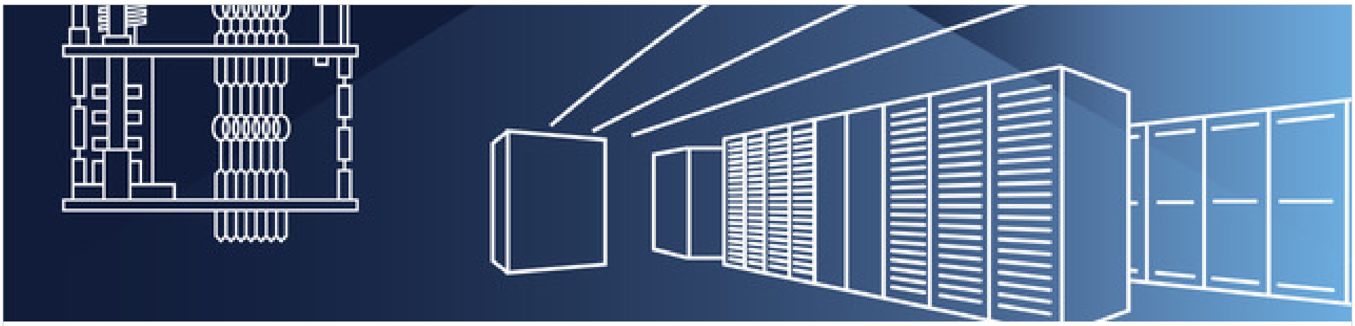


Integration of High Performance Computing and Quantum Computing

Sven Karlsson, DTU

HPCQC.org   nordiquest.net

DTU Technical University of Denmark   NordIQuEst

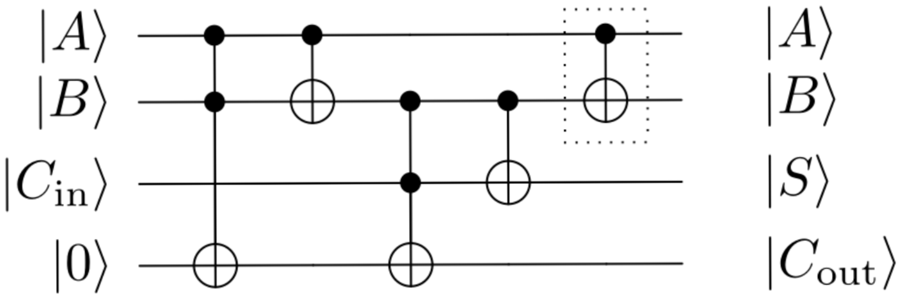
Why Quantum?

- Fundamentally changes what is computable
  - For some problems you need a quantum computer
    - Noted by Feynman in 1982
  - Some of what was previously intractable is with QC tractable
    - Chemistry, optimization, …
- Moore’s Law is ending
  - Quantum computing can help in continuing to increase performance
  - QC compute power can scale exponentially with the number of devices
- Quantum computing is radically different from “classical” computing
  - Thinking fresh and new is necessary
  - Can lead to new “classical” algorithms

Quantum simulator of physical system

- A quantum system is needed to efficiently simulate a quantum system
  - Noted by Feynman in 1982
- “Lets build an experiment where we use quantum effects to understand another system”
  - Leveraging the intristic quantum nature of quantum computers
- Use the quantum computer as an accelerator for quantum effects!

Quantum Gate Model Systems



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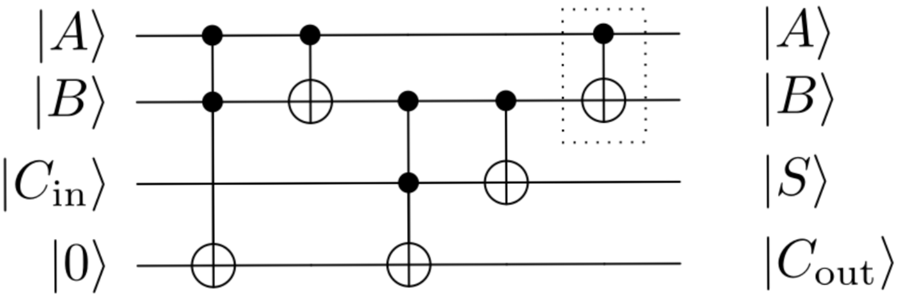
- More general quantum computers consists of quantum logic gates forming quantum algorithms
  - Above a quantum full adder

Quantum Gate Model Systems



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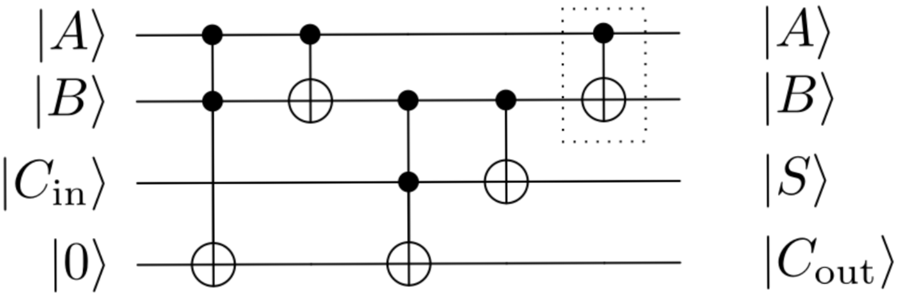
- **More general quantum computers consists of quantum logic gates forming quantum algorithms**
  - **Above a quantum full adder**
- **Gates are largely technology independent and are mapped to implementations using, often, proprietary tools**

Quantum Gate Model Systems, pt2



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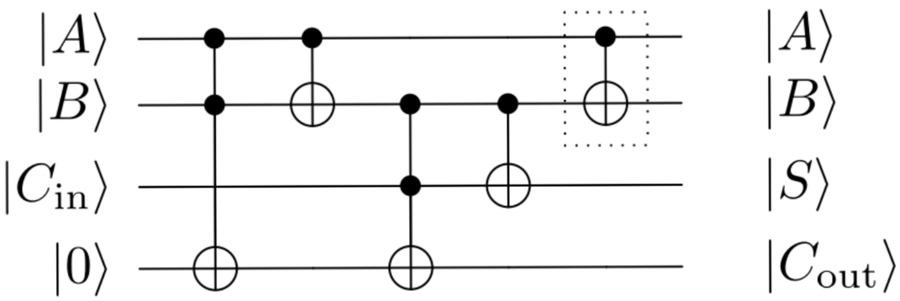
- **A number of technologies exists: Superconducting, Trapped ion, Diamond-based etc**
- **Gates typically are implemented by sending sequences of control signals**

- **Technology limitations means that the quantum state can only survive a limited time**
  - **Leads to limits on algorithm size**

Quantum Gate Model Systems, pt3



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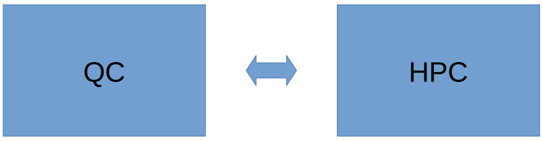
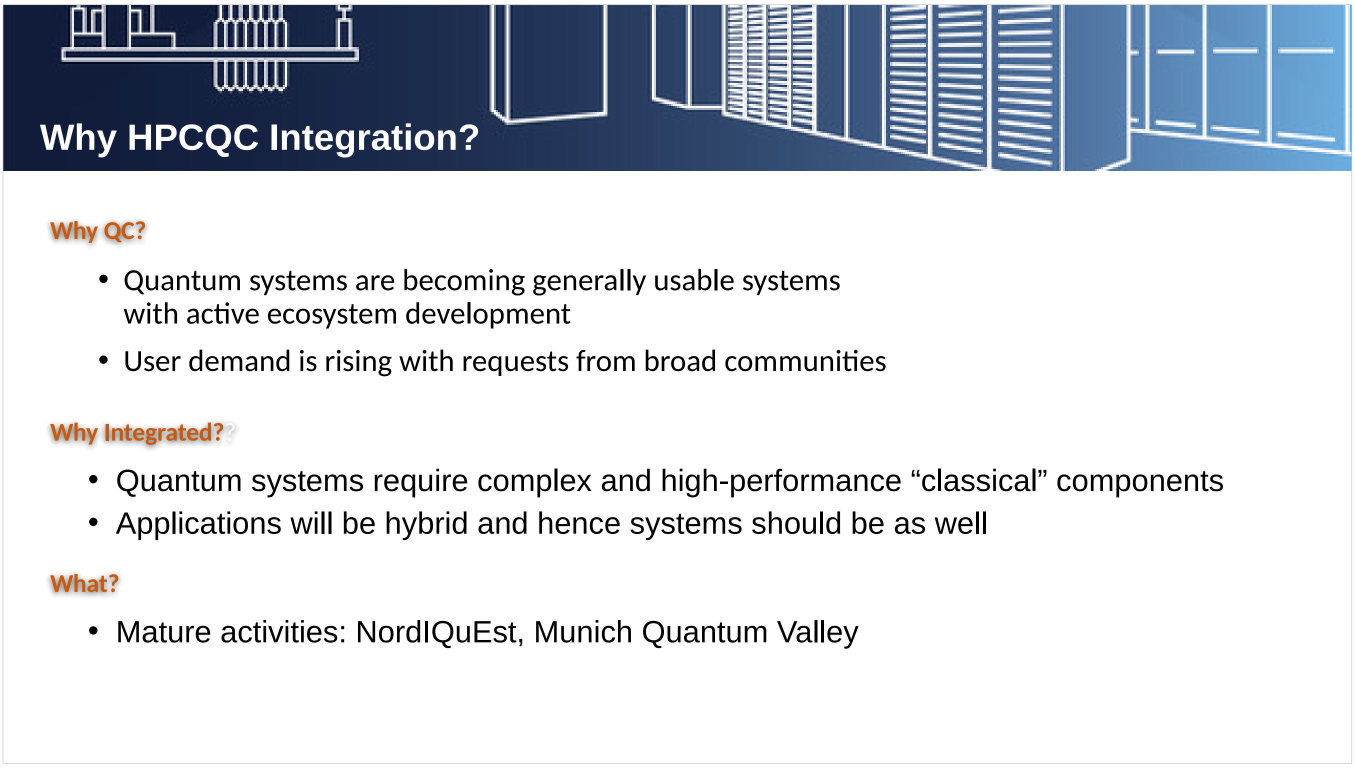
- A number of technologies exists: Superconducting, Trapped ion, Diamond-based etc
- Technologies develop rapidly
- Slowly working towards the holy grail: Fault tolerance
- We are currently in the NISQ era
  - Noisy Intermediate-Scale Quantum

QC and HPC Interplay



- QC will likely first be used as an accelerator of key HPC algorithms



Why HPCQC Integration?

Why QC?

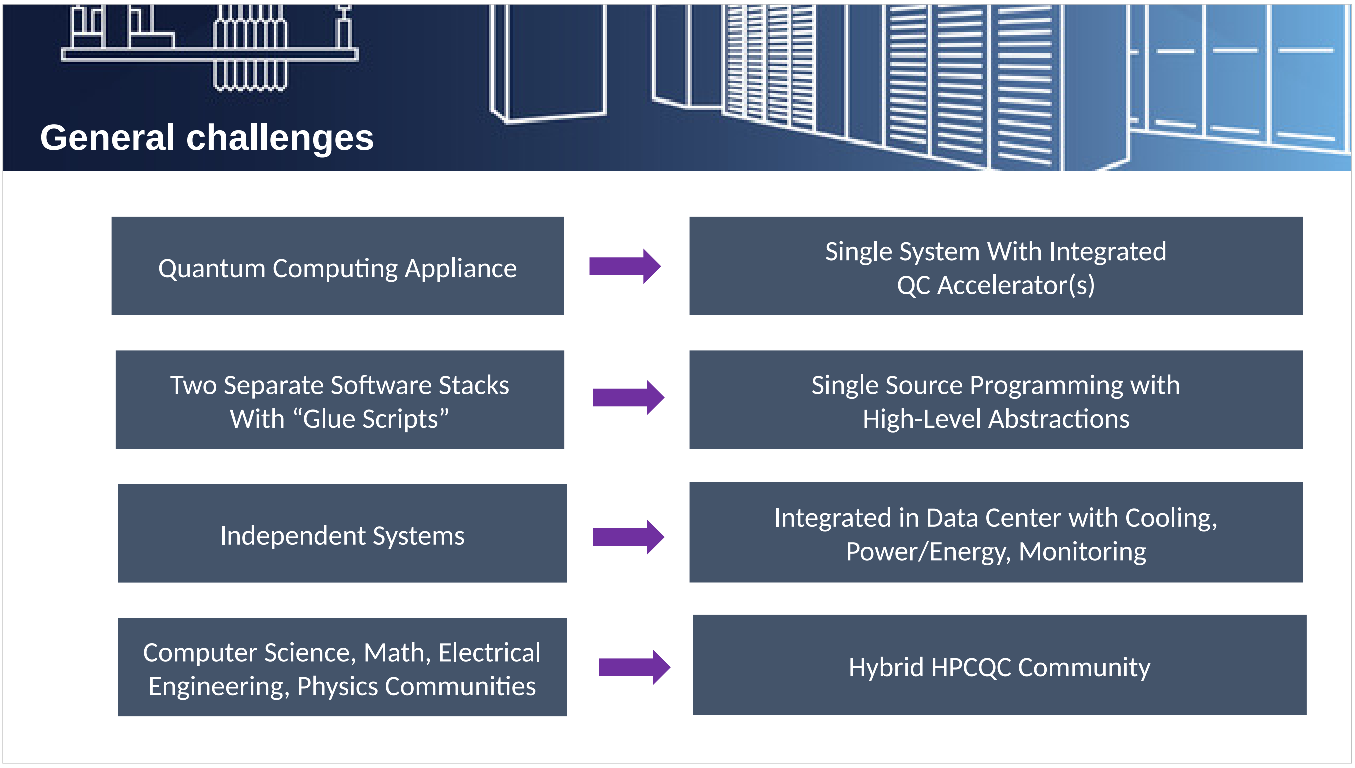
- Quantum systems are becoming generally usable systems with active ecosystem development
- User demand is rising with requests from broad communities

Why Integrated??

- Quantum systems require complex and high-performance “classical” components
- Applications will be hybrid and hence systems should be as well

What?

- Mature activities: NordIQuEst, Munich Quantum Valley



General challenges

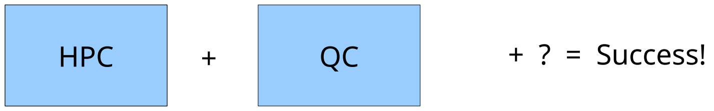
Quantum Computing Appliance → Single System With Integrated QC Accelerator(s)

Two Separate Software Stacks With “Glue Scripts” → Single Source Programming with High-Level Abstractions

Independent Systems → Integrated in Data Center with Cooling, Power/Energy, Monitoring

Computer Science, Math, Electrical Engineering, Physics Communities → Hybrid HPCQC Community

The Challenge

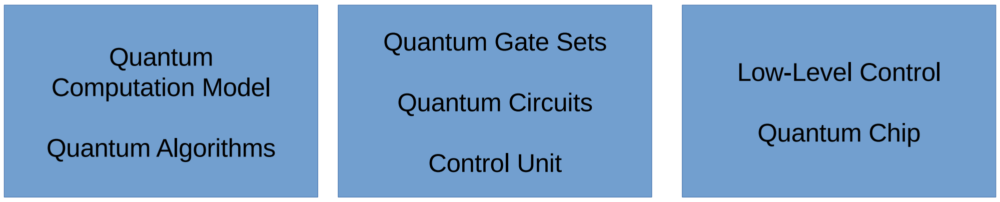


HPC + QC + ? = Success!

- Open question: How to integrate quantum devices into classical systems.

- Software? Programming models? Compilers?
- Workflows?
- System software? Tools?
- Hardware / Software co-design, classical and quantum
- Computer architecture?
- Hardware integration?

Technology stack



Quantum Computation Model

Quantum Algorithms

Quantum Gate Sets

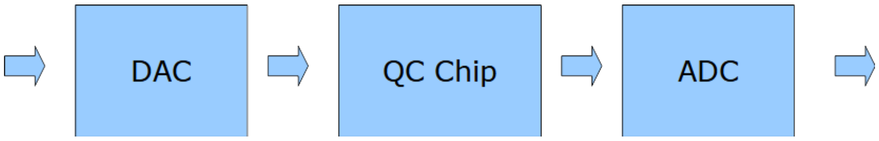
Quantum Circuits

Control Unit

Low-Level Control

Quantum Chip

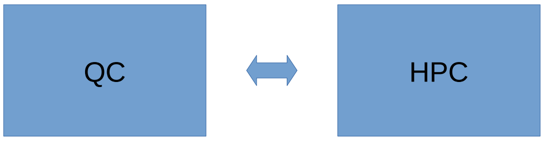
The Quantum Chip is “Analog”


DAC

QC Chip

ADC

QC and HPC Interplay


QC

HPC

- **QC will likely first be used as an accelerator of key HPC algorithms**
- **QC for HPC but also**
- **HPC for QC**

HPC for QC

Quantum
Computation Model

Quantum Algorithms

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Quantum Chip

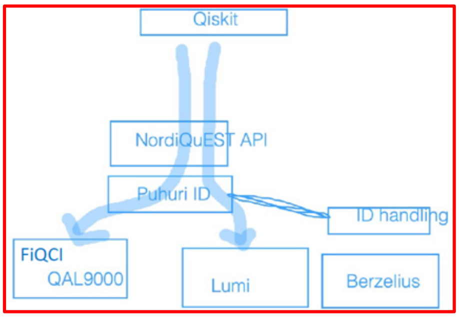
NordIQuEst

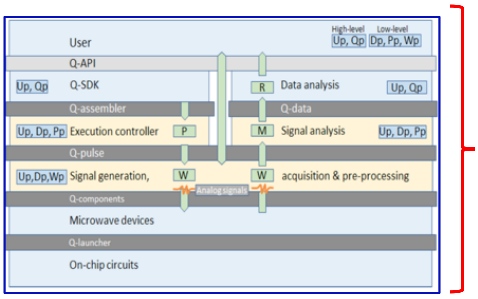
The NordIQuEst Mission

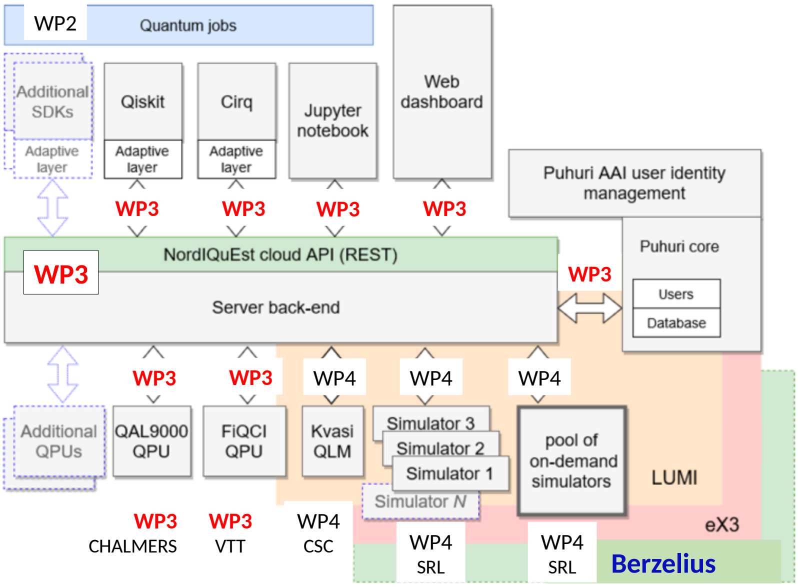
- **NordIQuEst** will deliver user and computer **interfaces**, quantum program **libraries**, **training** and **education** events and material, as well as user **support**.
- **Pooling of resources and collaboration** for reaching critical mass, **providing access** to several Nordic quantum computers (QC) (q-HW) and QC simulators (SW)
- **Chalmers** and **VTT** will **connect** their current QCs to the **NordIQuEst 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

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



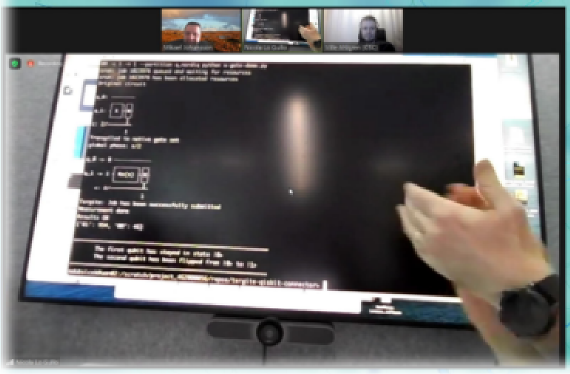


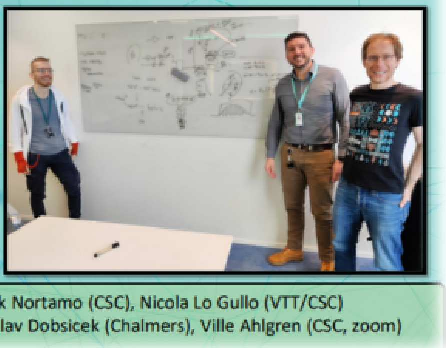


Nordic-Estonian Quantum Computing e-Infrastructure Quest

30.3.2022: First quantum job submitted through the LUMI queueing system

- Connected one LUMI-C node in Finland to the QAL 9000 QC in Sweden, and *successfully ran a cross-border quantum job*





Henrik Nortamo (CSC), Nicola Lo Gullo (VTT/CSC)
Miroslav Dobsicek (Chalmers), Ville Ahlgren (CSC, zoom)

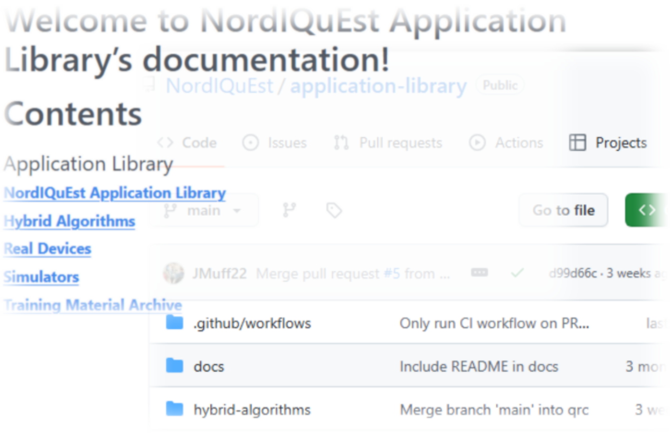
The NordIQuEst Application Library

What?

- Practical approach - collect documented and curated material
  - Algorithms
  - Examples
  - Experiences
- For use cases
  - Practical aspects
  - Theory aspects
  - Notebooks or code

https://nordiquest.net/application-library/

- Also on GitHub
- Clone and get all information
- We want your pull requests!
  - Library is growing



Welcome to NordIQuEst Application Library's documentation!

Contents

Application Library

NordIQuEst Application Library

Hybrid Algorithms

Real Devices

Simulators

Training Material Archive

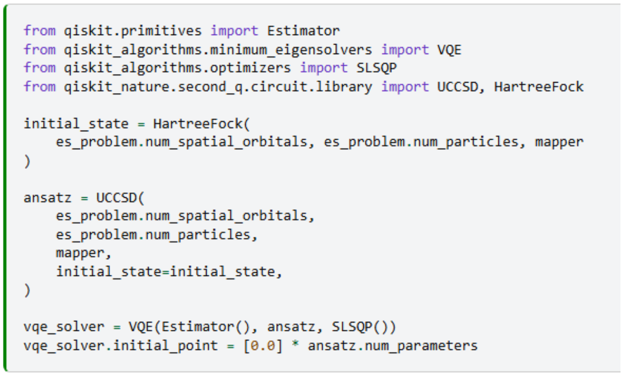
NordIQuEst / application-library Public

JMuff22 Merge pull request #5 from ... d99d66c · 3 weeks a

.github/workflows	Only run CI workflow on PR...	las
docs	Include README in docs	3 mo
hybrid-algorithms	Merge branch 'main' into qrc	3 we

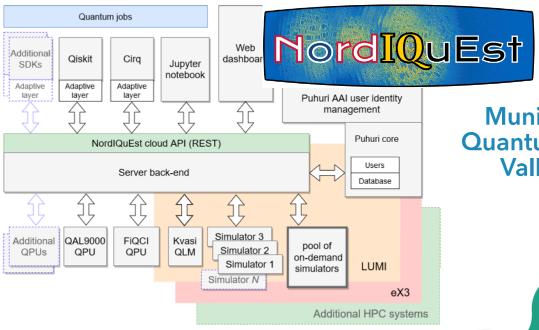
Quantum Chemistry Example

- Overview
  - Software requirements
  - Theory
    - Both for the problem domain
    - … and the Quantum implementation
  - Worklist
    - What are the steps required
  - Notebook

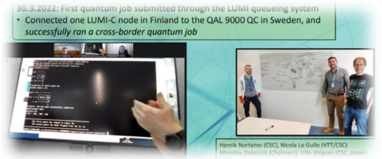


```
from qiskit.primitives import Estimator
from qiskit_algorithms.minimum_eigensolvers import VQE
from qiskit_algorithms.optimizers import SLSQP
from qiskit_nature.second_q.circuit.library import UCCSD, HartreeFock

initial_state = HartreeFock(
    es_problem.num_spatial_orbitals, es_problem.num_particles, mapper
)

ansatz = UCCSD(
    es_problem.num_spatial_orbitals,
    es_problem.num_particles,
    mapper,
    initial_state=initial_state,
)

vqe_solver = VQE(Estimator(), ansatz, SLSQP())
vqe_solver.initial_point = [0.0] * ansatz.num_parameters
```

Selected projects



Munich Quantum Valley



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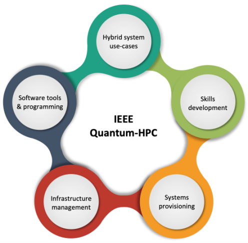
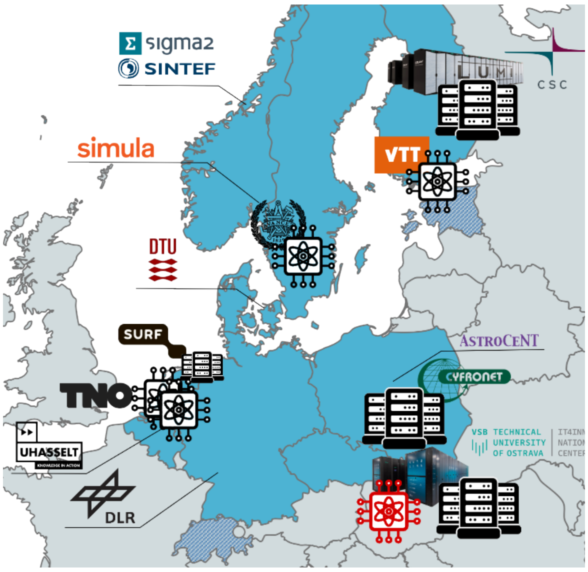

IEEE Quantum-HPC
Hybrid system use-cases
Skills development
Systems provisioning
Infrastructure management
Software tools & programming


sigma2
SINTEF
simula
DTU
LUMI
CSC
VTT
SURF
TNO
UHASSELT
DLR
ASTROCENT
CYFRONET
VSB TECHNICAL UNIVERSITY OF OSTRAVA
IT4INN
NATION
CENTER