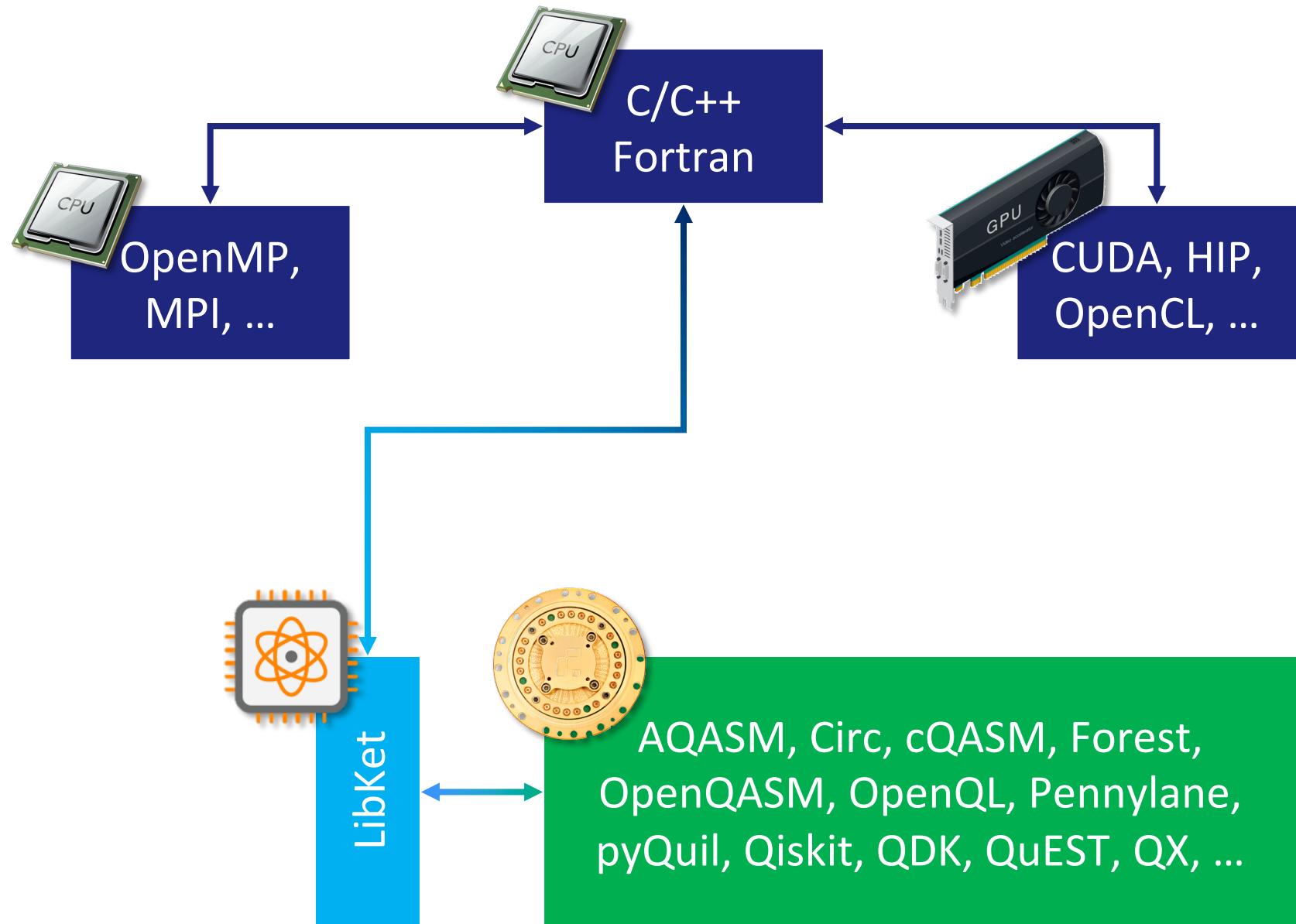
IBM Quantum



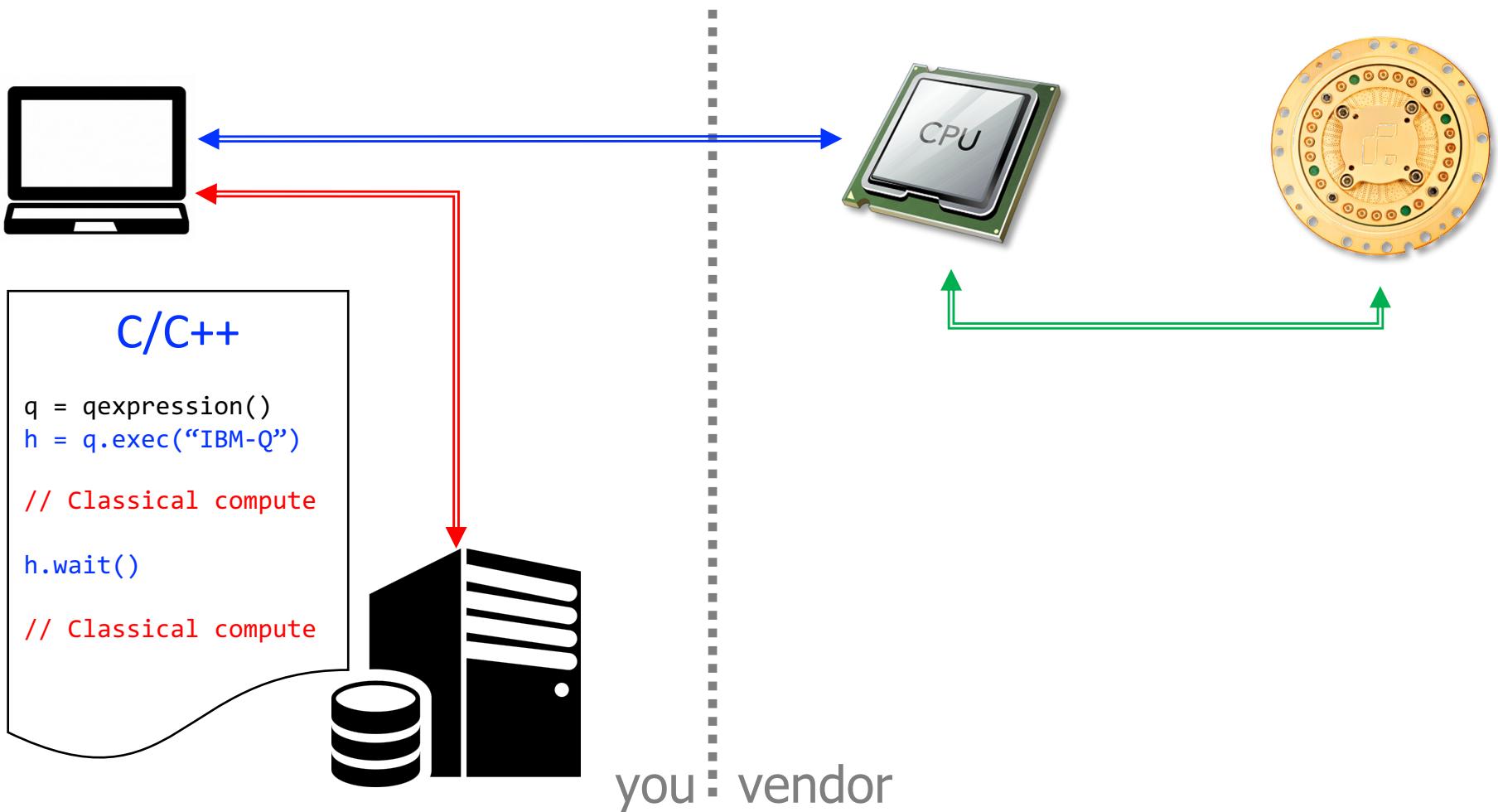
Scientific Computing



Quantum-accelerated Scientific Computing



Workflow



Workflow

