science + computing

SOLID

EVIDEN

q-solid.de

# HPC/QC Use Case Study

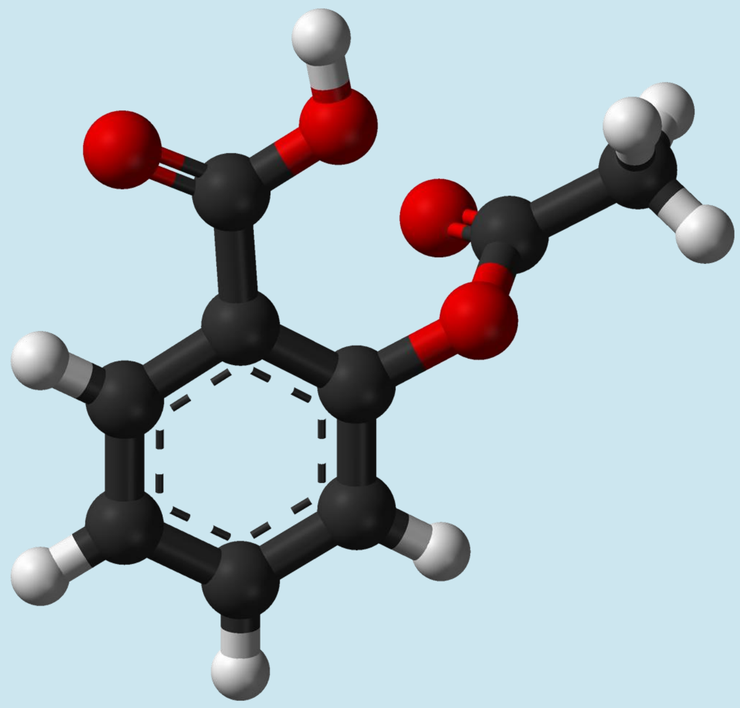
## Geometry Optimization of Acetylsalicylic Acid (ASA)

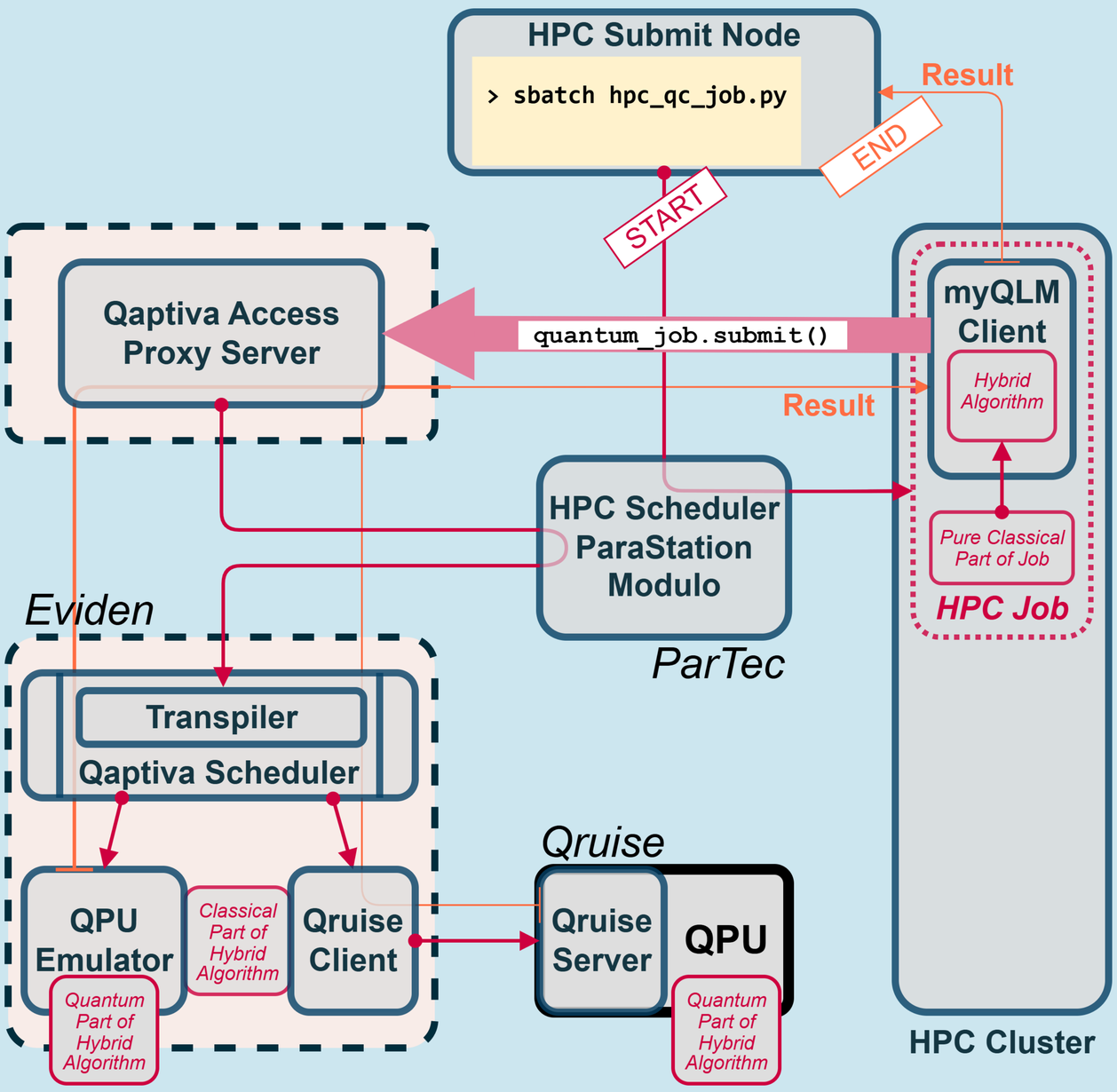
**Why Geometry Optimization is a good HPC/QC Use Case:**

- HPC use case that benefits from offload to QPU of certain parts
- Exact ground state geometry of a molecule or protein is crucial for getting precise results such as the ground state energy
- Typical chemistry Ansatz: computational less expensive methods (e.g. density functional theory, DFT) combined with more accurate methods (e.g. unitary coupled cluster, UCC)
- ASA optimization:
  - Non-reactive, large part: computation on HPC cluster
  - Smaller reactive part: outsourced to QPU

**Using this approach could lead to faster and more precise geometries compared to performing geometry optimization solely on an HPC cluster**

Demo notebook on how to use UCC with myQLM






### Optimization Workflow of ASA with myQLM / Qaptiva

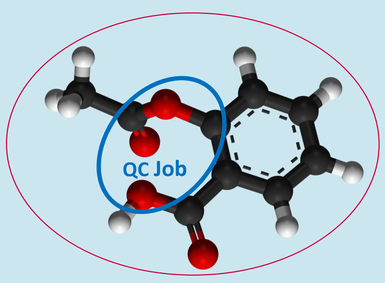
Take arbitrary geometry as input and perform optimization with ASE until ground state geometry is reached:

- Step 1 (HPC): Run DFT for entire molecule with PySCF
- Step 2 (HPC): Run DFT for active part of molecule with PySCF
- Step 3 (QPU): Run UCC for active part of molecule
  - Define molecular Hamiltonian
    `myQLM: qat.fermion.chemistry.MolecularHamiltonian`
  - Generate UCC circuit
    `myQLM: qat.fermion.chemistry.ucc.construct_ucc_ansatz`
  - Compile circuit to QSolid gateset (4 qubits / depth approx. 180)
    `Qaptiva: qlmaas.plugins.QSolidTranspiler`
  - Run circuit via Qaptiva:
    - Emulated QPU: `qlmaas.qpus.EmuQSolidQPU10`
    - Real QPU: `qlmaas.qpus.QSolidQPU10`
- Step 4 (HPC): Addition of results gives total energy and interatomic forces

### QSolid Job Flow Diagram

- Simple user access to real QPU
- Use case can be applied to emulated and real QPUs

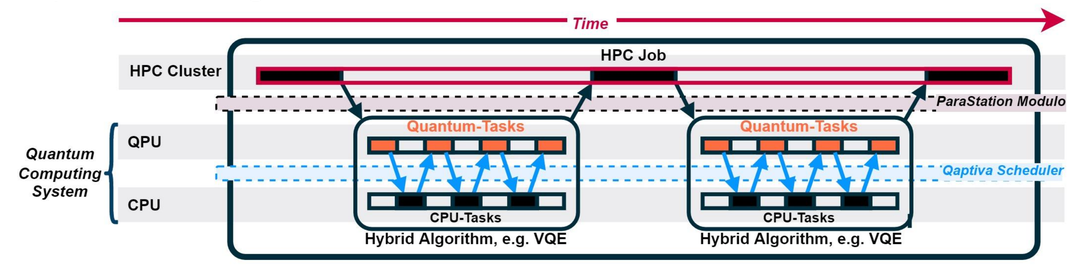
Recorded video of running job examples




Classical HPC calculation

### Scalable QC HPC Scheduling

Example for Heterogeneous Quantum-Classical Job




Task flow of heterogeneous quantum-classical job with hybrid algorithms on high performance computing (HPC) system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