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Solving Hard Problems with Quantum and High-Performance Computing in The Cloud

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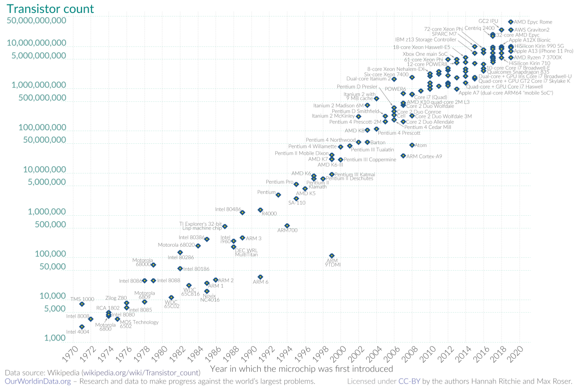
(Quantum) software architect with a PhD in quantum physics

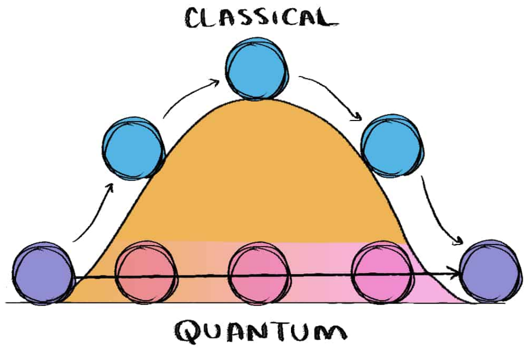
Computer are becomming so small that quantum effects become relevant

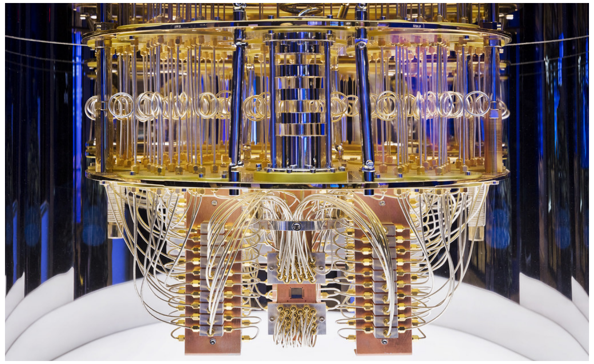
Moore's law expects doubling the number of transistor every 2 year

However, transistors are becomming too small. Quantum effects are starting to play a role

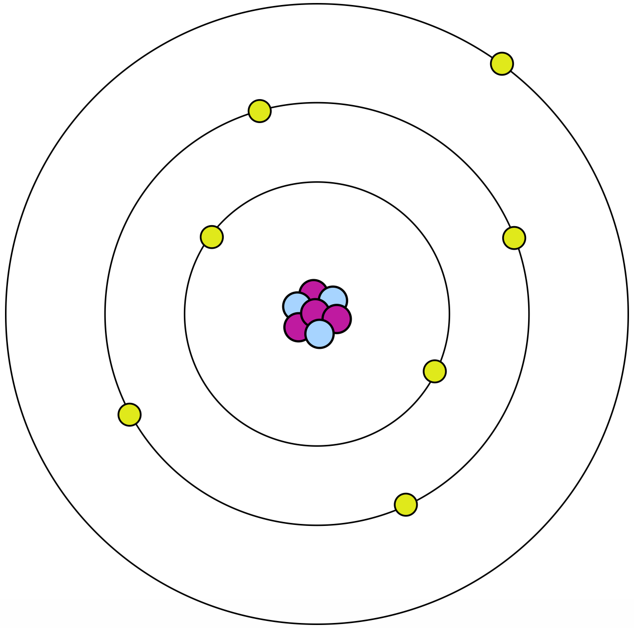
Incorporate quantum effect as part of the computer

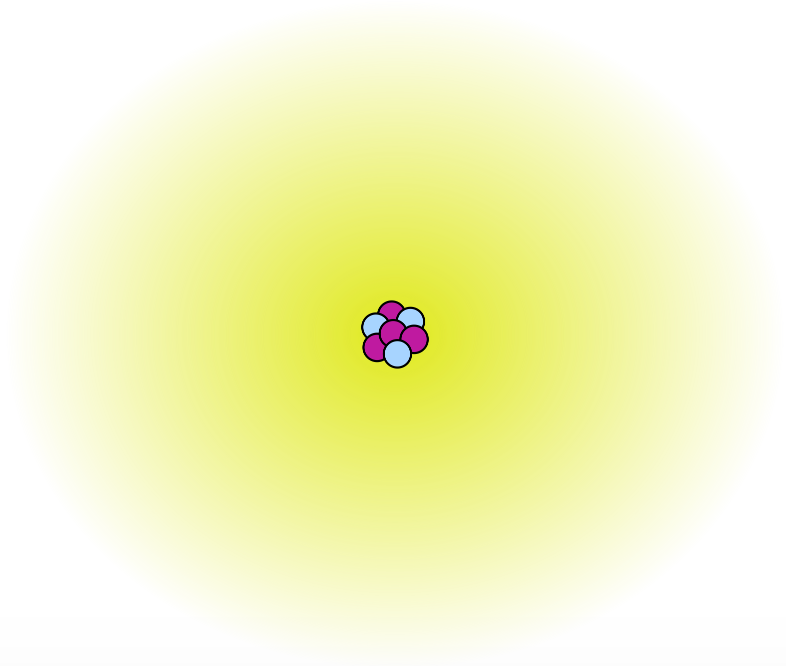






Quantum mechanics are the laws which rules the atomic world

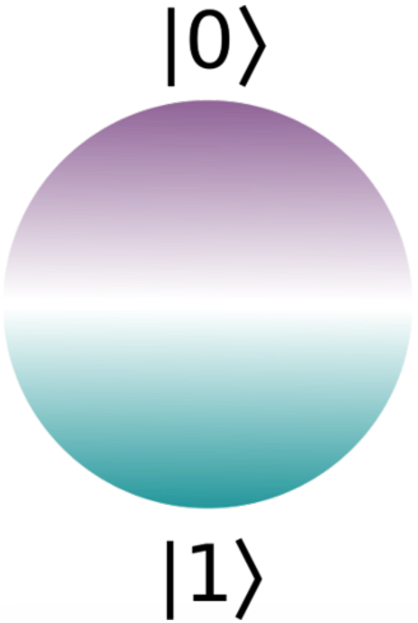




Classical atomic model electrons move as planets around a sun

Quantum atomic model the electrons position is determined by a wave function describing the *probability* of finding the electron at a given position

In quantum computers we harvest this property to make quantum bits



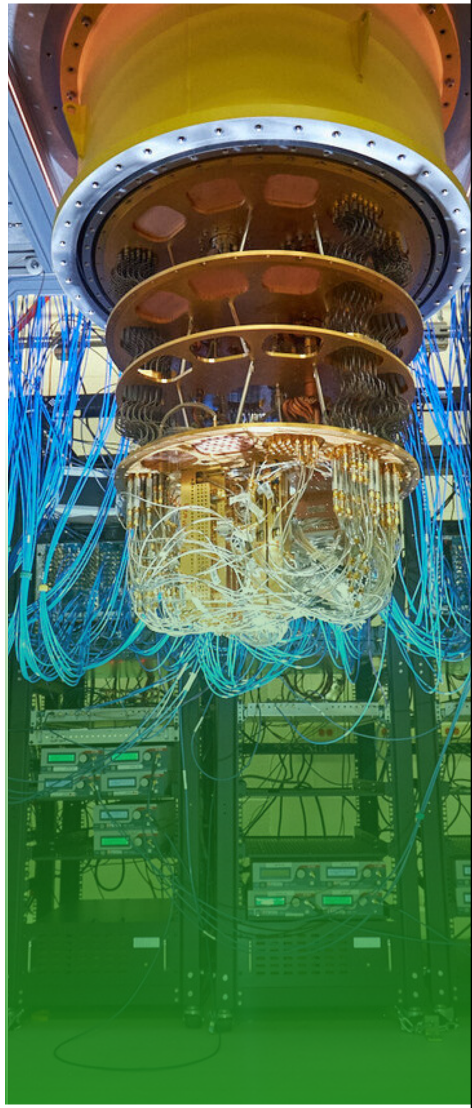
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Classical bit states are well defined in either 0 or 1

Quantum bit (qubit) states are a superposition of 0 *and* 1

There are still several platforms competing to build the best qubit

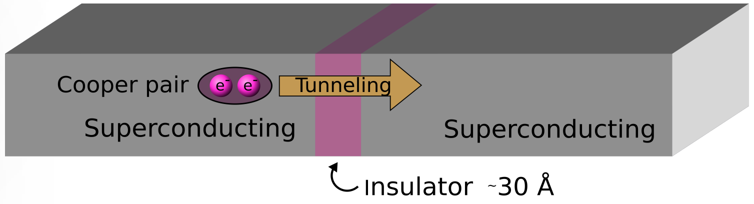
- Superconducting circuits — IBM Q, rigetti, Google, Alibaba
- Ion traps — IONQ, Honeywell, QUANTINUUM
- Rydberg atoms — PASQAL, |QuEra> COMPUTING INC.
- Photonics — XANADU
- Silicon quantum dots — intel
- Topological qubits — Microsoft

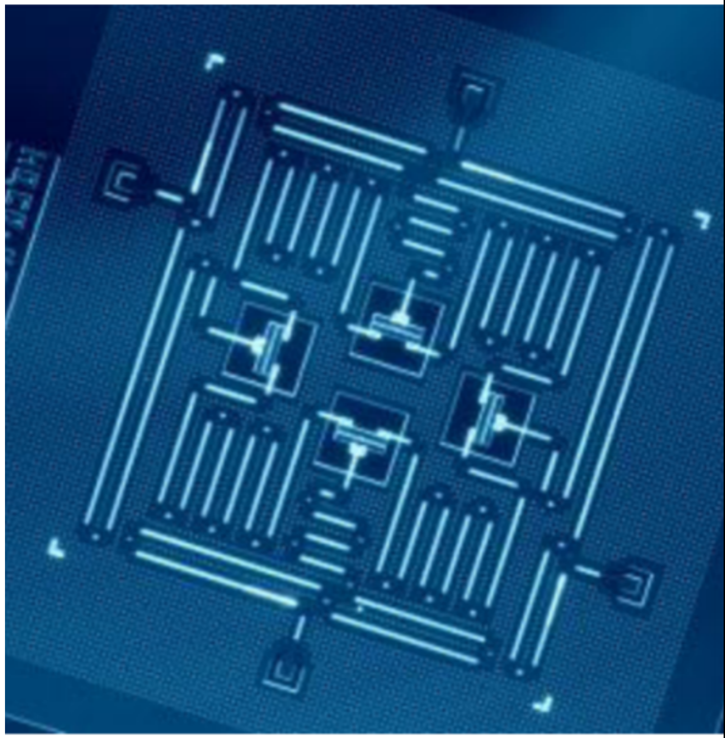


Source: Company webpages

Superconducting circuits are a prominent but cold platform

IBM Q	433 qubits
rigetti	80 qubits
Google	53 qubits
Alibaba	12 qubits





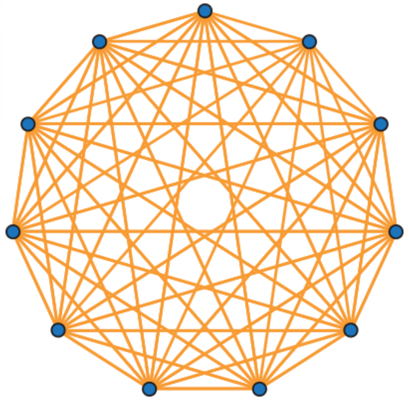
Jay M. Gambetta, Jerry M. Chow & Matthias Steffen
https://www.nature.com/articles/s41534-016-0004-0

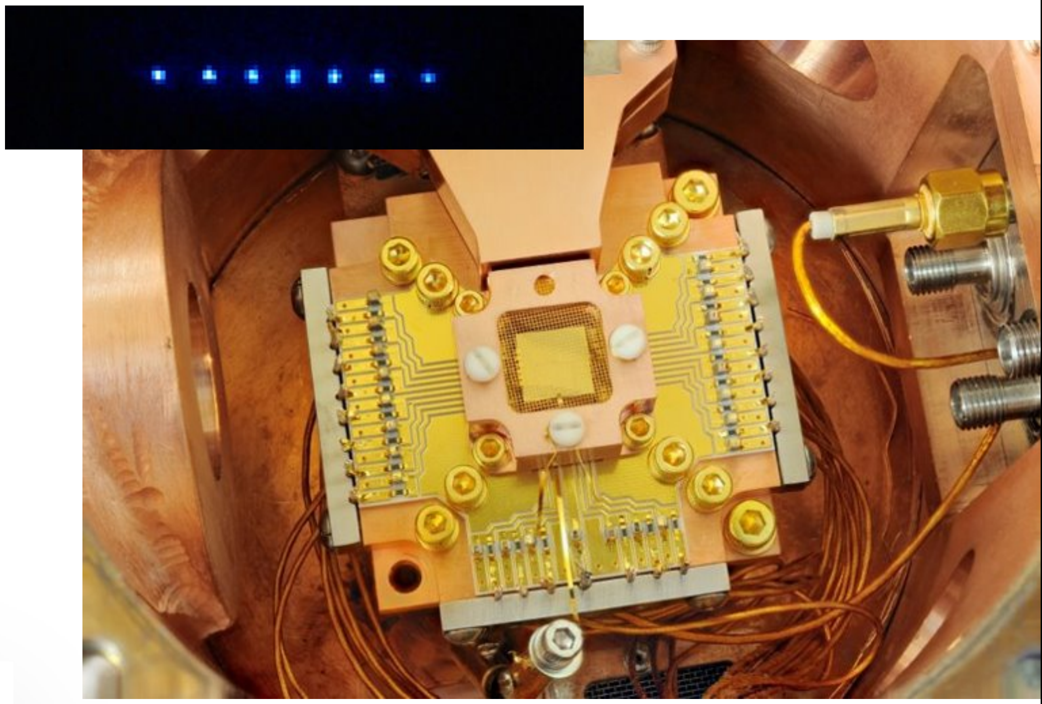
Build using Josephson junctions cooled to -273°C, which allows for tunneling

Fast (MHz) but difficult to connect

Trapped ions allow for full connectivity but are quite slow

Honeywell	32 qubits
IONQ	25 qubits



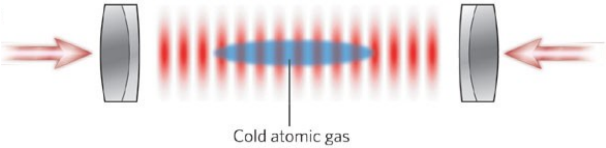


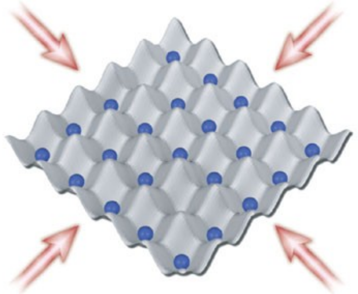
Build by trapping charged ion in magnetic fields

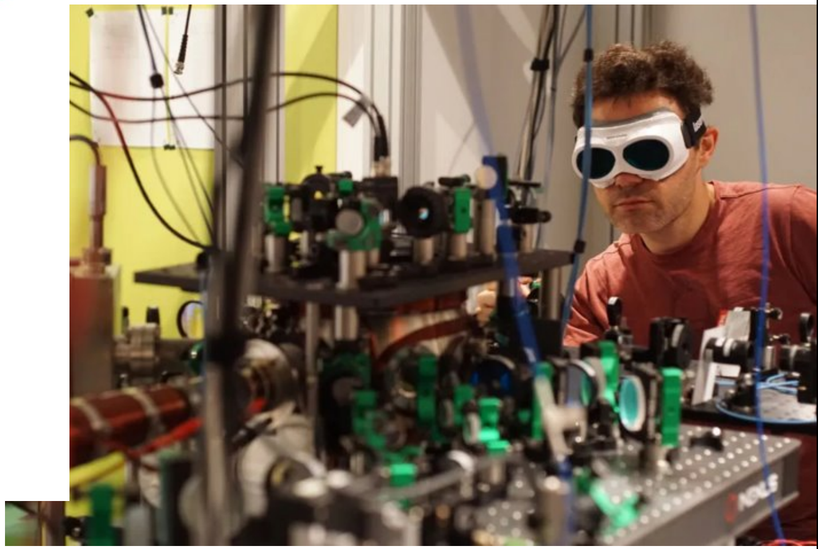
Slow (kHz) but with full connectivity

Rydberg atoms can trap many qubits but lacks connectivity

PASQAL	324 qubits
|QuEra>	256 qubits







Build by trapping large neutral atoms using laser light

Fast (MHz) but lack connectivity

Other platforms are currently lacking behind

XANADU	216 qubits	Photonics (light)
intel	10 qubits	Silicon quantum dots (chips)
Microsoft	0 qubits	Topological qubits (theoretical)

Some are difficult to build, others are difficult to connect

However, they might be the next big thing

The number of qubits are expected to increase **exponentially**

IBM Q	2018	2019	2020	2021	2022	2023 (FUTURE)	2025 (FUTURE)
Qubits	16 qubits	27 qubits	65 qubits	127 qubits	433 qubits	1121 qubits	4158 qubits
Processor		Falcon	Hummingbird	Eagle	Osprey	Condor	Kookaburra

source: https://www.ibm.com/quantum/roadmap

Not all bits are created equally: Most qubits are quite prone to errors

Classical bits are almost perfect; 1 (uncorrectable) error every ~10 year

Majority vote error correction helps this low error rate:
If 9 out of 10 bits agree the last bit is probably wrong

Current quantum bits are *not* perfect; Many errors each second

Error-free qubits are still working progress, but highly needed

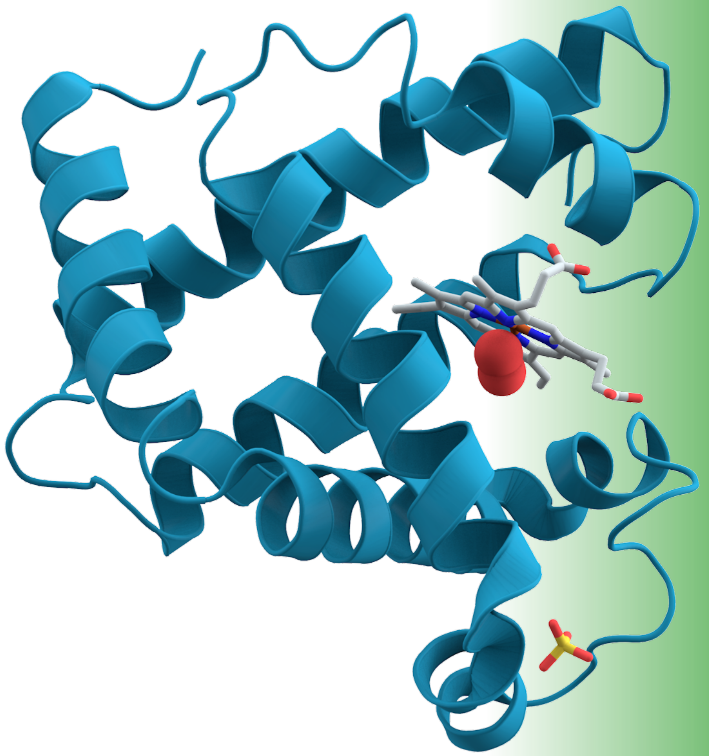
0011101 → Error → 0010101

Use case: Quantum chemistry on a quantum computer

Molecules are quantum mechanical by nature

Discovery of new drugs are very resource consuming

Battery development on quantum computers could help the green transition



Use case: Discovering a new pencilin on a quantum computer

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e.g., computing power needed to discover the next penicillin

A classical computer with more transistors (10^{86}) than there are atoms in the observable universe

A quantum computer with 286 qubits

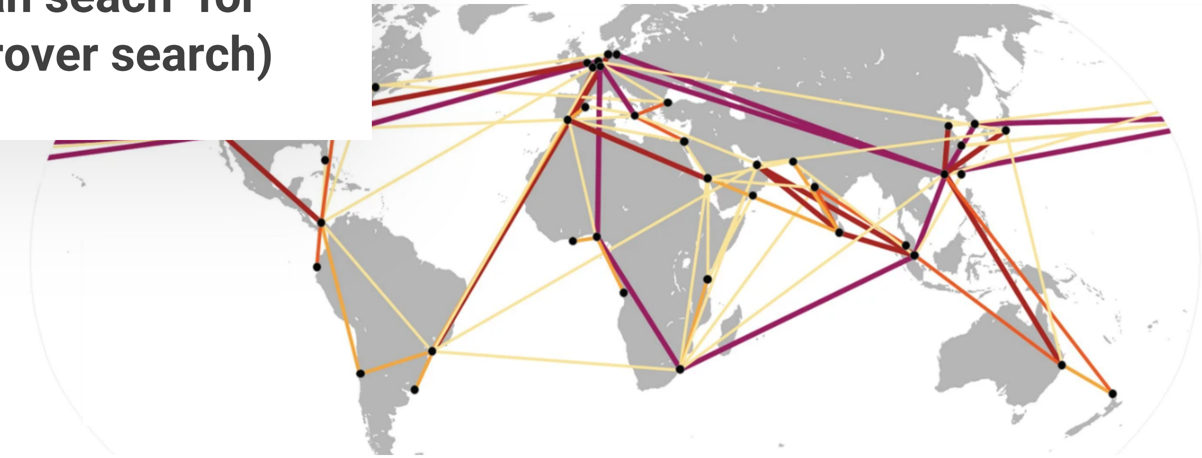
Source: Slide originally by Rigetti Computing Inc. Insight from "Will Quantum Computing Transform Biopoharma R&D?", BCG 10. Dec 2019.

Use case: Logistics optimization is quite suitable for quantum computers

Why is this difficult? Assume 1 ship has to visit 10 harbors out of 100 harbors

More than **10,000 billions** (10^{13}) combinations

On a **quantum computer** we can seach for the optimal path in parallel (Grover search)

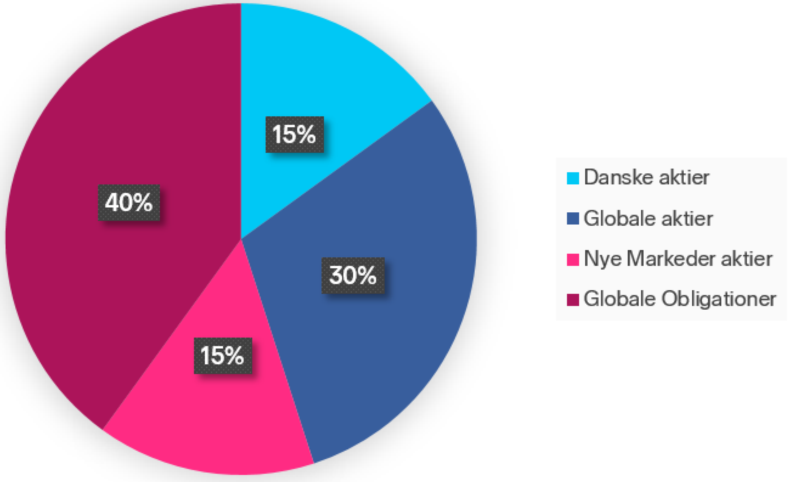


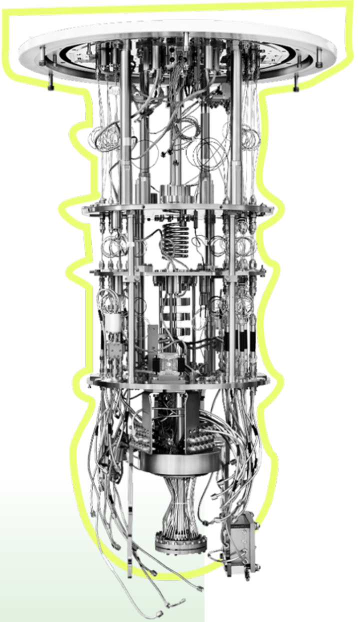
Use case: Financial optimization is suitable for quantum computing

Portfolio optimization and mitigating **financial risk** is increasingly complex

Assume you have 1000 stocks and want to **buy 100 stock for maximum profit**

Again a **quantum computer** can search in parallel





Quantum computing in Denmark recieve increased attention in 2022

March: Kvantify is founded

April: NATO announces quantum technology accelerator based in Copenhagen

September: Novo Nordisk foundation announces 1,5 billion DKK investment


novo nordisk fonden

Milliardinvestering skal udvikle Danmarks første fuldt funktionelle kvantecomputer


Regeringen

Ansvar for Danmark

Det danske samfund skal gøres mere robust i mødet med fremtidens trusler, udfordringer og kriser. Derfor vil regeringen tage initiativ til at styrke organiseringen og prioriteringen af samfundsberedskab, krisestyring, kritisk infrastruktur og forsyningssikkerhed.

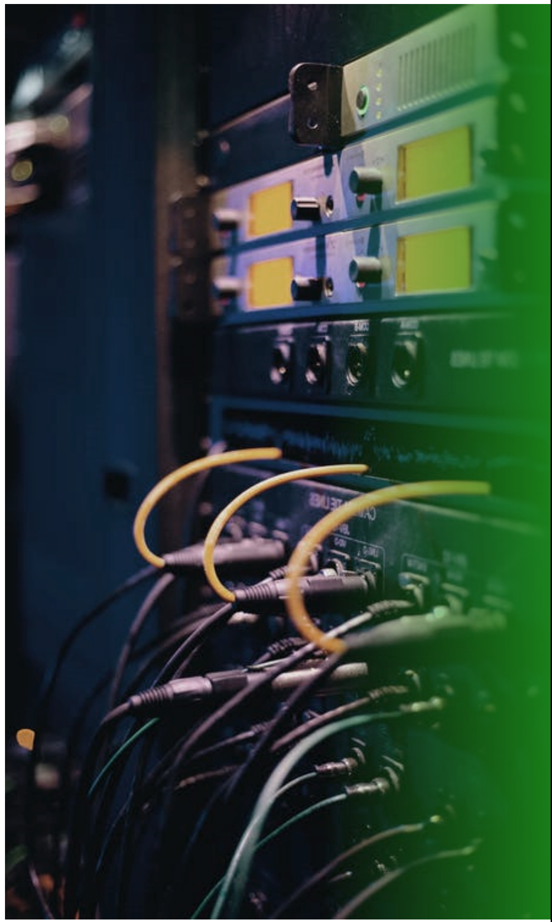
Vi er samtidig en del af en bredere global kamp om indflydelse, viden og ressourcer. Og om selve værdierne bag den internationale retsorden. Sammen med vores partnere og allierede skal vi sikre adgang til kritiske ressourcer, være på forkant med den teknologiske udvikling på f.eks. kvanteområdet og beskytte os mod trusler fra cyberangreb.

Vi skal styrke Udenrigstjenesten og det danske diplomati og dermed sikre Danmark en stærkere stemme globalt. Det gælder både om at udbygge samarbejdet med især ligesindede lande, og det gælder om at fremme indsatsen for at skabe frihed og menneskerettigheder verden over. Og regeringen vil arbejde målrettet for, at Danmark opnår valg til FN's Sikkerhedsråd i perioden 2025-2026.

December: Newly formed DK government foundation includes development of quantum tech

Kvantify is a rapidly evolving software company

- We develop software solutions for demanding computations (HPC / Quantum)
- 30+ employees in Aarhus and Copenhagen, majority with PhDs (condensed matter, chemistry, cosmology, math, etc.)
- Collaborations across EU, expanding towards a global scope (Universities, hardware developers, clients)
- Founded in March 2022, all three founders with PhD from AU



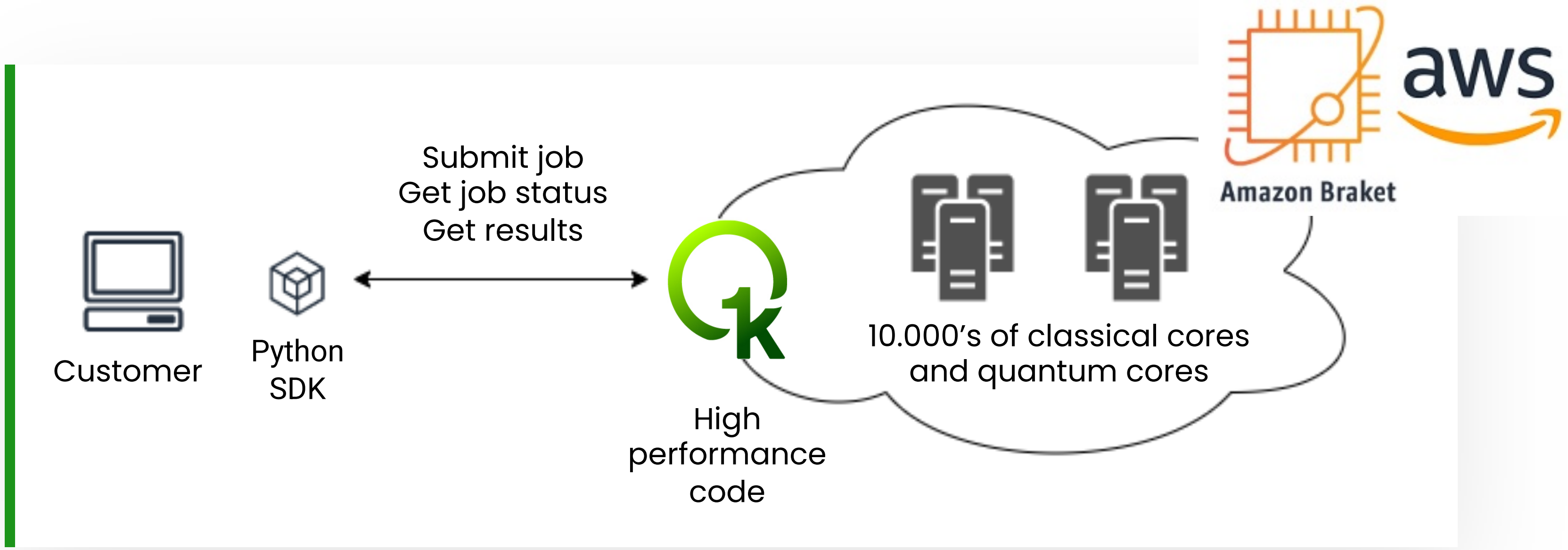
At Kvantify we do (quantum) software

- Quantum computers are difficult of operate and program
- We develope software-as-a-service to companies
- We access quantum computers and high-performance computers via AWS Braket or Azure Quantum

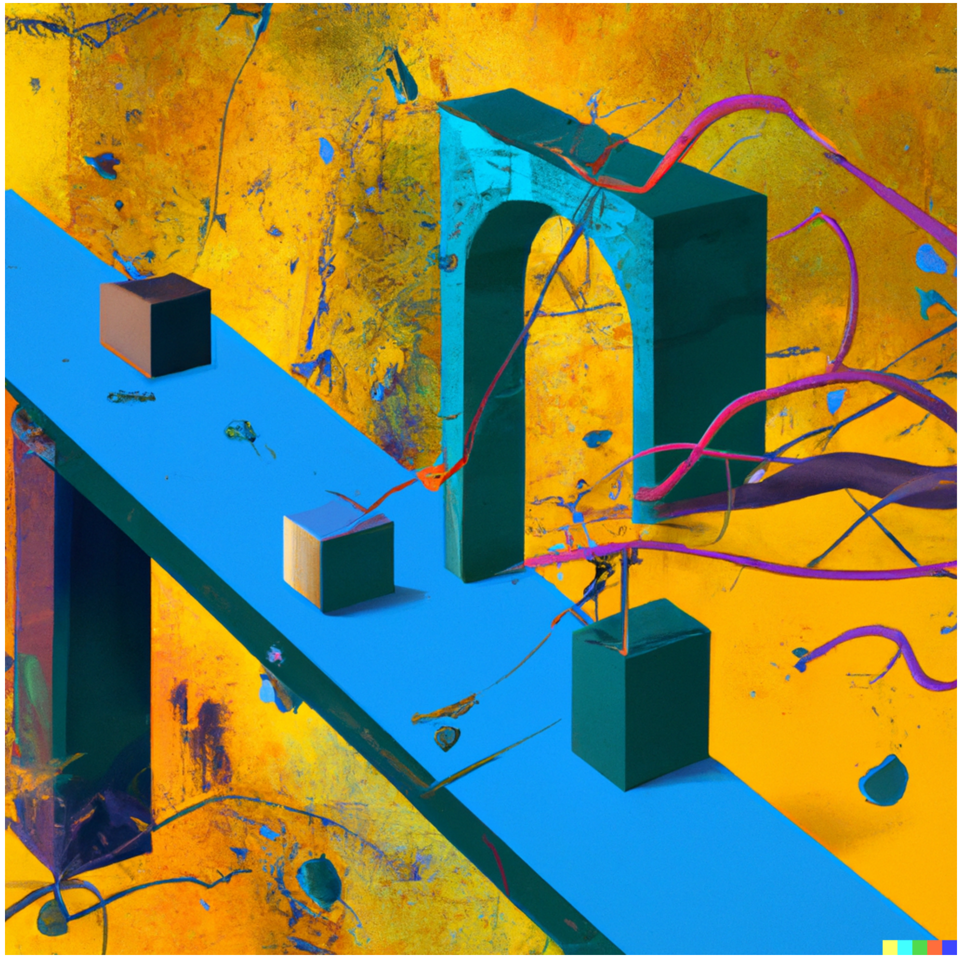
aws
Amazon Braket

Azure Quantum

Our approach to quantum and cloud computing



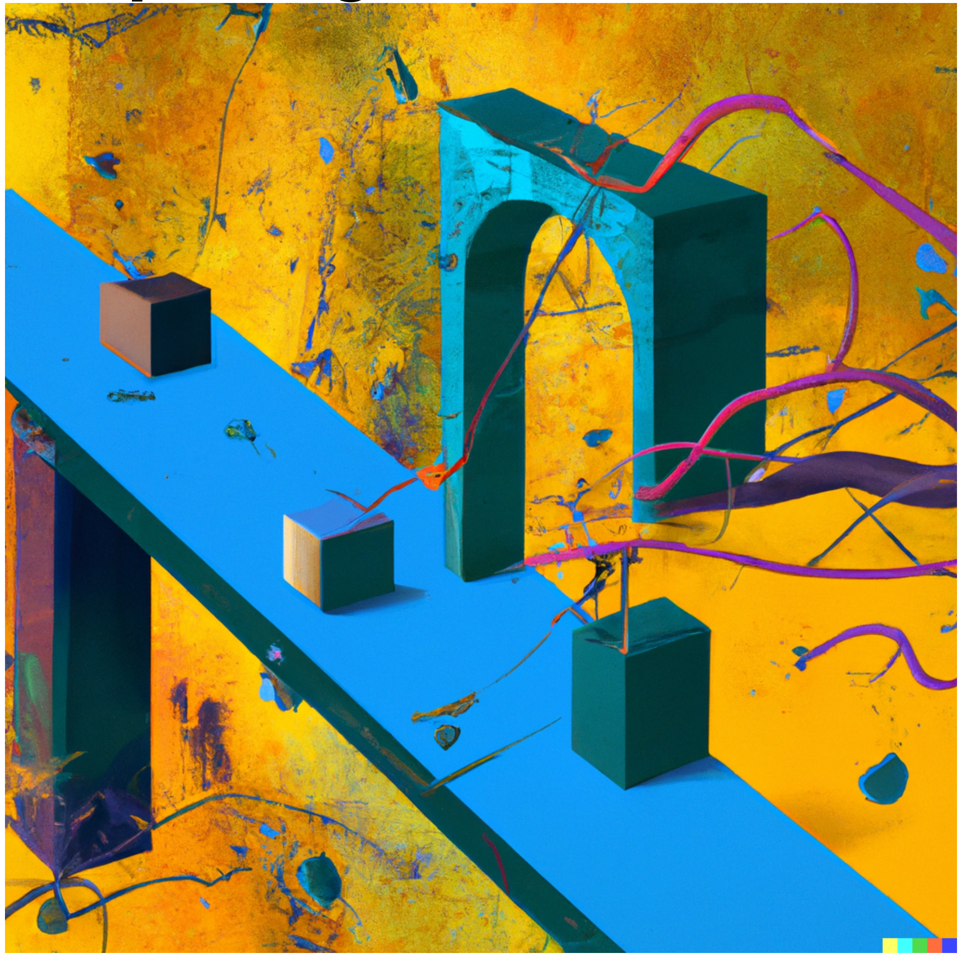
What can Kvantify do now?



DALL-E2: "A bridge going from classical to quantum computers in the style of Dali"

Kvantify: High performance computing as a service

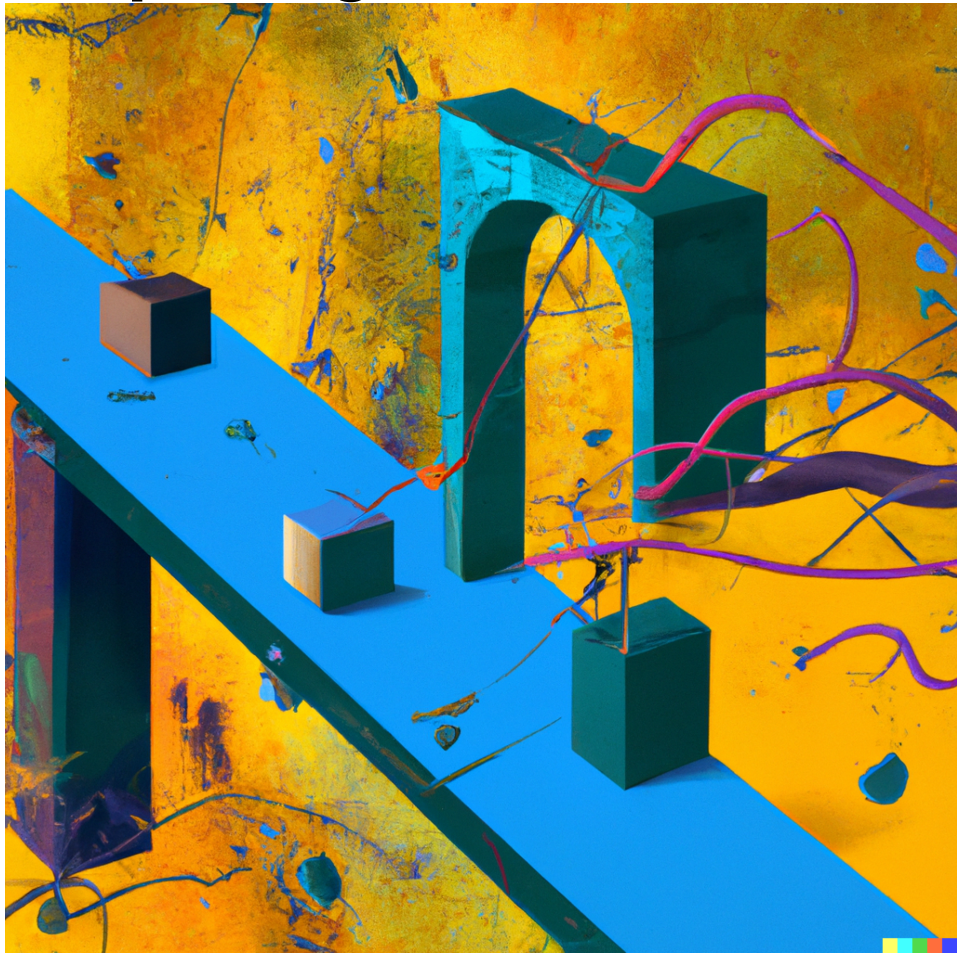
- Traditional HPC solutions
  - Often hard to use
  - Often unstable and poorly tested
  - Unclear how to integrate quantum computers
- Quantum computers are only available as cloud services



DALL-E2: "A bridge going from classical to quantum computers in the style of Dali"

Kvantify: High performance computing as a service

- Deliver HPC-services through cloud computing
- We are a software company
  - High quality software
  - Automated tests
  - Robust
  - Continuous integration and deployment
  - Cloud-native
  - Rapid iterations



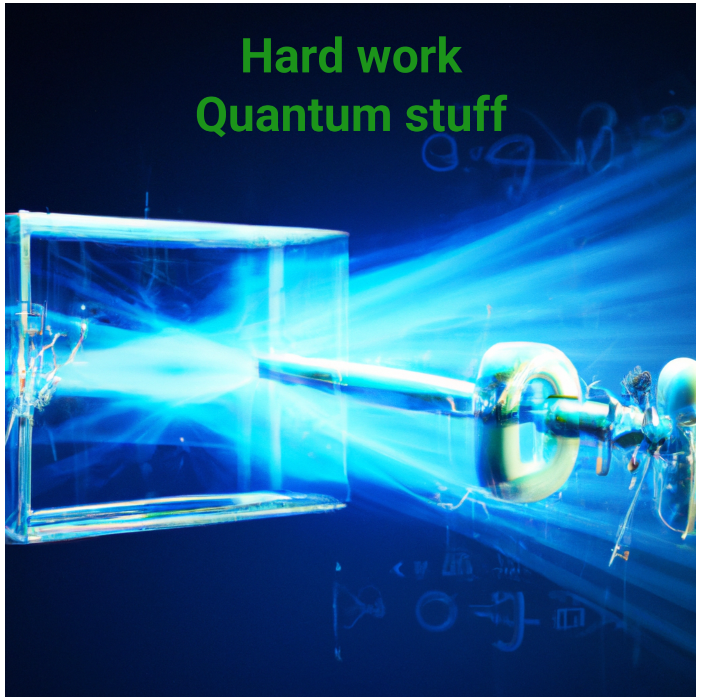
DALL-E2: "A bridge going from classical to quantum computers in the style of Dali"

Deep dive: Our first project

Problem definition

$\sqrt{1000000}$

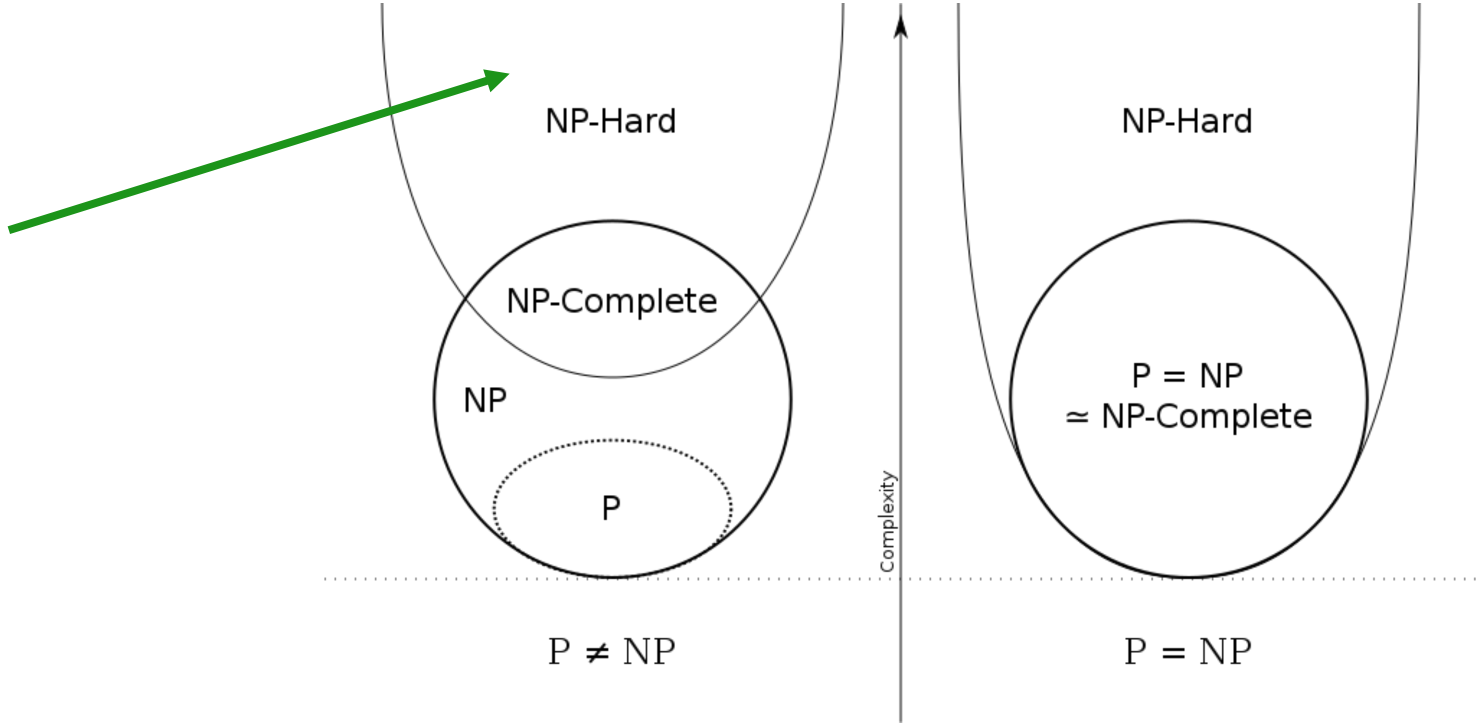
API



1000

Deep dive: Our first project

- A (large) optimisation problem from finance (risk management)
  - 10^2000 combinations
  - No way to check solution is optimal
  - NP-hard
  - Approximating the solution is NP-hard



Timeline

Numerical prototype	CI, CD, Cloud Robustness testing	Fix robustness	Polish
March 2022	August 2022	Dec-Feb 2022	March 2023

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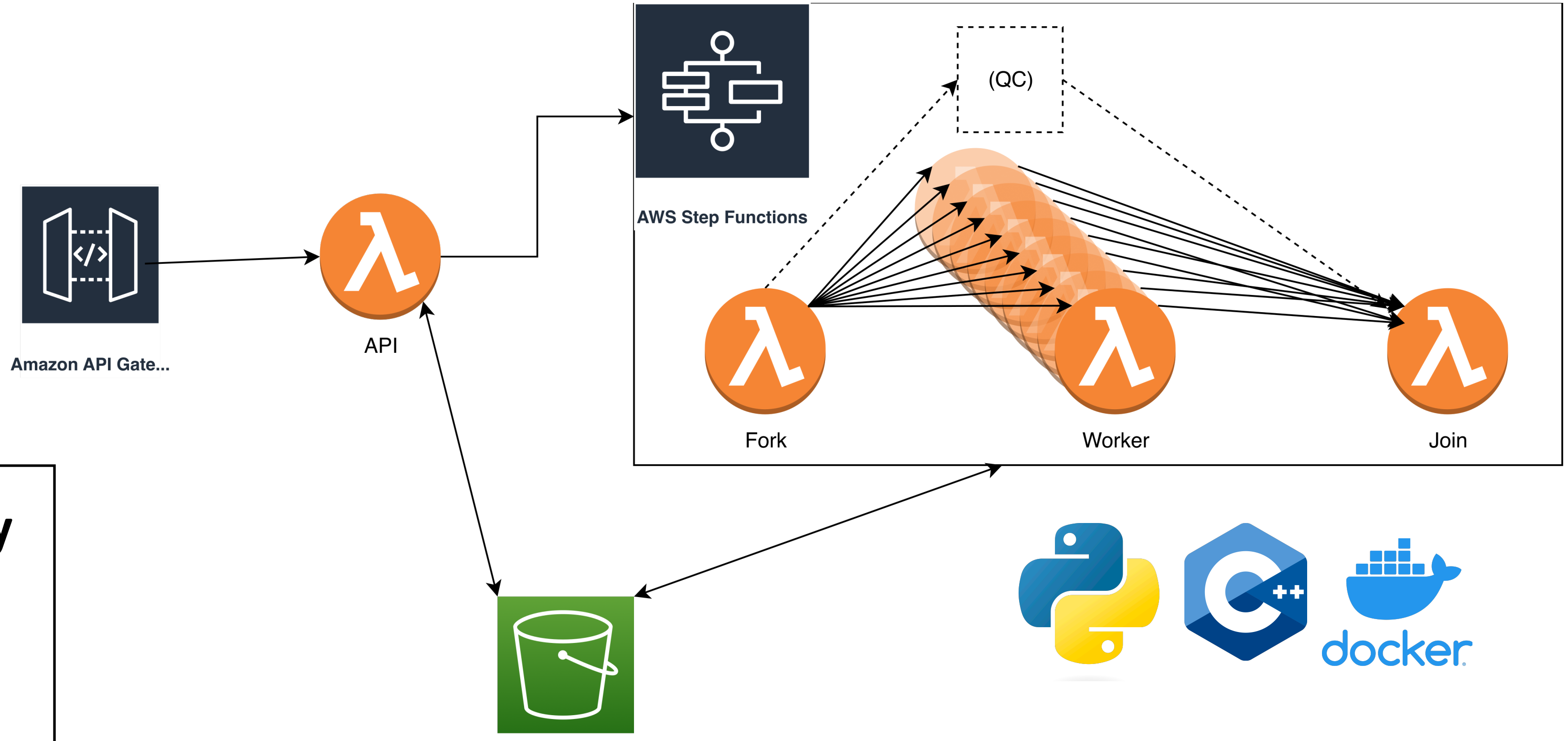
What kind of tech stack does it take?

- Quantum computers
  - Python
  - AWS, Azure, IBM
- Numerics, algorithms
  - Python, C++
- Infrastructure:
  - Python, (Go)
  - AWS, Azure

All sorts of stuff:
Linear algebra,
Monte Carlo
Optimisation (Global, stochastic, convex, …)
Compiler optimisation (for QC)
Machine Learning
…

Architecture



Continuous integration and deployment

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Build

Test

Deploy

aws docker

Distribute

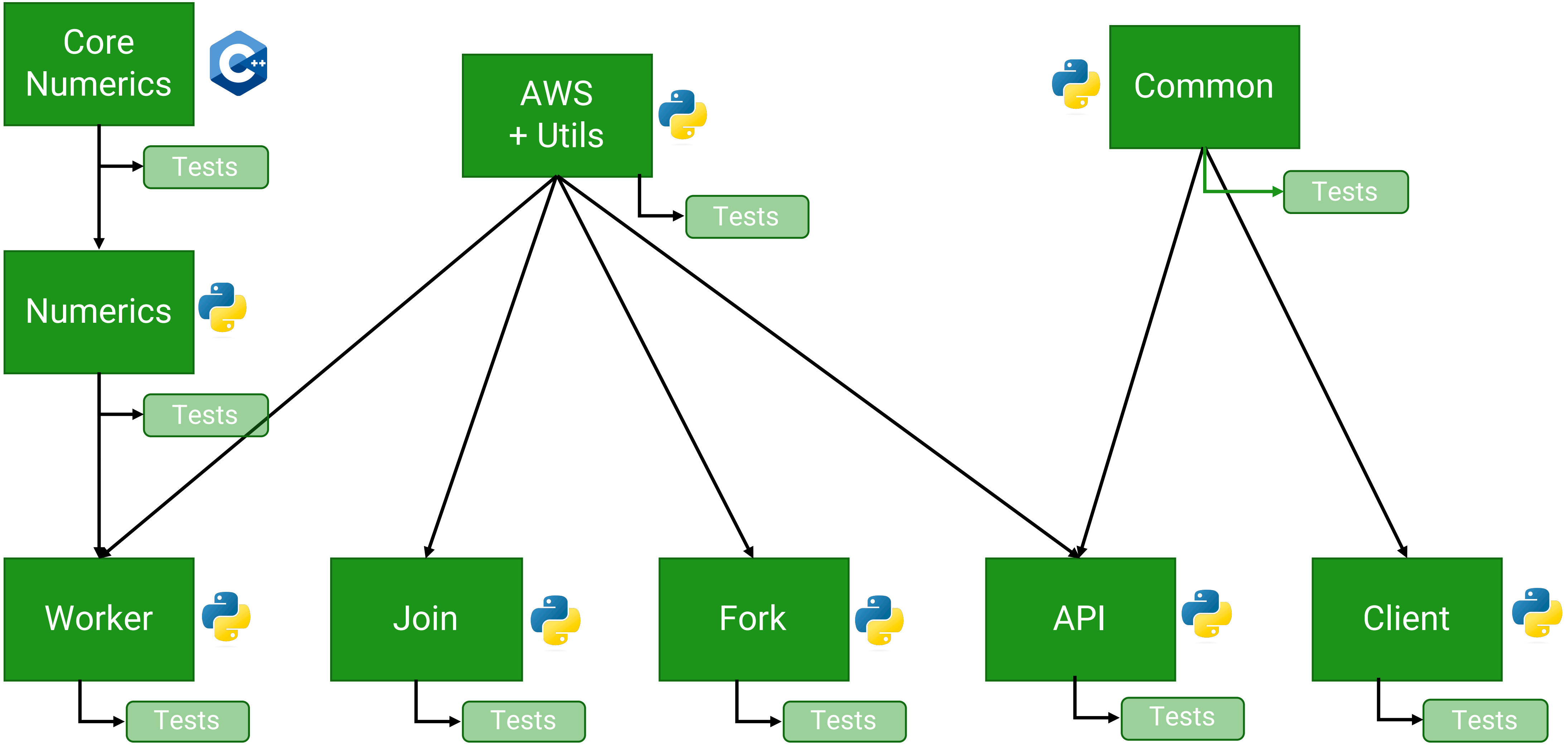
Azure

docker

Poetry (python)
CMake (c++)
Makefiles (coordination)
Docker (deployment+dev)
Autoconf, vcpkg (C++ dep)

Super slow.
Brittle.
Small codebase

Why brittle and slow?



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Enter bazel

- Monorepo build tools seems to fit the bill:
  - bazel, meson, buck2, gradle, …
- Tracks dependencies across languages!
- Tracks test dependencies
- Settled on bazel with
  - C++ toolchain for linux and mac (clang)
  - Python
  - Rules for building docker images
  - Rules for packaging python bundles
  - All third party dependencies pulled using bazel and explicit versions

Bazel

Enter bazel

- Huge improvement in developer experience
  - Very stable
  - Almost no setup for new developers (just works)
  - Encourages modularization on module level
  - Encourages tests at module level
  - CI/CD went from 30 minutes to 2 minutes (for one project)
- Just run `bazel test //...`
  - Fetches dependencies (including C++ compiler)
  - Builds everything including dependencies
  - Tests everything (python and C++ tests)

Robustness

Numerical prototype

CI, CD, Cloud
Robustness testing

Fix robustness

Polish

March 2022

March 2023

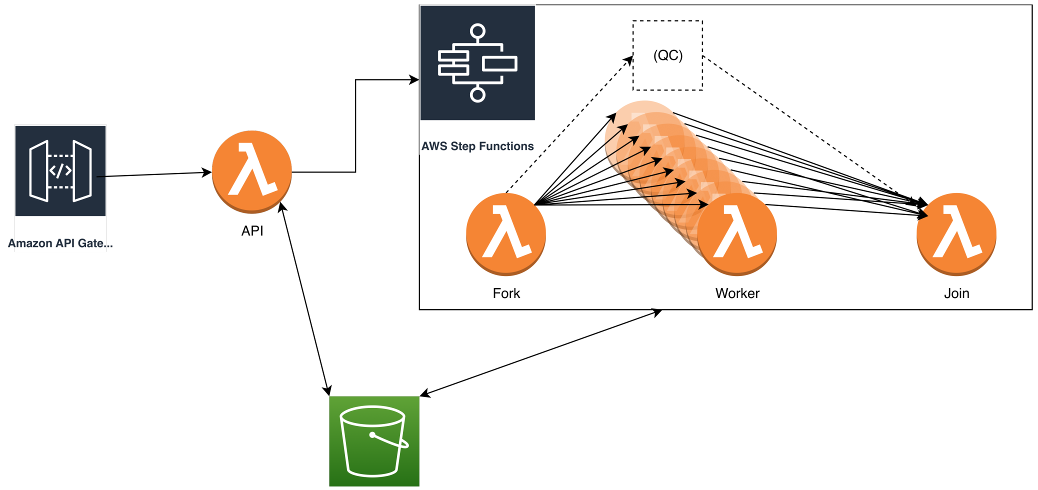
3 months
Testing
Corner cases
Rewrote numerics

Testing numerical calculations

- Testing HPC/QC applications can be quite difficult
  - HPC
    - Not always possible to test in isolation
    - An integration test can cost many $
    - Unknown true answers
  - QC: cannot run the program at any reasonable size in tests
    - Formal verification methods?
    - Simulation (expensive)
    - An integration test can cost many many many $

Final solution

1. User starts a job using the API
2. The API implementation starts an AWS step function
3. Step functions starts 1500 lambda instances in a few seconds
4. The 1500x6 threads runs our C++ simulation with different seed for 5 minutes (~10 TFLOPS)
5. Results are combined and returned to the user



- A lot of compute power delivered on demand for a short time.
- Existing system:
  - Very approximate calculation
  - 6 hours
- Our:
  - More accurate
  - 5 minutes

THANK YOU

www.kvantify.dk

Join the quantum revolution.
We are hiring.

Contact Søren Bendlin Gammelmark or Casper Kirkegaard on LinkedIn