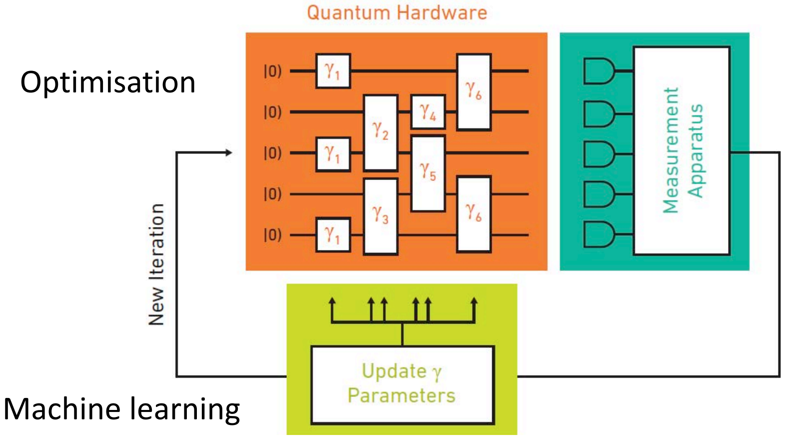
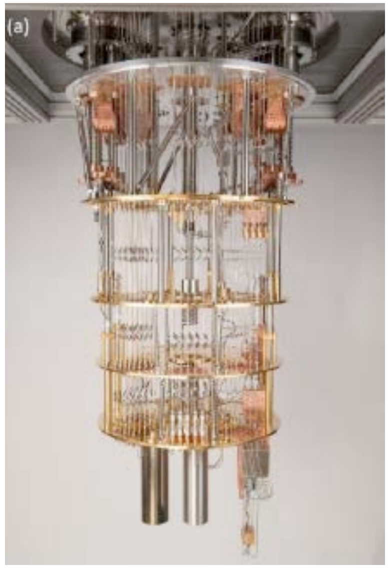
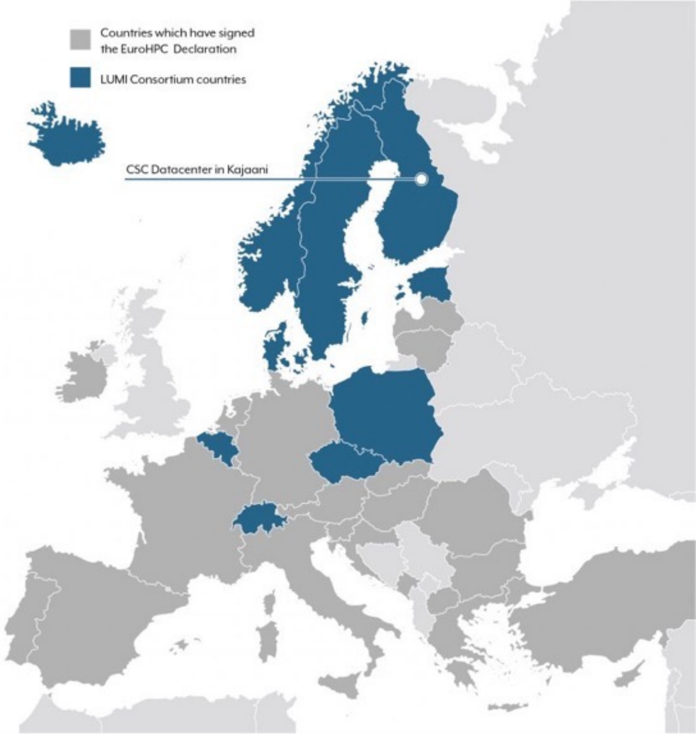
Nordic-Estonian Quantum Computing e-Infrastructure Quest

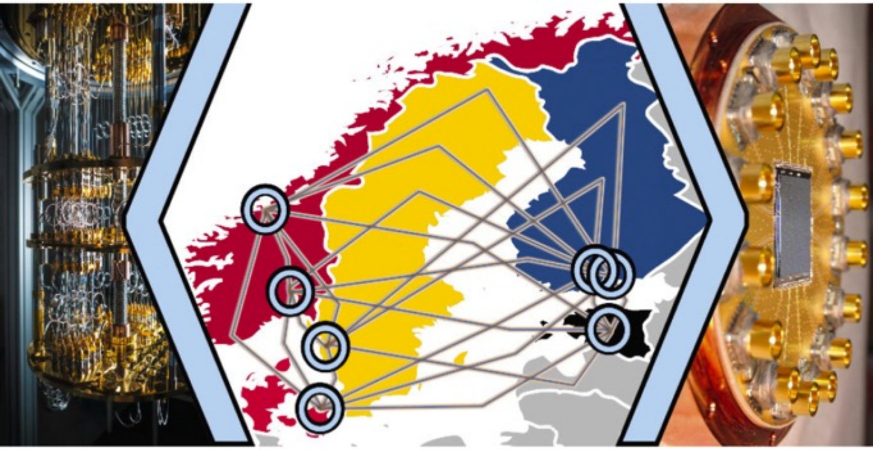




NordIQuEst

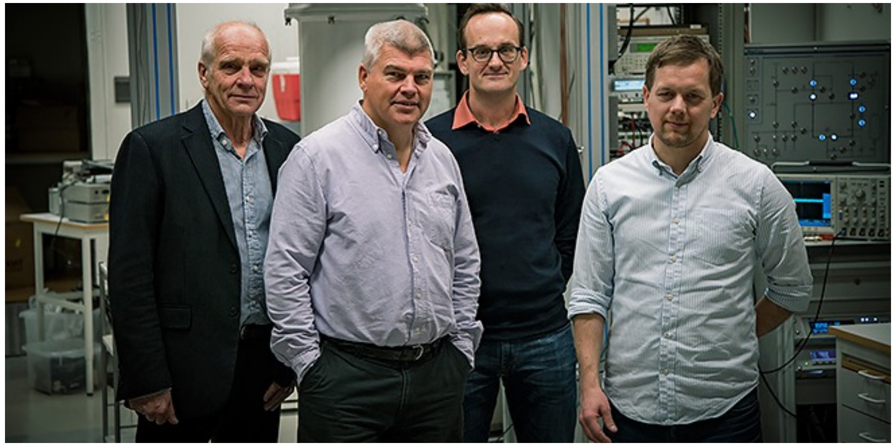
Göran Wendin
Quantum Technology Lab
Microtechnology and Nanoscience,
Chalmers



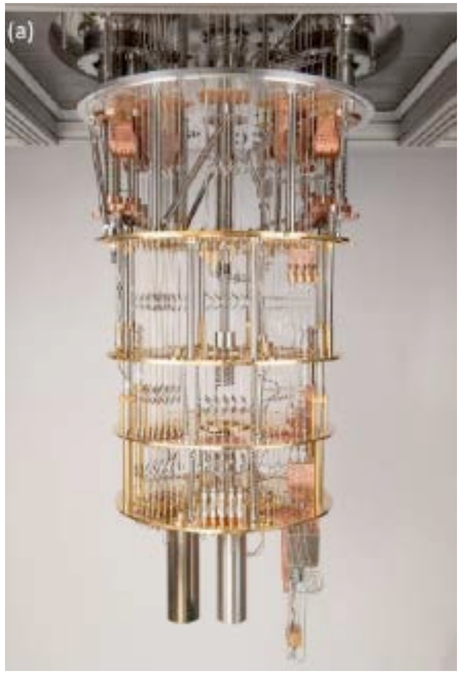


What happens at Chalmers ….. ?

Wallenberg Centre for Quantum Technologies
WACQT, 2018-2029   MC2, Chalmers U of Tech, Sweden



Cryostat
≈ 10 mK

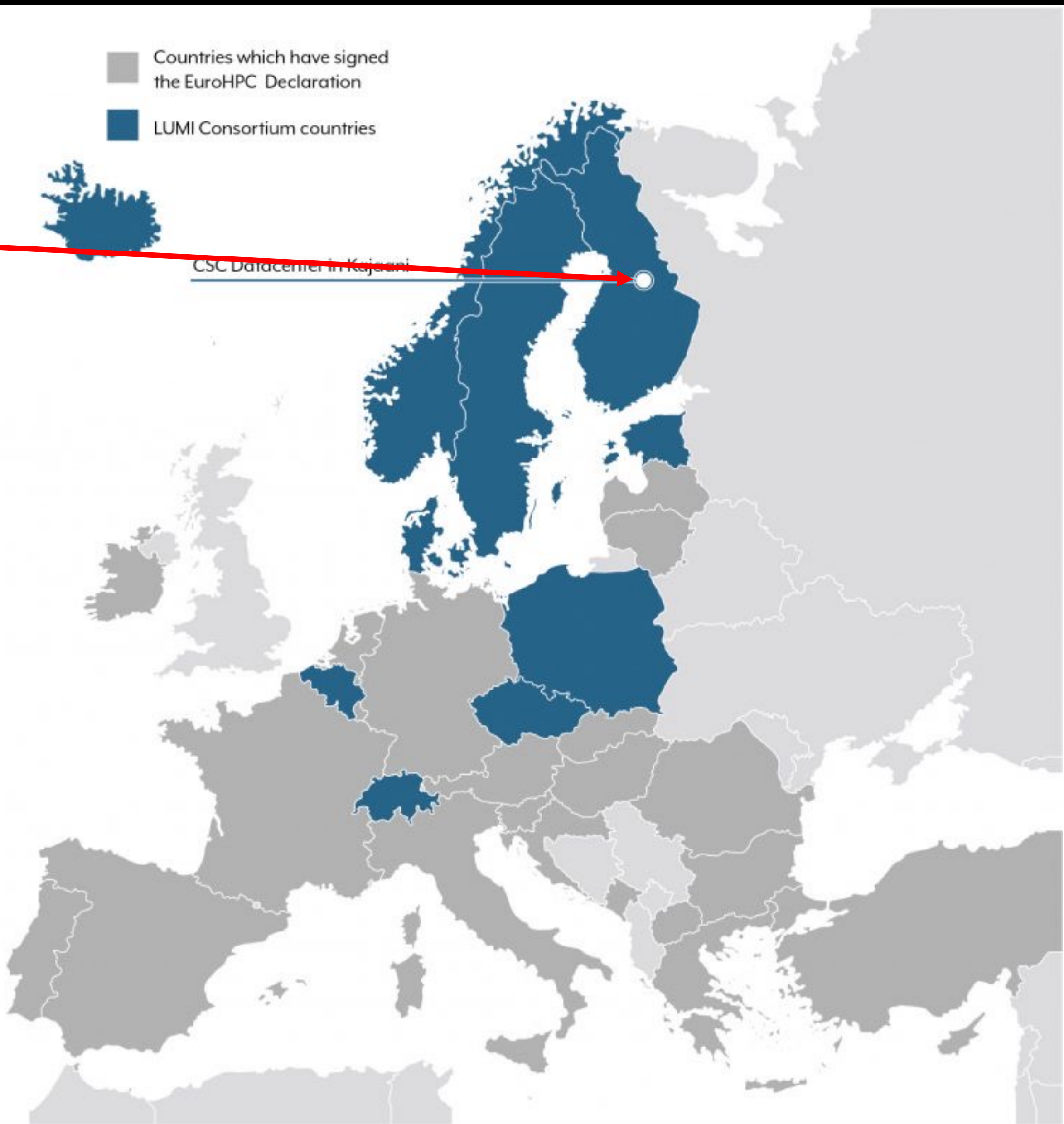


Mission: to build a quantum processor
with 100+ superconducting (Transmon) qubits

OpenSuperQ → OpenSuperQPlus (EU Quantum Flagship)
Mission: to build a 100+q full-stack QC by 2025 (and 1000+ by 2029 ….)

What happens in super HPC ….. ??

pre-exascale LUMI
EuroHPC JU



LUMI consortium partners:
Belgium: Belgian Science Policy Office
Czech Republic: VSB –Technical University of Ostrava, IT4Innovations National Supercomputing Center
Denmark: Universities Denmark
Estonia: Estonian Scientific Computing Infrastructure
Finland: CSC – IT Center for Science Ltd.
Iceland: University of Iceland
Norway: UNINETT Sigma2 AS
Poland: AGH University of Science and Technology, Academic Computer Centre Cyfronet AGH
Sweden: Swedish Research Council, Vetenskapsrådet
Switzerland: ETH Zürich

What happens in super HPC-QC …. ???

LUMI-Q

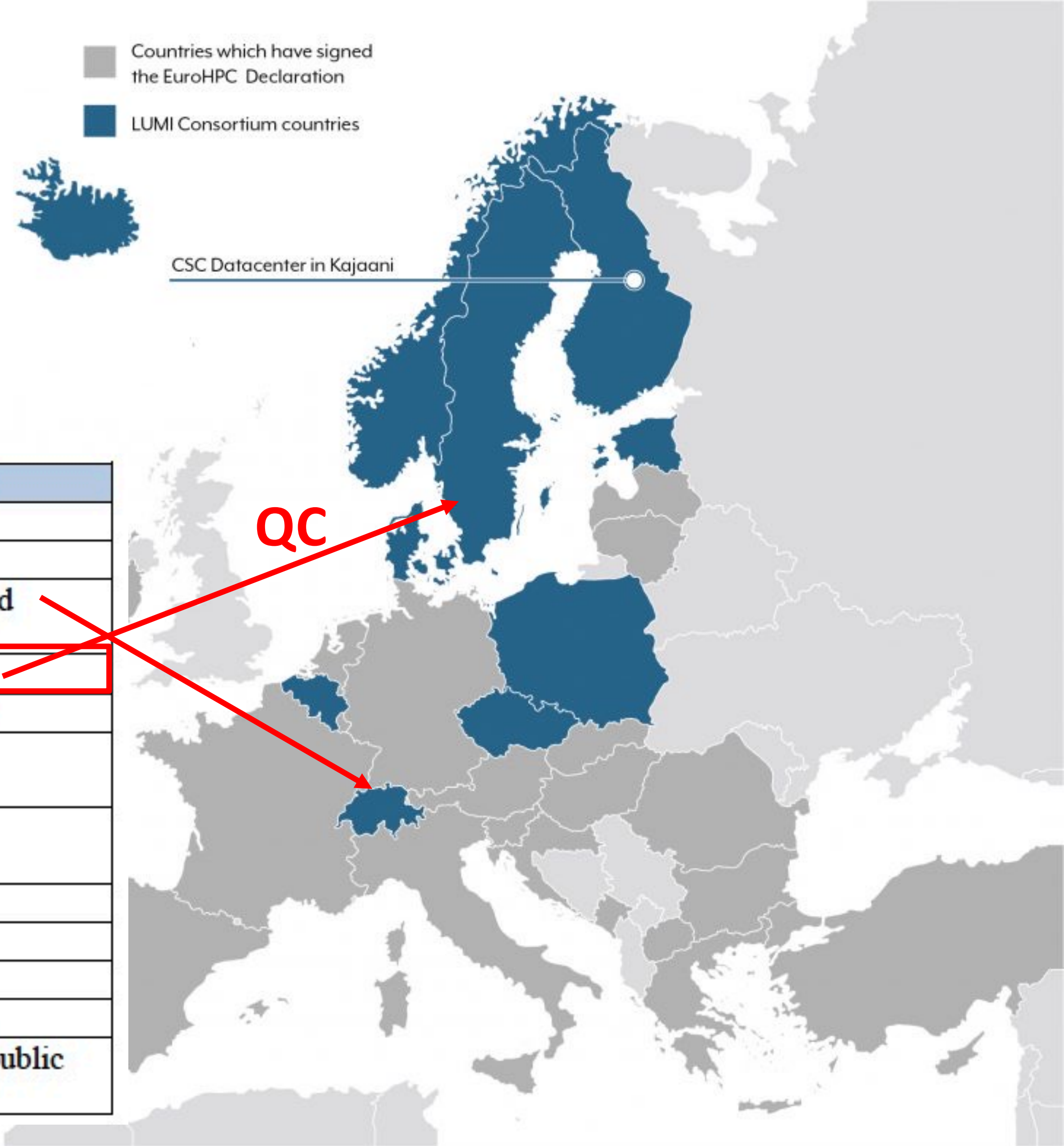
Sections 1-3

Proposal full title	LUMI-Q: The EuroHPC Quantum Simulation Infrastructure
Proposal acronym	LUMI-Q
Topic identifier	EuroHPC-2020-01-b
Type of action	EuroHPC-RIA
Coordinator	CSC – IT Center for Science Ltd
Person in charge of the proposal	Dr. Kimmo Koski, kimmo.koski@csc.fi Managing Director CSC – IT Center for Science Ltd

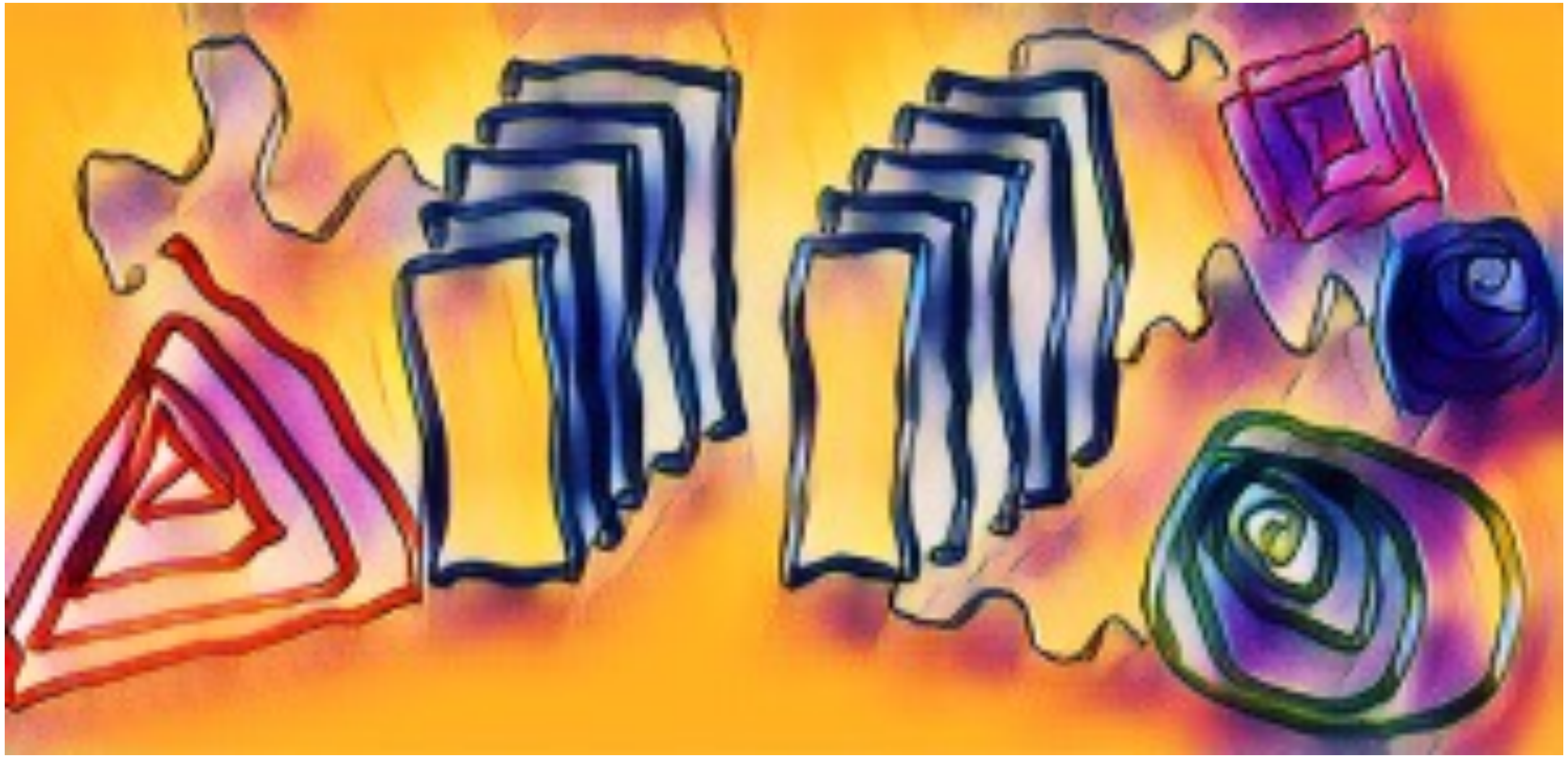
EuroHPC JU proposal autumn 2020

"almost succeded"

#	Partner full name	Short name	Country
1	CSC-TIETEEN TIETOTEKNIIKAN KESKUS OY	CSC	Finland
2	TEKNOLOGIAN TUTKIMUSKESKUS VTT OY	VTT	Finland
3	EIDGENOESSISCHE TECHNISCHE HOCHSCHULE ZUERICH	ETHZ	Switzerland
4	CHALMERS TEKNISKA HOEGSKOLA AB	CHALMERS	Sweden
5	TECHNISCHE UNIVERSITAET MUENCHEN	TUM	Germany
6	CENTRUM ASTRONOMICZNE IM. MIKOLAJAKOPERNIKA POLSKIEJ AKADEMII NAUK	NCAC	Poland
7	AKADEMIA GORNICZO-HUTNICZA IM. STANISLAWA STASZICA W KRAKOWIE	Cyfronet	Poland
8	TARTU ULIKOOL	UTARTU	Estonia
9	SINTEF AS	SINTEF	Norway
10	SIMULA RESEARCH LABORATORY AS	SRL	Norway
11	UNIVERSITEIT HASSELT	UHASSELT	Belgium
12	VYSOKA SKOLA BANSKA - TECHNICKA UNIVERZITA OSTRAVA	IT4I	Czech Republic

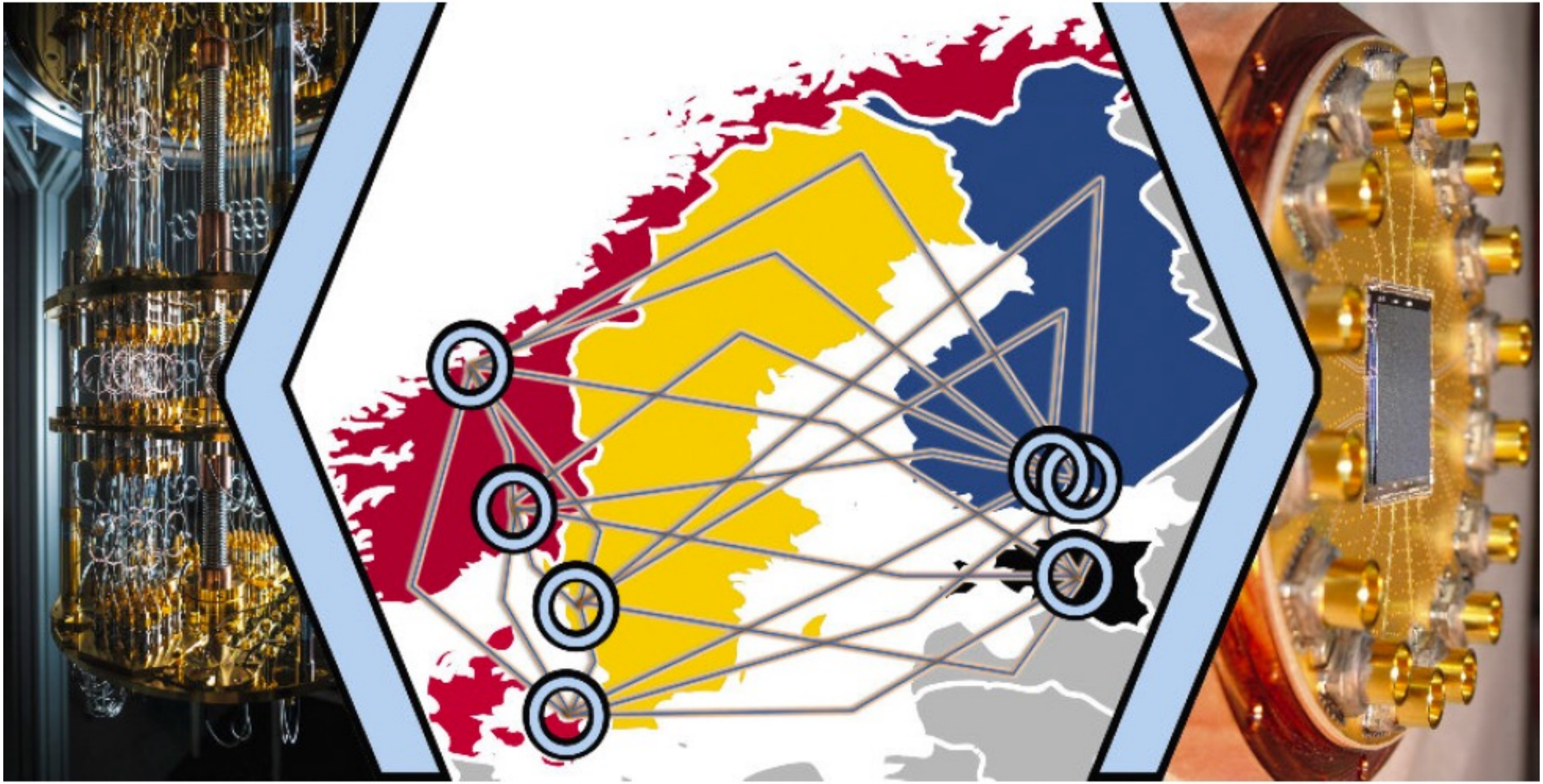


The LUMI-Q concept



Depiction of the LUMI-Q concept, where several different quantum computing solutions are integrated with the LUMI supercomputing ecosystem.

The NordiQuEst result !!



Nordic-Estonian Quantum Computing e-Infrastructure Quest

Ir	
C	
C	
D	
S	
SRL	
UTartu	of.
VTT	Team Leader

NordIQuEst

Start 1 Feb 2022, 3 years

Göran Wendin Project Manager

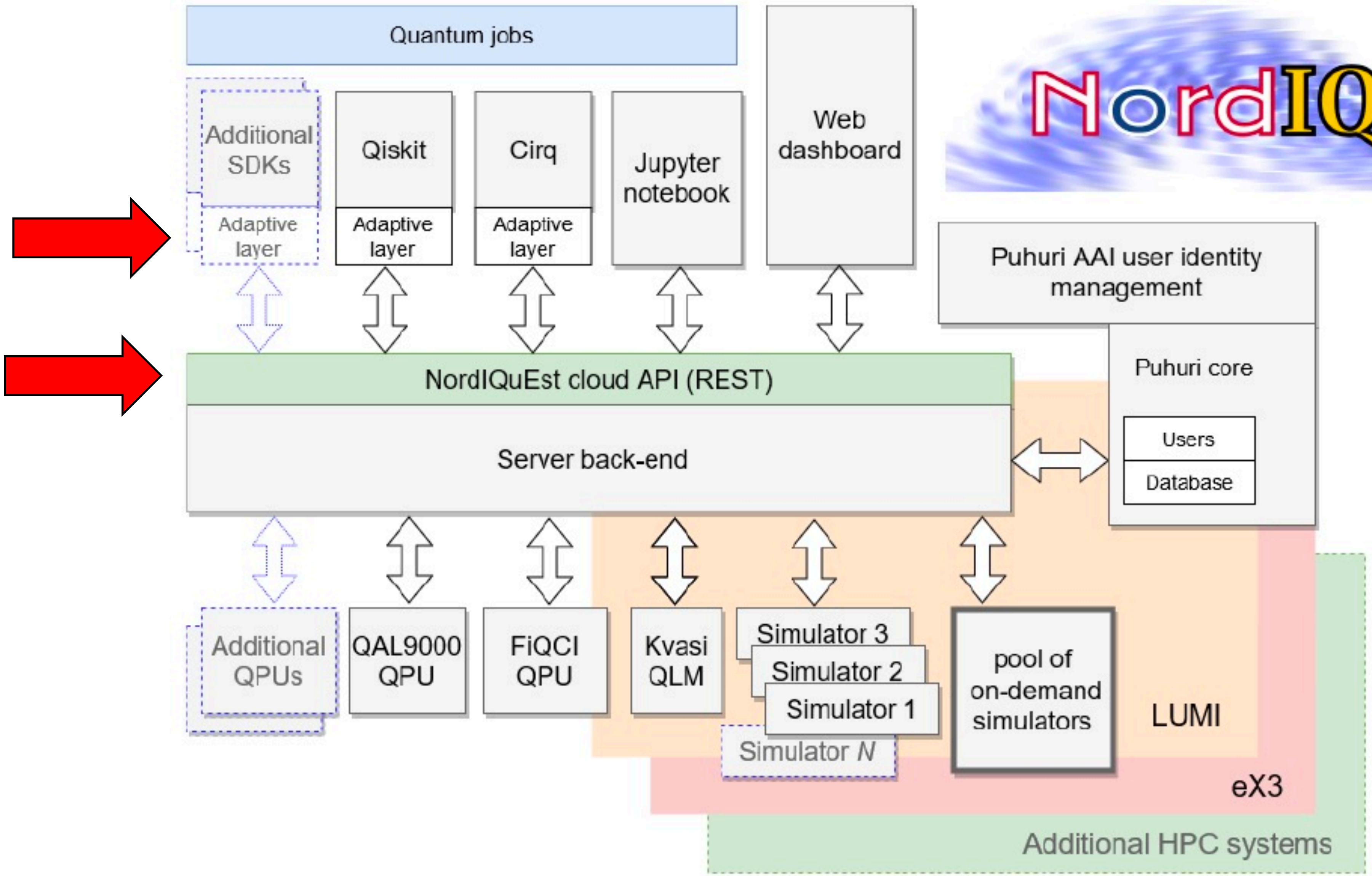
Nordic-Estonian Quantum Computing e-Infrastructure Quest

Institution	Country	Contact person	Position
CHALMERS	Sweden	Göran Wendin	Professor
CSC	Finland	Mikael Johansson	Technology Strategist
DTU	Denmark	Sven Karlsson	Assoc. prof.
SINTEF	Norway	Franz Fuchs	Research Scientist
SRL	Norway	Shaukat Ali	Professor
UTartu	Estonia	Dirk Oliver Theis	Assoc. prof.
VTT	Finland	Ville Kotovirta	Research Team Leader

The NordIQuEst Mission

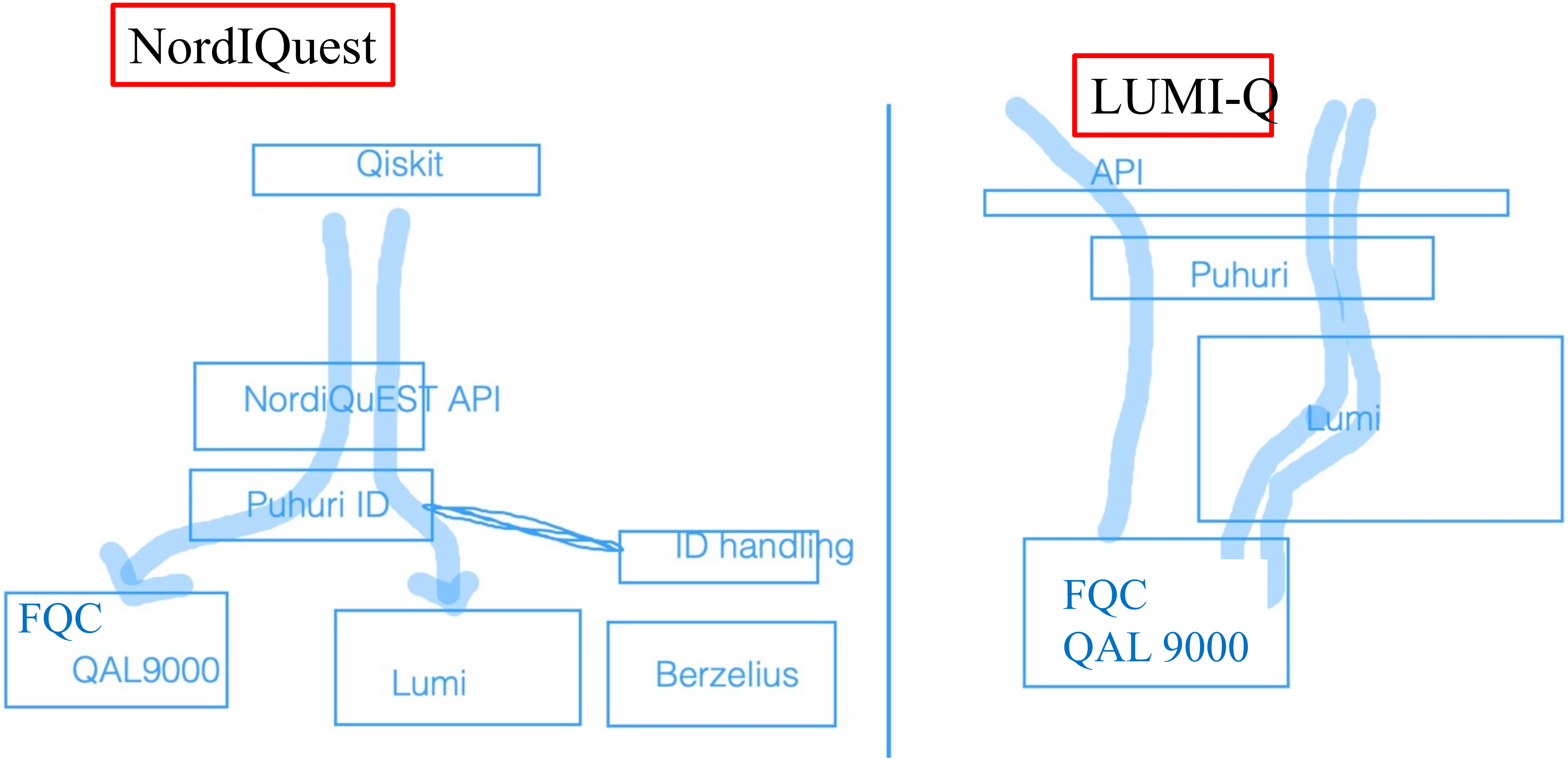
- **NordIQuEst** will deliver user and computer **interfaces**, quantum program **libraries**, **training** and **education** events and material, as well as user **support**.
- **Pooling of resources and collaboration** for reaching critical mass, **providing access** to several **Nordic quantum computers (QPU)** and **QC simulators (SW+HPC)**
- **Chalmers** and **VTT** will **connect** their current QCs to the **NordIQuEst Rest API**
- **CSC** will **connect LUMI** and **the Atos QLM** quantum simulator to the **NordIQuEst API**
- By the end of this project, a **sustainable functioning, truly multi-purpose Nordic quantum computing ecosystem** will be established and ready to be further exploited

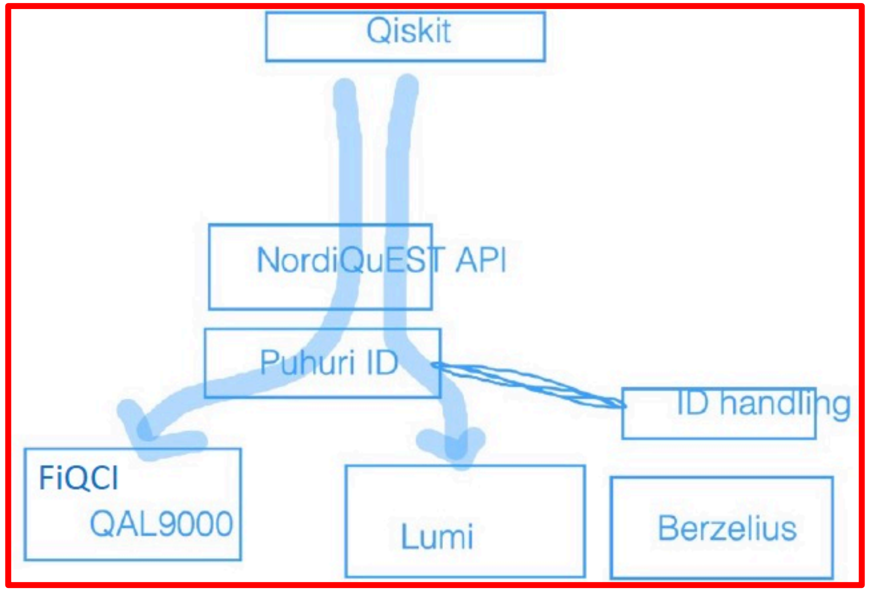
NordiQuEst in a nutshell

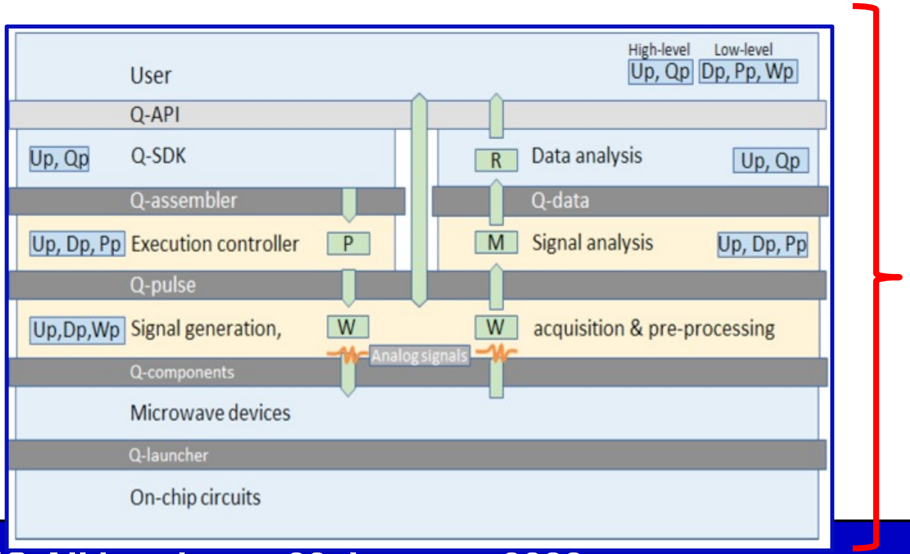


NordIQuEst

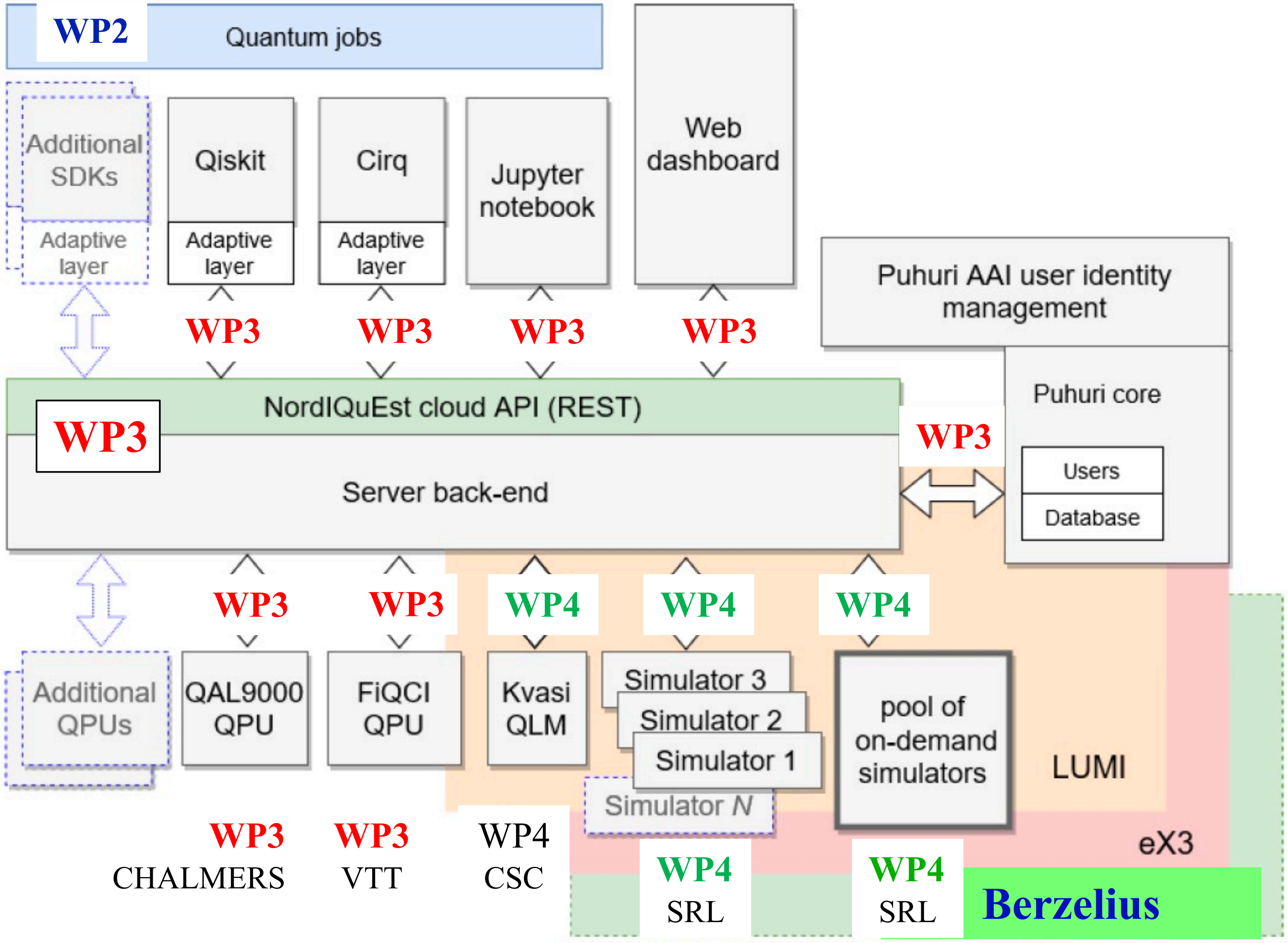
The difference between NordIQuEst and LUMI-Q and the meaning of "**connect**"







WP2: Library of use cases:
QAOA, VQE, …..



MD1.1 Presentation material on the opportunities of and for quantum computing prepared
MD1.2 First report on the user-base
MD1.3 Final report on the user-base, including progress and change report
MD2.1 Installation of quantum programming frameworks
MD2.2 Sample QAOA application library
MD2.3 **Problem library with rules**
MD2.4 Testing and debugging framework
MD3.1 The **NordIQuEst API defined**, access vetted through **Puhuri**
MD3.2 **Real quantum computers connected**
MD3.3 Adaptive layers for Qiskit and Cirq created
MD4.1 Kvasi, the **Atos** Quantum Learning Machine **connected**
MD4.2 Large and accelerated simulators connected
MD4.3 Pool of smaller on-demand simulators, suitable for **education connected**
MD5.1 NordIQuEst home page
MD5.2 FAQ section
MD5.3 **User guides**
MD5.4 Training and presentation material
MD5.5 Blog posts and other topical issues
MD6.1 Detailed plan on training and education
MD6.2 Training events and course material for various target groups
MD6.3 Guest lectures

NordiQuEst KPIs …. for the Project Manager ….

CHALMERS

Service or tool	Description	DK users	EE users	FI users	IS users	NO users	SE users	Nordic users (in total)	Int. users
Kvasi	The Atos Quantum Learning Machine (QLM) advanced quantum computer simulator appliance at CSC	0 (150)	0 (50)	50 (500)	0 (20)	0 (150)	0 (150)	50 (1020)	10 (50)
Qiskit + IBM-Q	Using Qiskit for research in quantum information processing, either with local simulator, IBM Q simulator, or IBM Q quantum devices.	20 (100)	30 (50)	20 (100)	5 (20)	15 (100)	50 (500)	140 (870)	ca 200,000
Qiskit + NordIQuEst	New service, alongside Qiskit + IBM-Q.	0 (500)	0 (50)	0 (500)	0 (50)	0 (500)	0 (500)	0 (2150)	0 (500)
Cirq locally	Using Cirq for research in quantum-computational chemistry (OpenFermion) or quantum machine learning (TensorFlow Quantum). Only possible with a local simulator, i.e., restricted to tiny emulations; no quantum device access.	10 (100)	10 (30)	10 (100)	5 (20)	10 (100)	5 (10)	50 (360)	ca 20,000
Cirq + NordIQuEst	New service, Replaces using Cirq with local simulator, making realistic-size emulation as well as computations on quantum devices available to researchers.	0 (250)	0 (30)	0 (250)	0 (25)	0 (250)	0 (250)	0 (1075)	0 (500)
QHub	University of Tartu Physics Institute's high-end GPU+multi-core quantum emulation compute server used for teaching and research.	0 (10)	20 (30)	0 (10)	0 (5)	0 (10)	0 (10)	20 (75)	0 (0)
OQC	Open source algorithm library developed by the Gemini center https://github.com/OpenQuantumComputing	0 (100)	0 (10)	0 (100)	0 (10)	20 (100)	0 (100)	20 (440)	2 (50)
FiQCI QPU	The Finnish Quantum-Computing Infrastructure (FiQCI) is based on the first Finnish quantum computer developed in the leadership of VTT, and the computing infrastructure provided by CSC. FiQCI provides quantum-computing resources and services and aims at accelerating the development of quantum computing knowhow and applications in academia and industries.	0 (200)	0 (50)	0 (500)	0 (25)	0 (200)	0 (200)	0 (1075)	0 (50)
QAL9000 QPU	QAL9000 is a Swedish superconducting quantum processor (QPU) developed within the WACQT project with support from OpenSuperQ (EU). It is currently at the 5 qubit level, and will operate 20 qubits by mid-2022 using the API- and Service-structure described in WP3. The structure already exists at the research level and will be used to operate present and upcoming generations of QPUs.	0 (100)	0 (40)	0 (50)	0 (10)	0 (100)	20 (1000)	20 (1300)	5 (50)
NordIQuEst service portal	The main entry point to the computing services set up by NordIQuEst	0 (500)	0 (100)	0 (500)	0 (50)	0 (500)	0 (800)	0 (2450)	0 (500)

Why do we need NordIQuEst ?

→ We need QC for **exponential speed-up**
to solve (approximately!) **hard problems** with finite resources (time, memory).
(to reduce energy consumption, if nothing else ...)

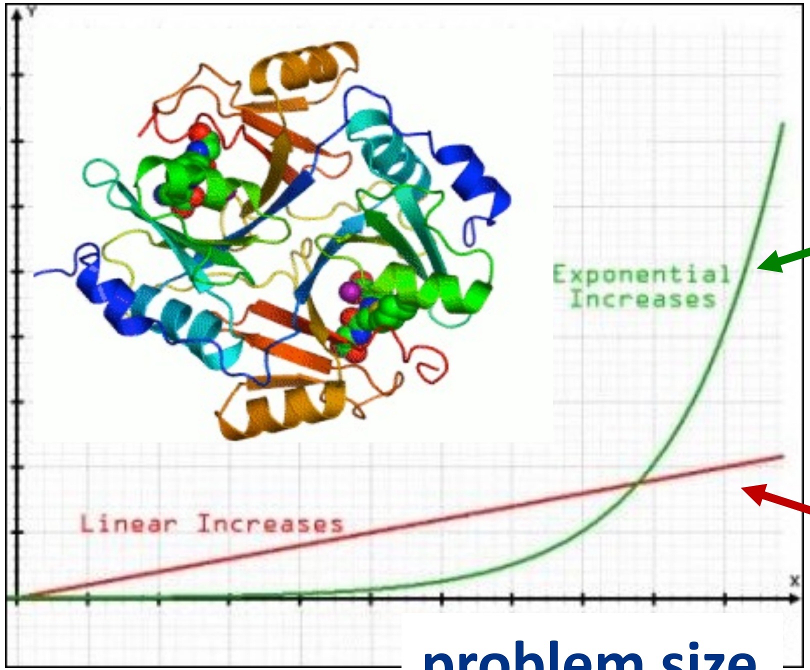
The original "killer application": Shor's algorithm for factorisation (1995)

Today, the typical killer applications are "use cases":

- **Quantum Chemistry** – designing enzymes and catalysers
- **Materials science** – describing strong electron correlations
- **Optimization** - logistics, scheduling, ...

Quantum computers offer, in principle, exponential speed-up for certain classes of hard problems

time



problem size

No Quantum Advantage

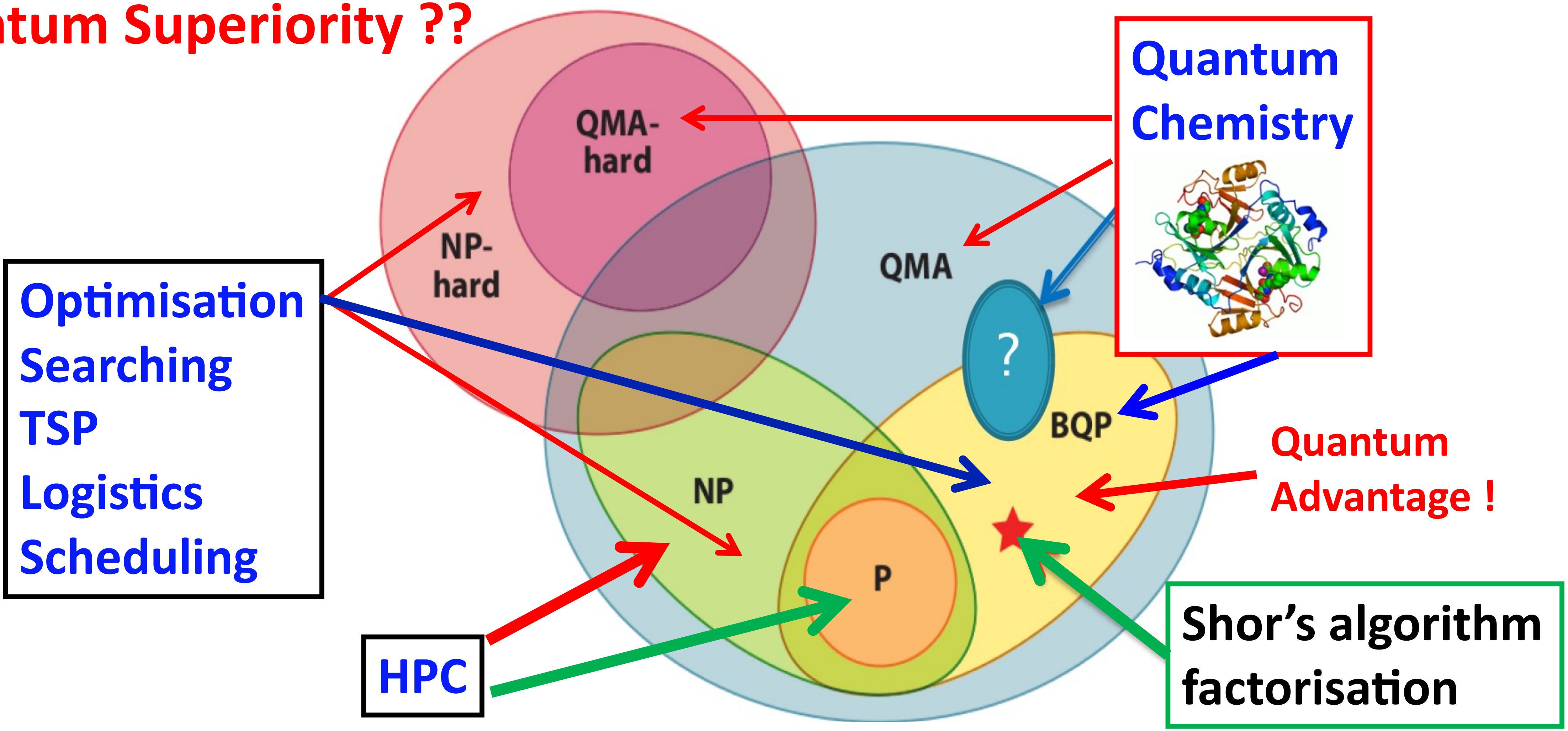
TTS (time-to-solution) for a HPC:
Grows exponentially

TTS for a quantum computer:
Grows linearly/polynomially

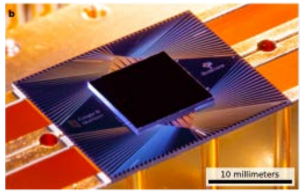
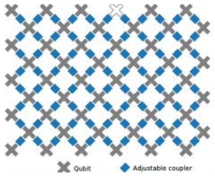
Complexity class landscape

Quantum Advantage ?

Quantum Superiority ??



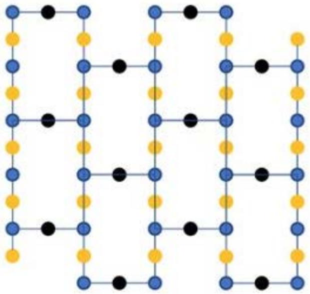
The HPC-QC STACK

Google,
54 transmon qubits

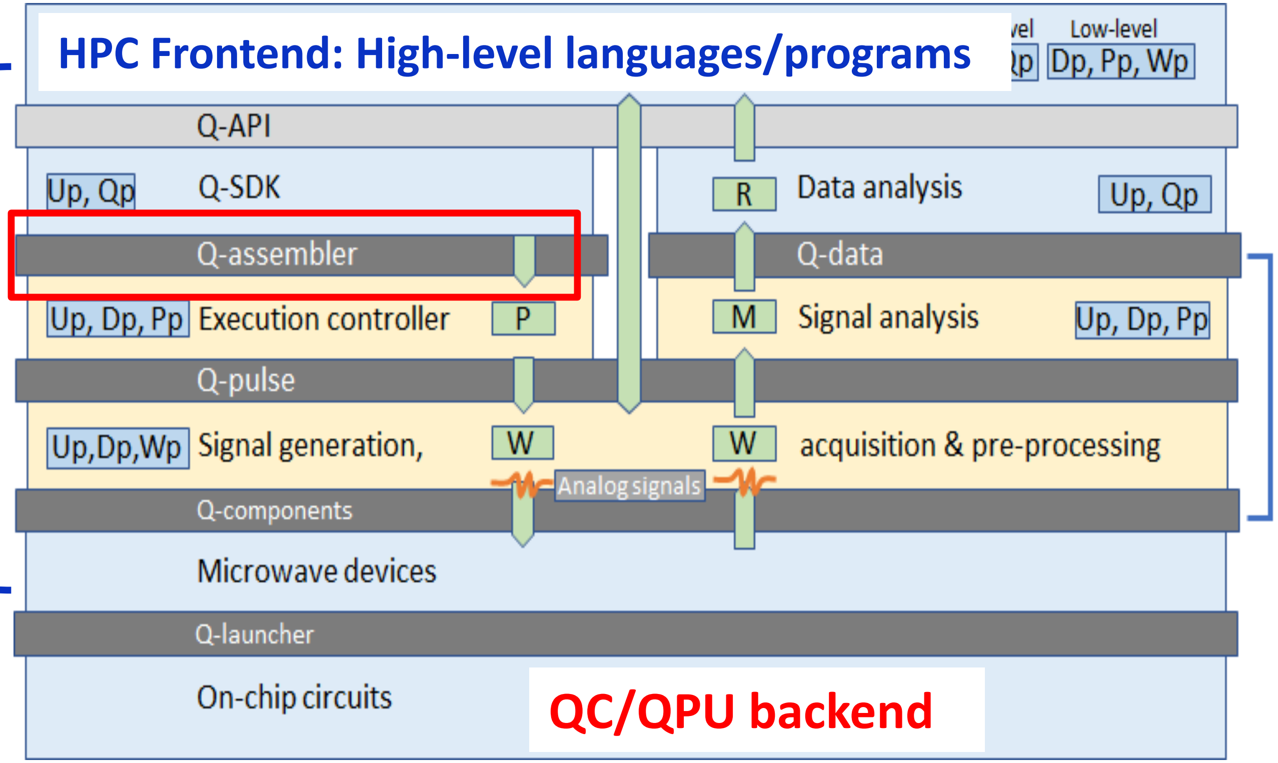
HPC (mainframe/control) + QC (accelerator/subroutines)

QT-Flagship/OpenSuperQ Full Stack



IBM,
65 transmon qubits

(H)PC control



Honeywell, 10 qubits (ion trap)

Qiskit (IBM)
Cirq (Google)
Forrest (Rigetti)

Qipper
……
……..
Microsoft
…….

IBM
Google
Rigetti
Alibaba
Baidu
ETH

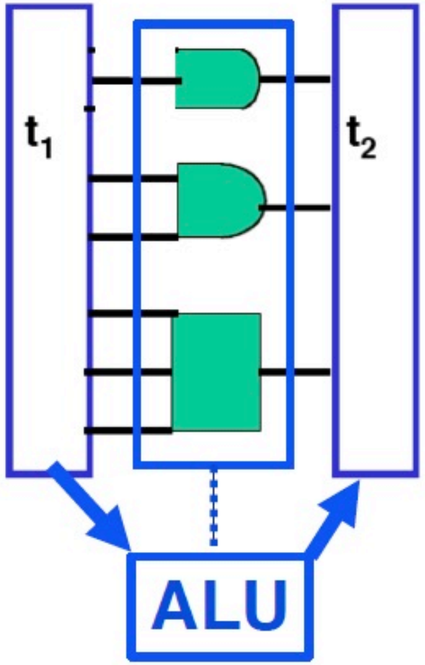
Innsbruck
IonQ
Sandia
Honeywell

HPC-QC = Hybrid classical computer + q-accelerator

HPC frontend

CC: Classical gates

C-register state | C-register state | Irreversible gates



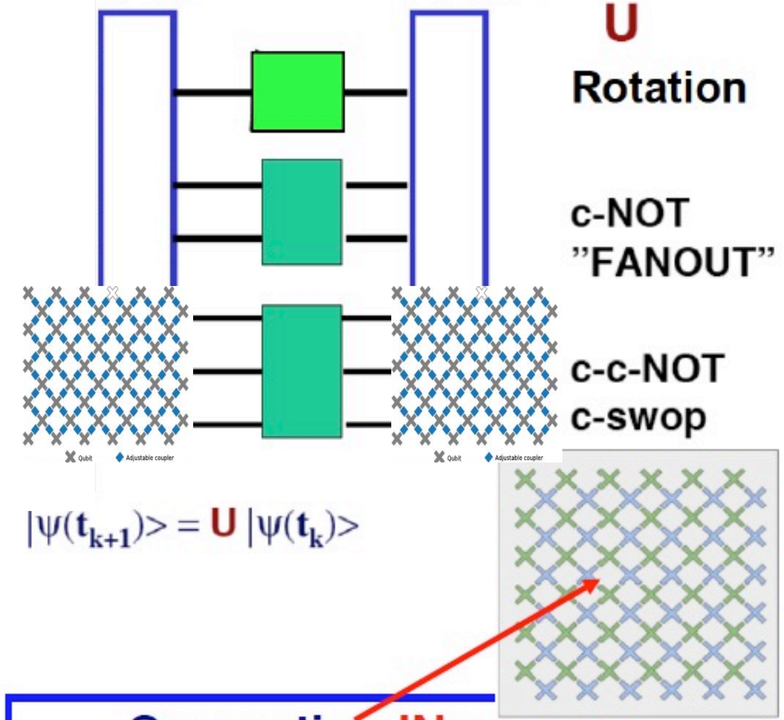
FANOUT
NOT,
AND,
OR,
XOR,
NAND,
NOR, ...

Computing FROM/TO memory
The memory is the storage

QC backend

QC: Quantum gates

Q-register state $|\psi(t_k)\rangle$ | Q-register state $|\psi(t_{k+1})\rangle$ | Reversible gates



U
Rotation

c-NOT
"FANOUT"

c-c-NOT
c-swop

$|\psi(t_{k+1})\rangle = U\,|\psi(t_k)\rangle$

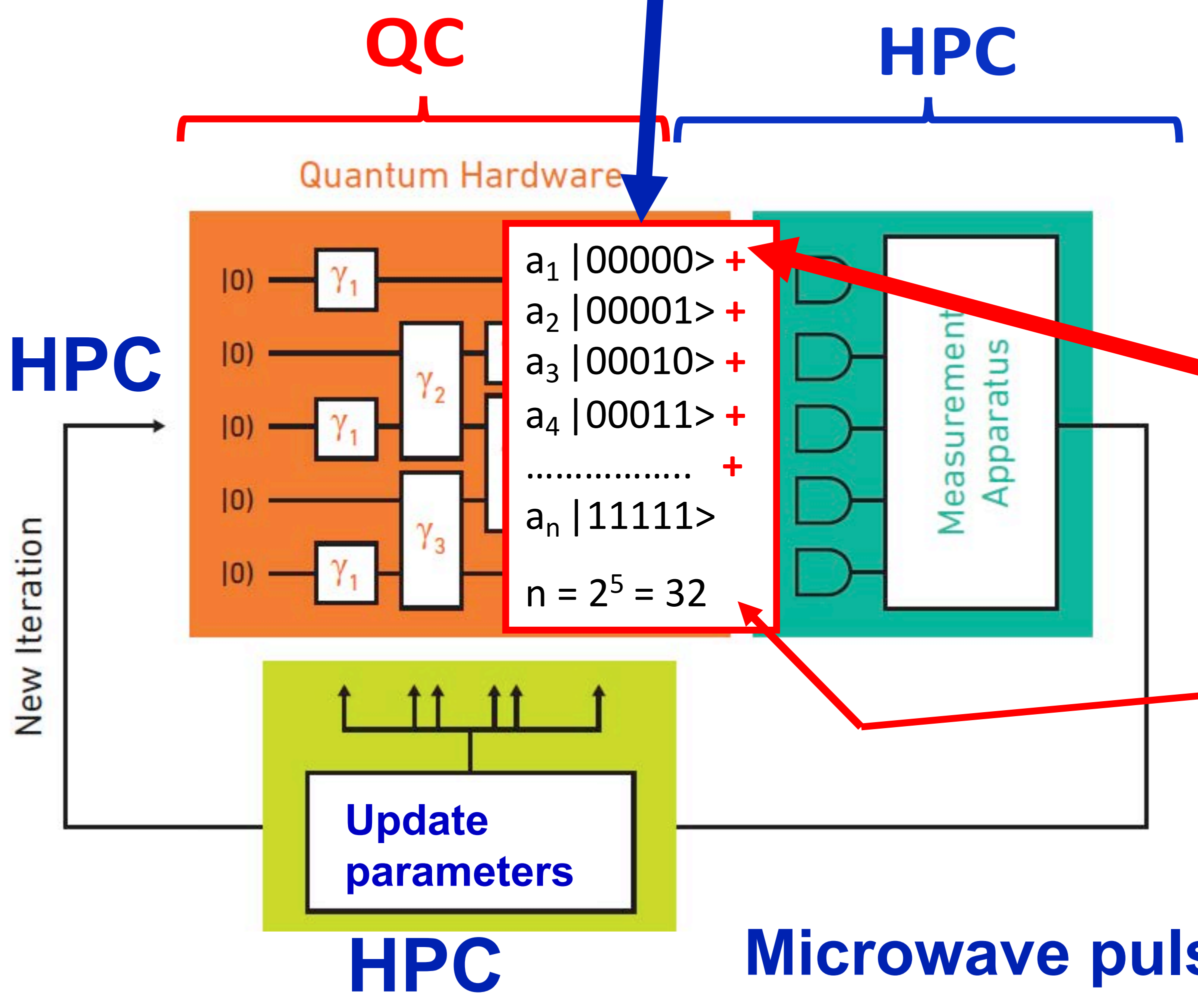
Computing IN memory
The memory is the computer

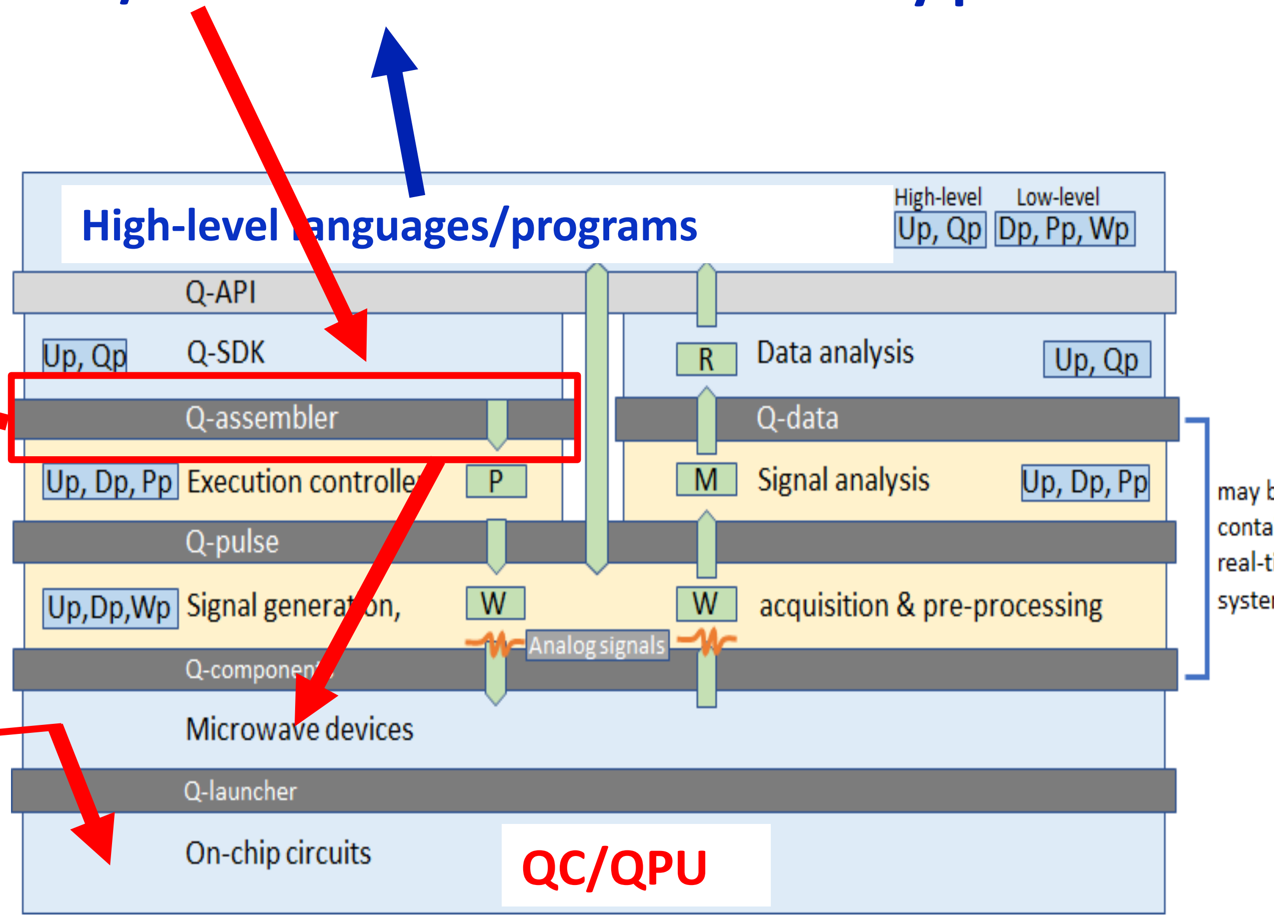
The HPC necessarily RUNS the QC

First created in HPC

May be NP-hard to create and run !!

Example: Qiskit outputs a quantum circuit/ state/wave function for a chemistry problem

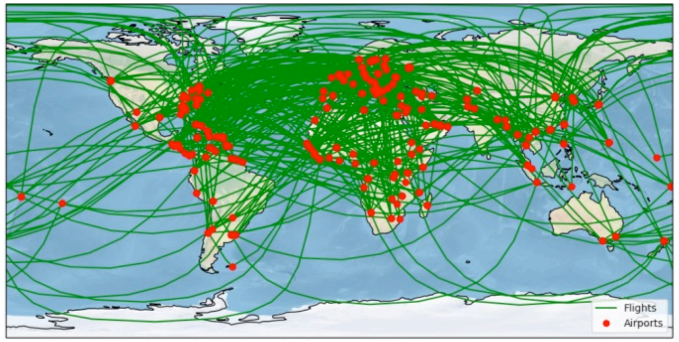


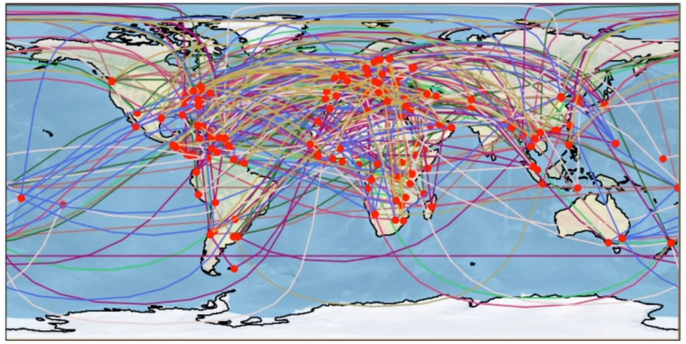


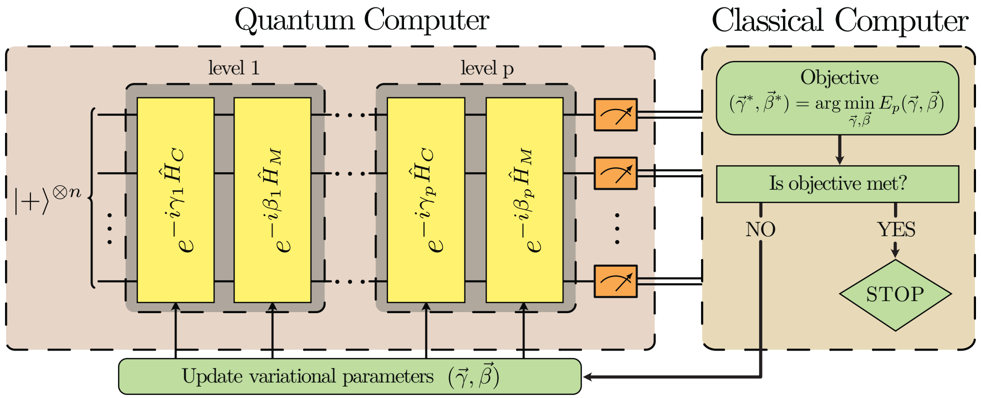
Microwave pulse train creates the Q-circuit in QPU HW

CHALMERS

QAOA - HPC simulation of QC   QT-Flagship/OpenSuperQ







Flight Optimization: QAOA for the Tail Assignment problem ("Traveling Salesman" **ExactCover**, NP-complete) on FZJ q-simulators

Problem instance of a tail-assignment problem.
-- the 472 flights between the airports that have to be performed;
-- unique solution with 9 routes covering the 472 flights exactly once.

Collaboration Chalmers/Jeppesen/FZJ;
HPC/GPU Q-simulation
40 qubits; unique ground state solution:

$|00000000010100100110010000001000000000110 >$

Each qubit represents a flight route.
The 9 1`s represent 9 routes covered exactly once

P. Vikstål et a., Applying the Quantum Approximate Optimization Algorithm to the Tail Assignment Problem, *Phys. Rev. Appl.* **14**, 034009 (2020). (**25q simulation)**

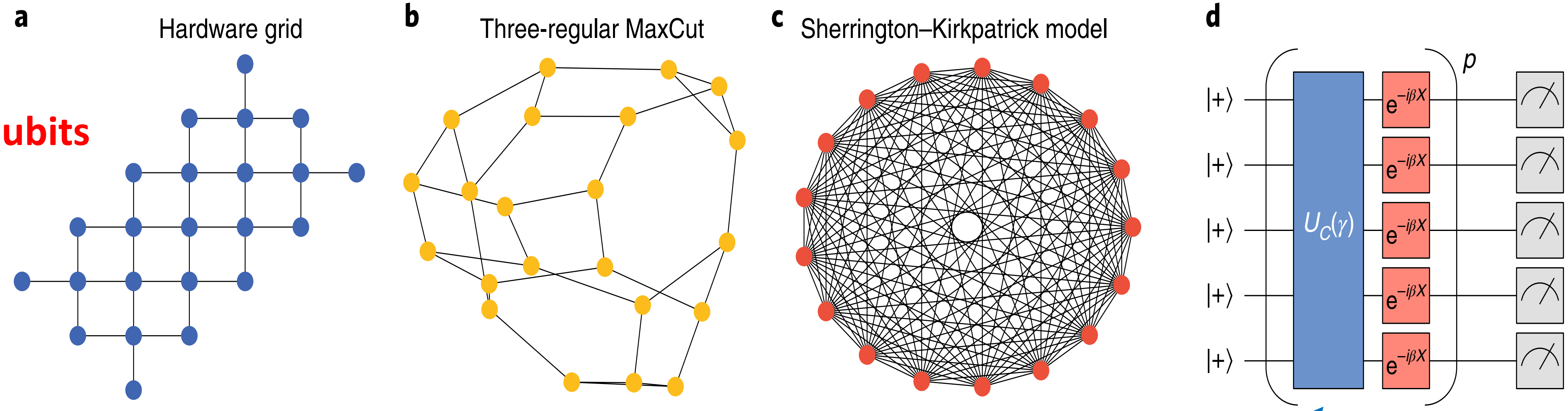
A. Bengtsson, et al. *Phys. Rev. Appl.* **14**, 034010 (2020).
Exp: 2 qubit processor.
N. Lacroix, ... A. Wallraff, *Phys. Rev. X Quantum* **1,** 110304 (2020).
Exp: 7 qubit processor.

QAOA - HPC simulation and QC execution (Google, 2021)

- Harrigan et al. (Google), *Quantum approximate optimization of non-planar graph problems on a planar superconducting processor*, Nature Physics **17**, 332–336 (2021)

(Theory & exp; 54 qubit superconducting QPU)

23 qubits



Cost function operator

Mixing operators

Quantum variational methods – iteration HPC <--> Q

Rayleigh-Ritz

$$E(\theta) = \langle\psi(\theta)|\hat{H}|\psi(\theta)\rangle \geq E_0; \quad \hat{H} = \sum_i \hat{H}_i$$

Superposition
Entanglement

Quantum circuit/ state function created by HPC !!

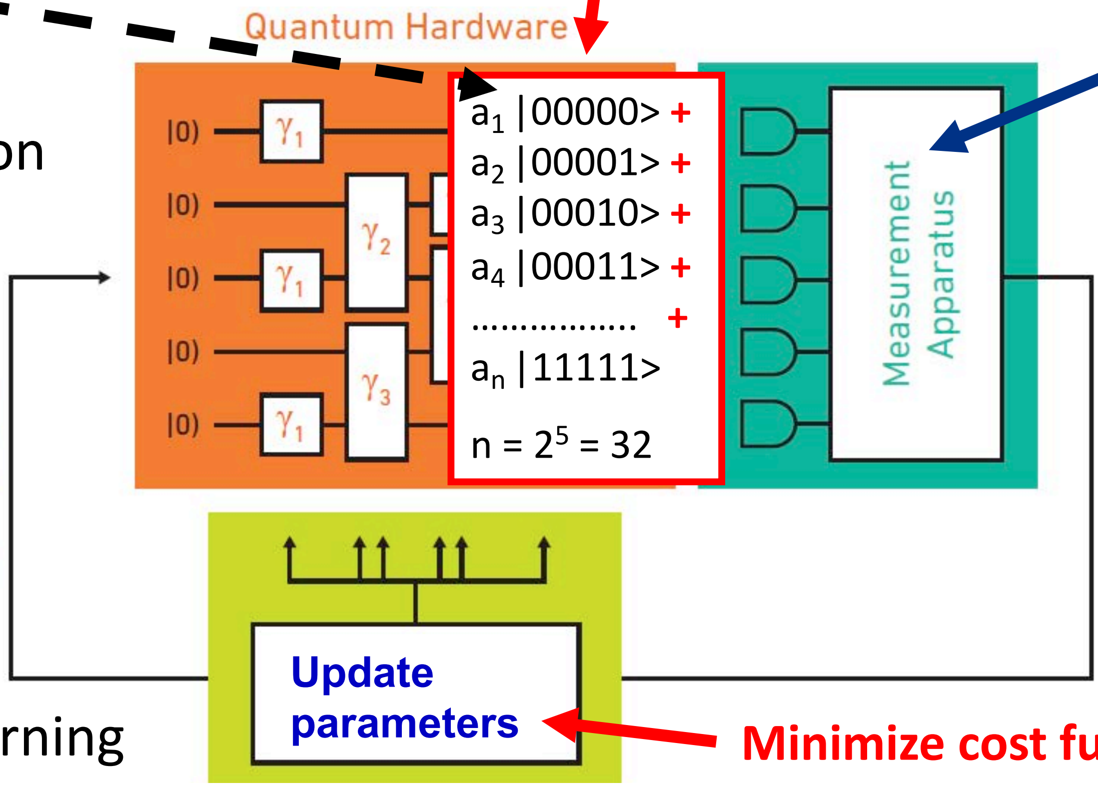
QC **HPC**

Quantum circuit trial function $|\psi(\theta)\rangle$

Optimisation

Quantum Approximate Optimization Algorithm **(QAOA)**

Quantum Variational Eigensolver **(VQE)**

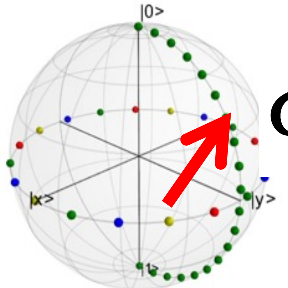


Quantum state tomography (exp)
Distribution via sampling

Evaluate cost function with sample distribution

Machine learning

Minimize cost function $\sum_i \langle\psi|\hat{H}_i|\psi\rangle$



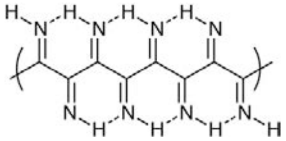
$\sigma_{i\alpha}$

Ising-type Cost function

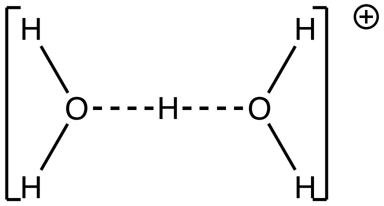
$$\hat{H} = \sum_{i\alpha} h_{i\alpha}\,\sigma_{i\alpha} + \sum_{i\alpha,j\beta} h_{i\alpha,j\beta}\,\sigma_{i\alpha}\sigma_{j\beta} + \sum_{i\alpha,j\beta,k\gamma} h_{i\alpha,j\beta,k\gamma}\,\sigma_{i\alpha}\sigma_{j\beta}\sigma_{k\gamma} + \ldots\ldots$$

Benchmarking VQE for "large" molecules

- H_2O (8q, 20q)
- HCN (15q, 33q, 69q)
- **Water clusters**: $[H_2O\text{-}OH]^-$, $[H_2O]_2$; $H^+[H_2O]_2$ (19-22q)
- **Water chains: Hydrogen bonding** and **proton transfer**
- HCN **isomerisation**: HCN → HNC
- HCN **polymerisation**: $HCNH^+$, $(CN)_2$, HCN-OH (17-25q)
- NC-CN (29q)
- N2 (64q)
- HCN (69q)
- C=C=C (98q)



Pople basis sets:
"Minimal": STO-6G
"Large": 6-31G, ...



Qiskit (IBM)
HF
VQE
|UCCSD>
SLSQP

Transpiler optimization level 1
----
iMac i9
8 cores
3.6 Ghz
128 GB RAM

HPC simulation

VQE
6-31+G*

- 16 847 variational parameters
- 6 784 465 gates (6 172 486 CNOT)
- Circuit depth 6 390 393)
- One quantum circuit: **Not possible, not even on (post)exascale HPC!! .**

QPU: Rough estimate: (50 ns 2q gate time)

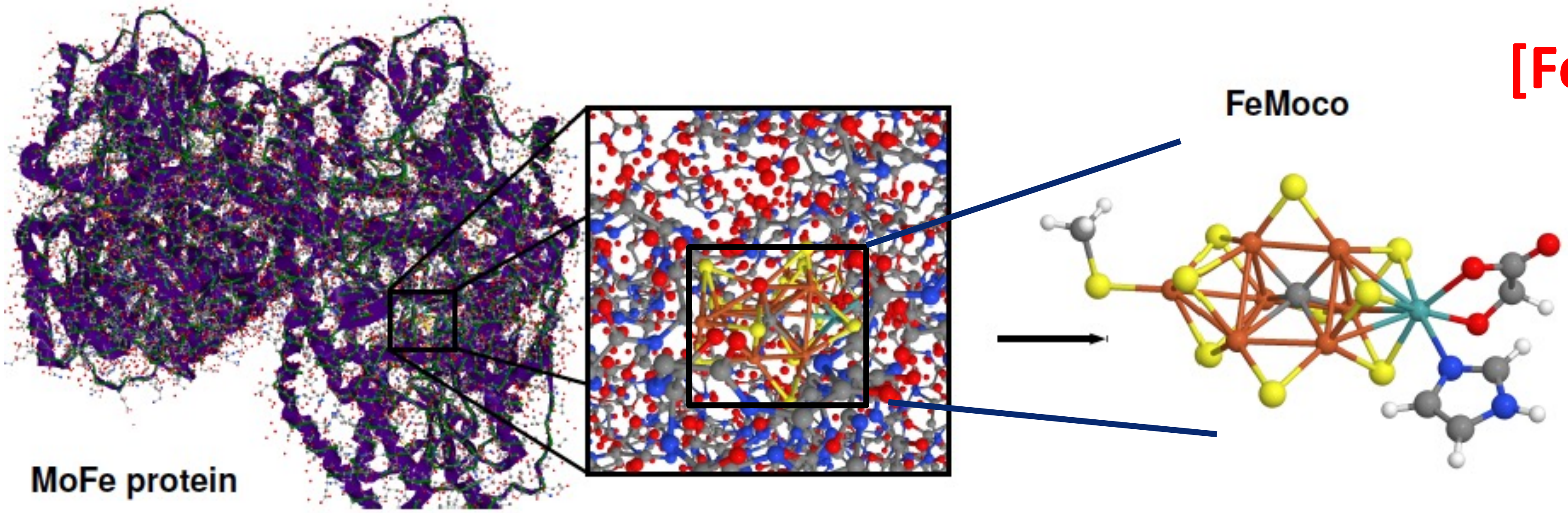
- **One single quantum circuit: minimum 300 ms**

→ Needs a 69q QPU coherent for > 300 ms
→ TTS: 0.3 x 16847 x 10 ≈ 15 hours (minimum)

P. Lolur, M. Rahm, M. Skogh, L. García-Álvarez, and G. Wendin, *AIP Conference Proceedings*, Vol. **2362** (2021); arXiv:2010.13578

Biological catalyzing enzyme

Nitrogenase protein: iron molybdenum cofactor FeMoco



$[FeS]_n$

Elucidating reaction mechanisms on quantum computers

M. Reiher, N. Wiebe, K. M. Svore, D. Wecker, and M. Troyer

PNAS **114**, 7555-7560 (2017)

That's All Folks!

Questions?

Comments?