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.
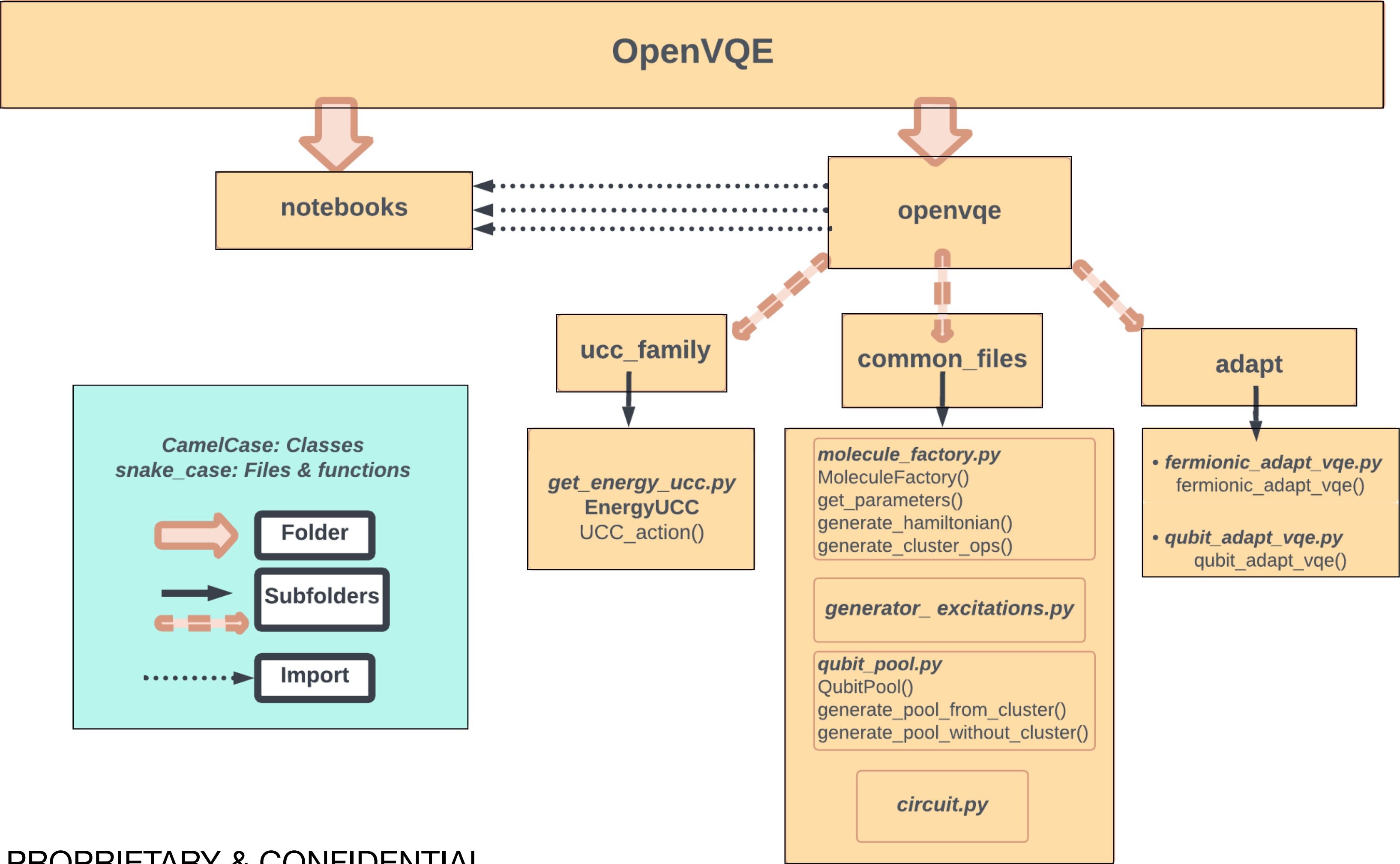
Why OpenVQE ?

An extremely efficient & well-structured variational quantum chemistry algorithms based on MyQLM - Eviden.

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

- Application in material sciences, drug discoveries, climate change and machine learning

- Non-profit organisation, aim for education

- **3** published papers from the author

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