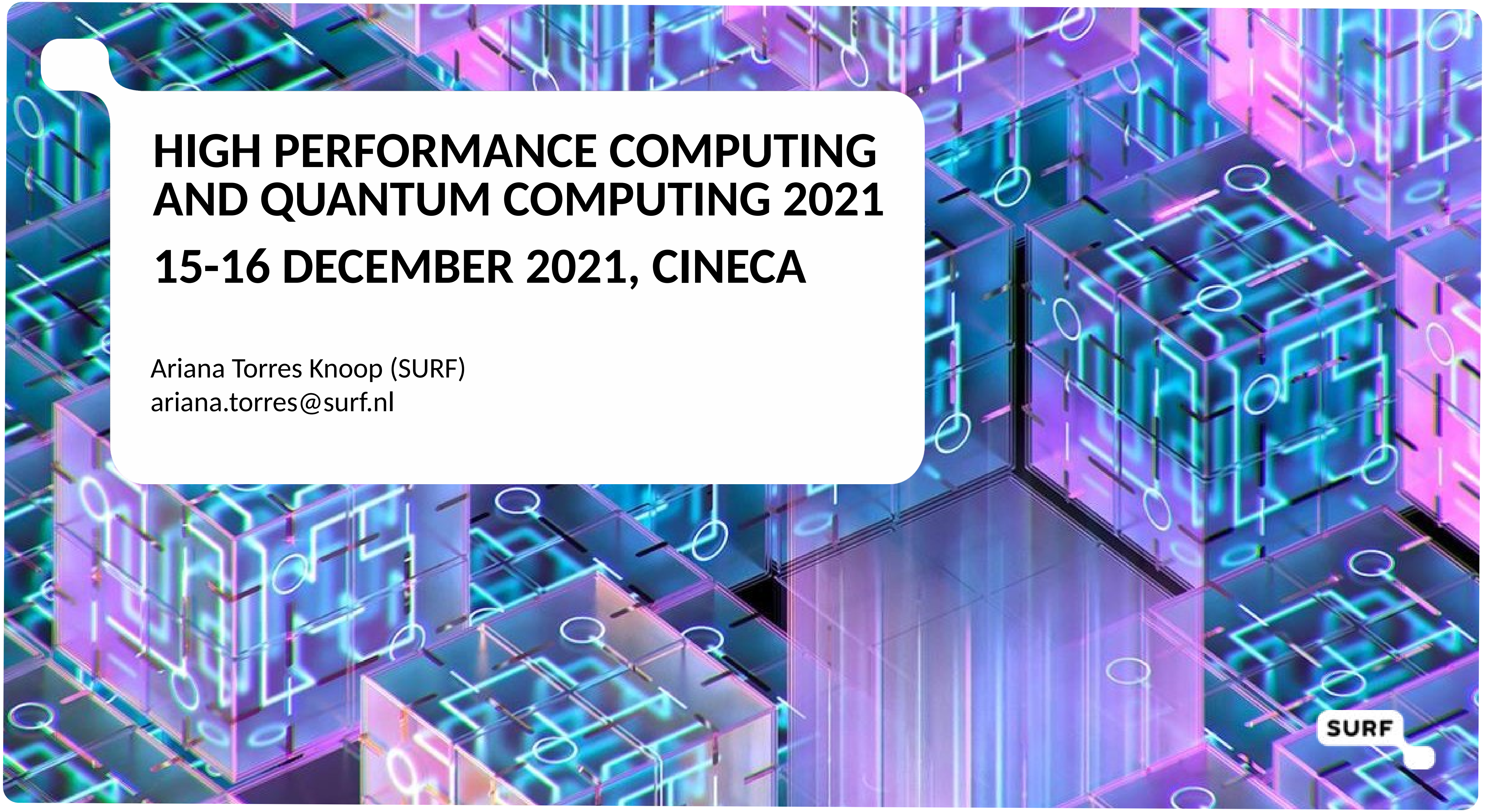

HIGH PERFORMANCE COMPUTING AND QUANTUM COMPUTING 2021

15-16 DECEMBER 2021, CINECA

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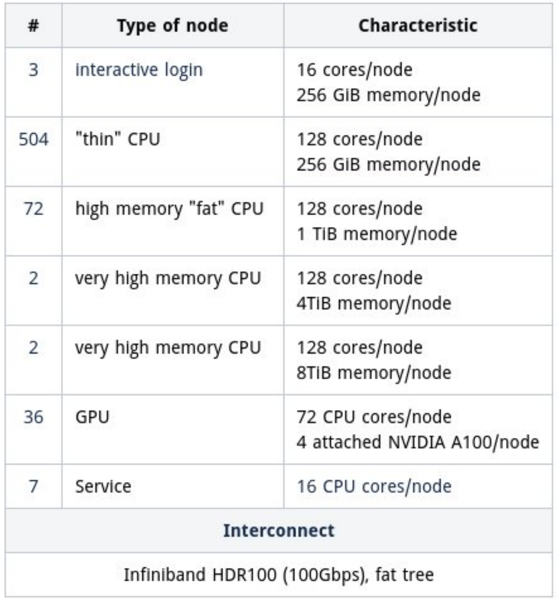
driving innovation together

SURF is the collaborative organization for ICT in Dutch education and research

- Data storage and management
- HPC access
(National Supercomputer and LISA cluster)
- Network infrastructure
- Education tools

https://www.surf.nl/en



#	Type of node	Characteristic
3	interactive login	16 cores/node 256 GiB memory/node
504	"thin" CPU	128 cores/node 256 GiB memory/node
72	high memory "fat" CPU	128 cores/node 1 TiB memory/node
2	very high memory CPU	128 cores/node 4TiB memory/node
2	very high memory CPU	128 cores/node 8TiB memory/node
36	GPU	72 CPU cores/node 4 attached NVIDIA A100/node
7	Service	16 CPU cores/node
Interconnect		
Infiniband HDR100 (100Gbps), fat tree		

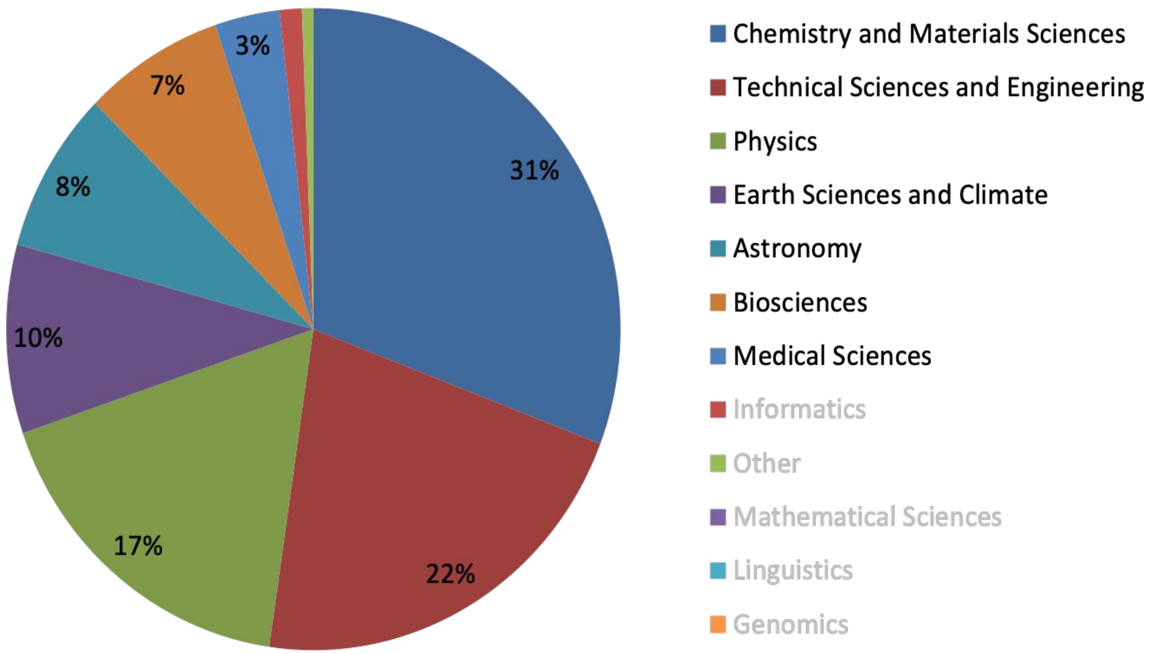
SURF

“We need to understand, update and grow with our users”

Chemistry and materials science is our largest pool of users

Machine learning growing rapidly in many of the other groups (astronomy, climate, medicine, etc.)

Where are these fields evolving towards?



Simulating quantum systems

driving innovation together

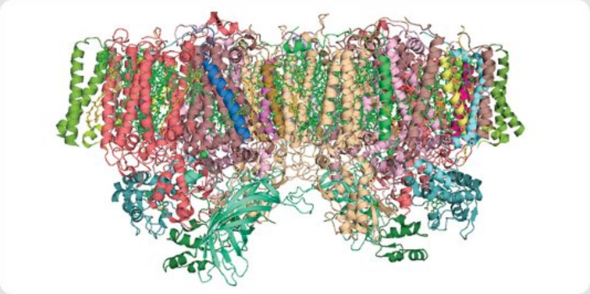
COMPUTATIONAL CHEMISTRY

Chemistry is quantum computing's killer app

Quantum computers could help chemists better understand and develop catalysts, photovoltaics, and more

by **Katherine Bourzac**

October 30, 2017 | A version of this story appeared in **Volume 95, Issue 43**



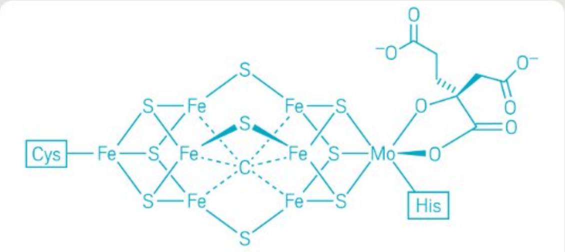
Photosystem II

This large enzymatic complex carries out some of the critical first steps in photosynthesis, using the energy from absorbed light to oxidize water and harvest electrons. Water oxidation occurs at a site called the manganese center, which future quantum computers could someday model. A deeper understanding of photosystem II's chemistry could enable

Solar-cell materials

Quantum computers could better simulate how charges move through the active materials in solar cells. Such information could enable researchers to predict and design new solar-cell materials that have different combinations of properties, such as low cost, flexibility, and high performance.

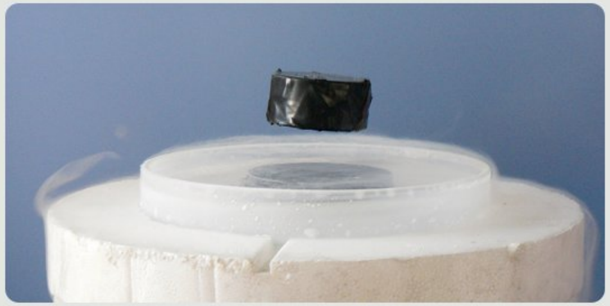
Credit: Shutterstock



Nitrogenase Fe-Mo cofactor

Nitrogenase

Bacteria use nitrogenase to fix atmospheric nitrogen into ammonia. Chemists would like to understand how the enzyme performs this catalytic feat to help design less-energy-intensive industrial processes for synthesizing nitrogen fertilizers. Quantum computers could one day model the enzyme's FeMoco metal cofactor to provide insight into its mechanism.



High-temperature superconductors

Powerful quantum computers could predict superconductors that work at room temperature. Such materials would enable advances in magnets, motors, the power grid, and more.

Credit: Wikimedia Commons

https://cen.acs.org/articles/95/i43/Chemistry-quantum-computings-killer-app.html

What is the role of HPCs in the quantum era?

Role of “classical” vs quantum

TODAY < 100 qubits

50 qubits 1000 qubits 1M qubits

QC (Quantum Computing):
- understand and characterize the hardware
    - reliability,
    - scaling,
    - performance

CC (Classical Computing):
- emulation of QC
    - simulation driven co-design of hardware (study noise, bottlenecks in hardware, asses hardware constraints, etc)
    - algorithms development and testing (debugging)
- quantum compilation

QC (co-processor):
- perform time consuming tasks from classical workflow

CC:
- perform hybrid algorithms with quantum subroutines
- pre/post processing of data
- state preparation
- QEC

QC (co-processor OR main processor):
- perform fault-tolerant algorithms

CC (co-processor):
- use of classical resources to accelerate the execution of quantum circuits (?)

HPC in quantum computing

- **Quantum accelerated classical computing**: to offload time consuming tasks from classical workflows into the quantum co-processor
- **Classical accelerated quantum computing**: use of classical resources to accelerate the execution of quantum circuits (eg. offload clifford based circuits). In this case the classical computer is the co-processor
- **Supported quantum simulation**: use of classical computing resources for pre-processing and/or post-processing of data

HYBRID COMPUTING

Hybrid workflows

Local < ~20 qubits

Workflow	Classical part	Quantum part	Use cases
Local-Local	Local	Simulation (Local)	Small experiments (prototyping)
Local-HPC	Local	Simulation (HPC)	Large quantum simulations that can not be run locally, eg. too many qubits and not enough memory or many repetitions needed
Local-QPU	Local	QPU	Small experimentation/exploration of hardware: effects of noise, crosstalk, etc
HPC-HPC	HPC	Simulation (HPC)	Multiple experiments, expensive classical and/or quantum part, high performance simulations
HPC-QPC	HPC	QPC	Well-defined multiple experiments, hybrid computation with expensive classical part

Developing cycle

One code should be portable to all scenarios!!!

Support and stimulate the transition to QC

Support **access** and use of quantum emulators as well as quantum simulators and physical quantum computers

Support the **integration** of the quantum and classical ecosystems

Stimulate and support the development of quantum applications

Support the **development** of required expertise and tools to ‘transform’ regular applications into quantum applications

Support research to take early and competitive **advantage** of Quantum computing

Example of initiatives at SURF “low hanging fruits”

- High memory nodes

- Access to emulators

- Singularity containers

- Access to QPUs

(QLM Atos)

- Close collaboration with QPU developers (Quantum Inspire)

- access
- scheduler/orchestration
- “standarization”

- Computing resources

- Human resources

- Help create/connect communities involved in the field

- Help find suitable problems

- Participate in development of QC emulators (QX, Netsquid)

- Hosting internships, MsC, BsC

- Create examples (Jupyter notebooks)

All of the before mentioned and more!

Some worked.. some did not

- QLM Atos: not enough users to “justify” it (pre myQLM) ✗
- “standard HPC access” ✗
- Singularity container ✗
- Interfaces (+/-)
- Internships ✓
- Financial support for use cases ✓
- Collaboration quantum Inspire ✓
- Access QPUs (?)

Multipurpose high memory nodes ✓

Jupyter Hub ✓

Easybuild installations ✓

…

Chemistry use case

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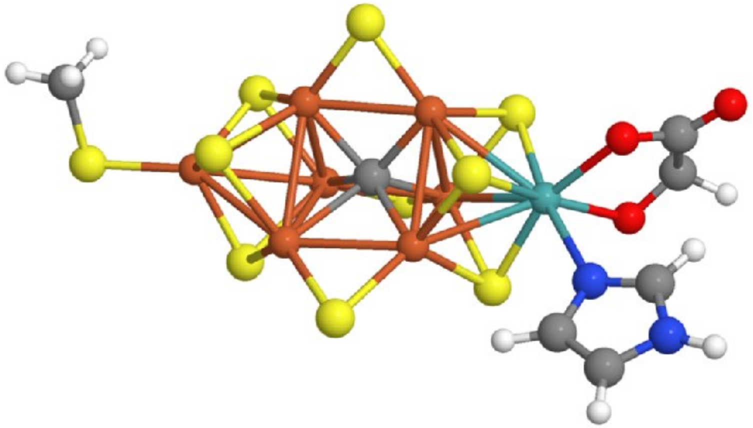
Quantum systems are especially challenging for classical computers because they are, by nature, uncertain.

Qubits, on the other hand, can more easily reflect the nature of a quantum system because they are themselves uncertain.



M. Reiher et al., Proc. Natl. Acad. Sci. USA 114, 7555 (2017)

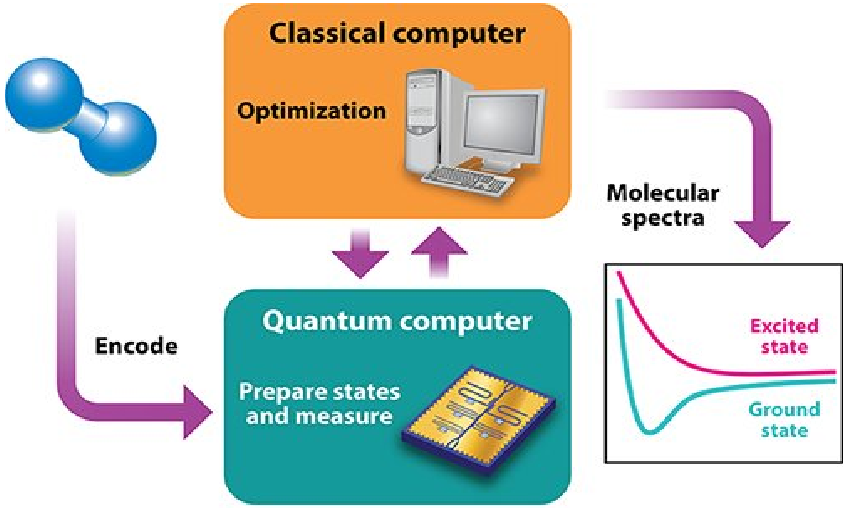
QC4QC

Support development of algorithms for quantum chemistry

- HPC resources and support
- human resources

(SURF employees time + PD 1 year)

Results



Sim et al., Quantum Computer Simulates Excited States of Molecule, Physics 11, 14, 2018

Reinforcement learning algorithm that autonomously explores the space of possible ansätze, identifying economic circuits which still yield accurate ground energy estimates.

VQE

1) Interfaces to classical software (OpenFermion)
2) Classical optimization
3) Ansatz optimization
4) Knowledge dissemination

Reinforcement learning for optimization of variational quantum circuit architectures
https://arxiv.org/abs/2103.16089

Other projects..

Ray tracing for atmospheric simulations

Patterns recognition and ray tracing in HEP

QNN for classification (Chemistry)

Benchmarking simulators

Integration with Quantum Inspire

ML methods for qubit routing

MsC. Quantum computing for PDEs (TuD)

Conclusions

- HPCs need to get ready for quantum
- There are some “simple” initiatives that we can start to stimulate and support QC developments
- Quantum computing will always be hybrid, we therefore need to focus on how to enable this in the best possible way

SURF

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