Open source variational quantum eigensolver (OpenVQE)

Extension of the quantum learning machine (QLM) for quantum chemistry

Tutorial: OpenVQE training session

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What is OpenVQE ?

Open Source Variational Quantum Eigensolver package for Quantum Chemistry that based on the tools provided in MyQLM-fermion package.
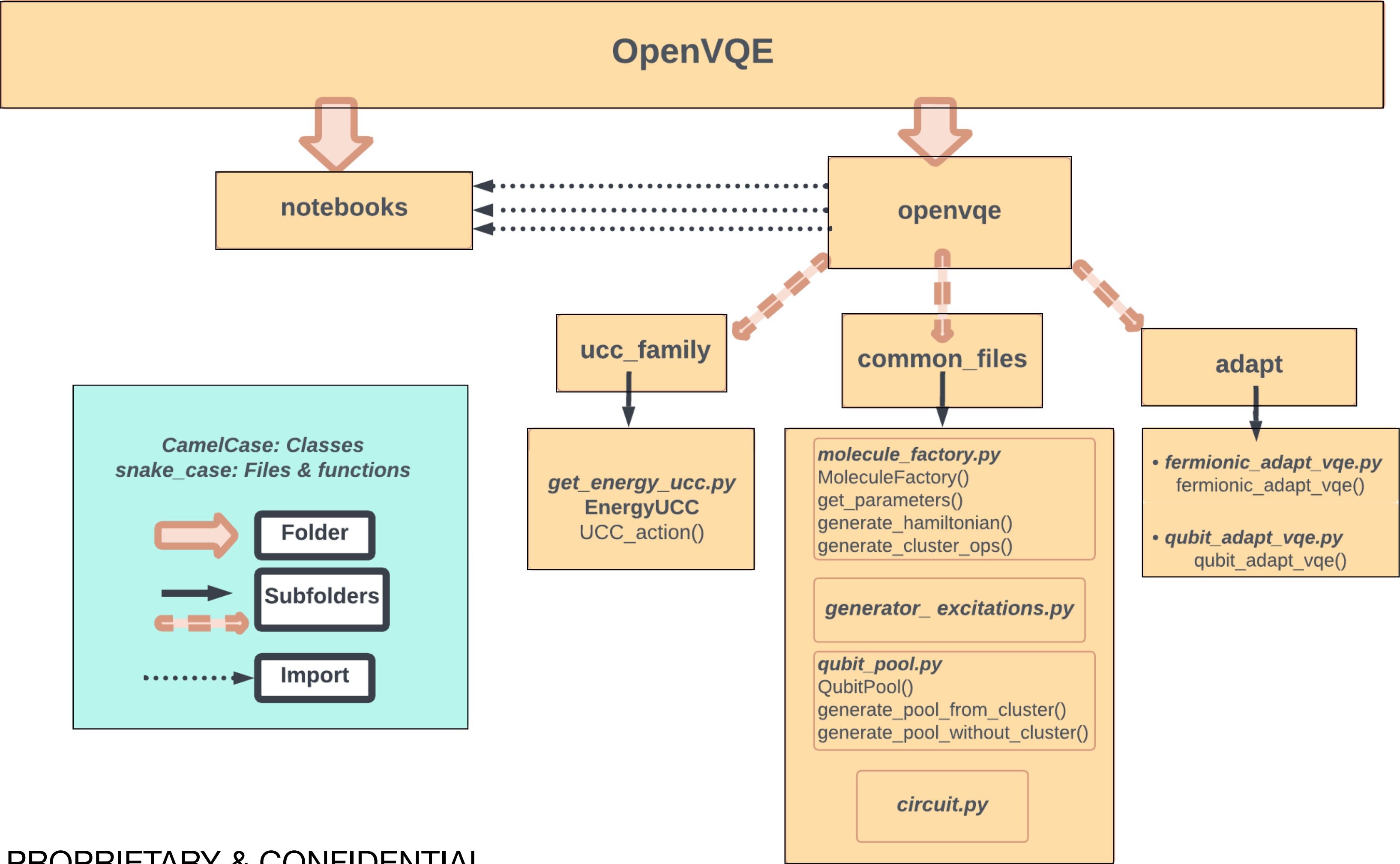
Why OpenVQE ?

The combined OpenVQE/
myQLM-fermion libraries facilitate
the implementation, testing and
development of variational
quantum algorithms.

Flowchart of the OpenVQE Package

The code is given in our Github repository and documentation

OpenVQE

notebooks

openvqe

ucc_family

common_files

adapt

CamelCase: Classes
snake_case: Files & functions

Folder

Subfolders

Import

get_energy_ucc.py
EnergyUCC
UCC_action()

molecule_factory.py
MoleculeFactory()
get_parameters()
generate_hamiltonian()
generate_cluster_ops()

generator_ excitations.py

qubit_pool.py
QubitPool()
generate_pool_from_cluster()
generate_pool_without_cluster()

circuit.py

• *fermionic_adapt_vqe.py*
fermionic_adapt_vqe()

• *qubit_adapt_vqe.py*
qubit_adapt_vqe()

State of the art

Empowering impactful projects via OpenVQE.

- More than **35** contributors from different countries: Europe, US, Asia

- Noiseless Schrödinger-style dense simulator can reach up to **41** qubits for any circuit

- **4** published papers from the author

- Non-profit organisation, aim for education

Wiley review **https://doi.org/10.1002/wcms.1664**