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Quantum Chemistry: from Simulators to QPUs

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European Research Council
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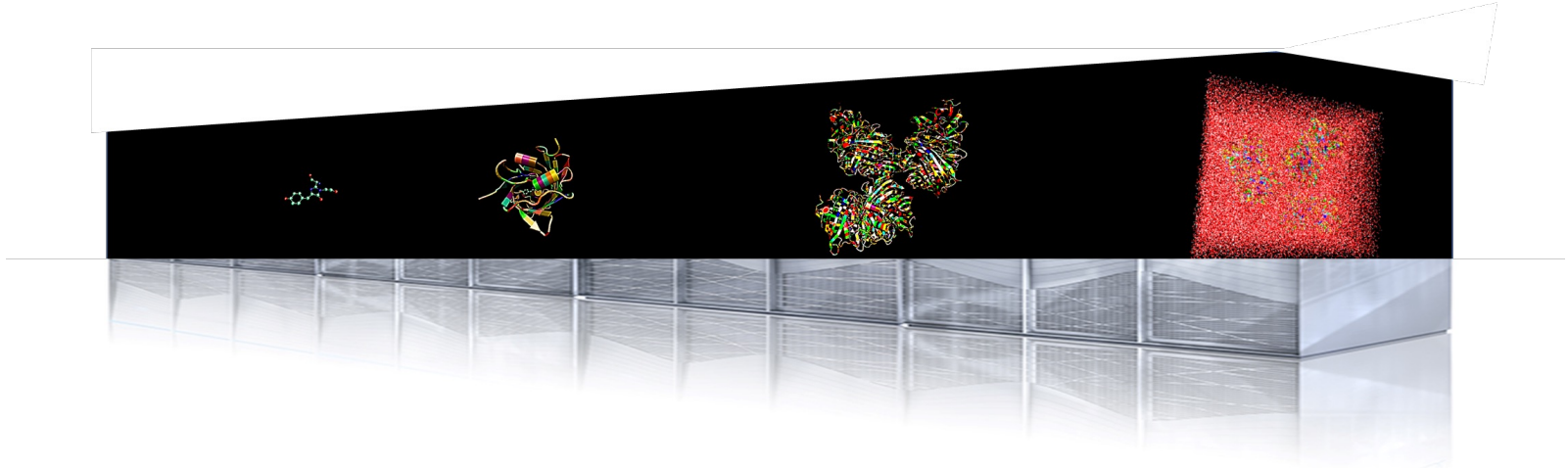
Extreme-scale Mathematically-based Computational Chemistry

The importance of hardware evolutions

Computational chemistry diversifies:

- **Quantum Chemistry**
- **Artifical Intelligence (neural networks …)**
- **Molecular dynamics**

- **Lots of possibilities for hardware now. CPUs, GPUs, QPUs, depending on the methodology. Although they are multi-purpose (and double precision), CPUs are not the standard anymore in many fields.**

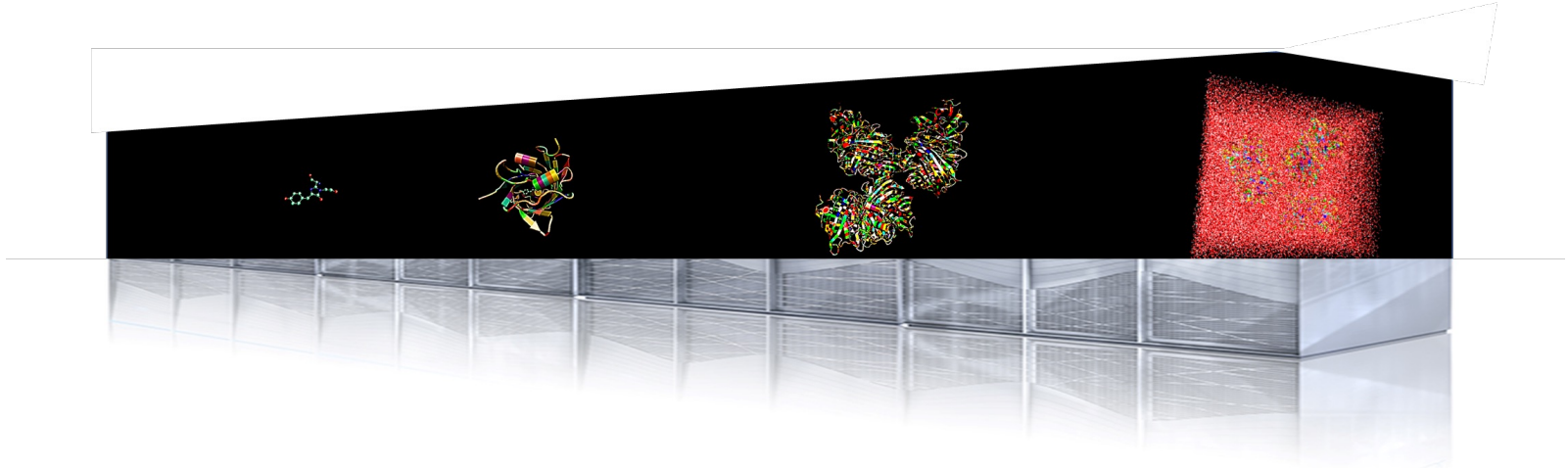


The importance of hardware evolutions

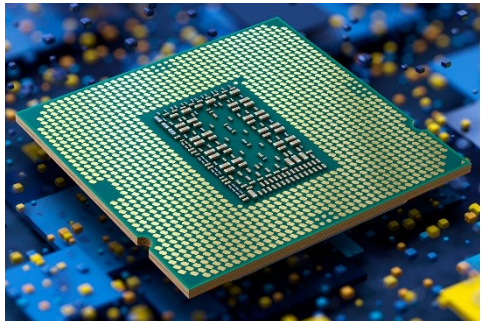
We tend to forget it but Computational Chemistry applications are always intrinsicaly related to the available HPC hardware and its evolution.

- Good news: HPC evolves quickly and goes stronger/faster
- Bad news: the community codes need to be adapted and it is not gonna stop…

- Modeling complex systems (i.e. very large and/or with lots of electrons) requires an HPC strategy, especially as computational chemistry diversifies.



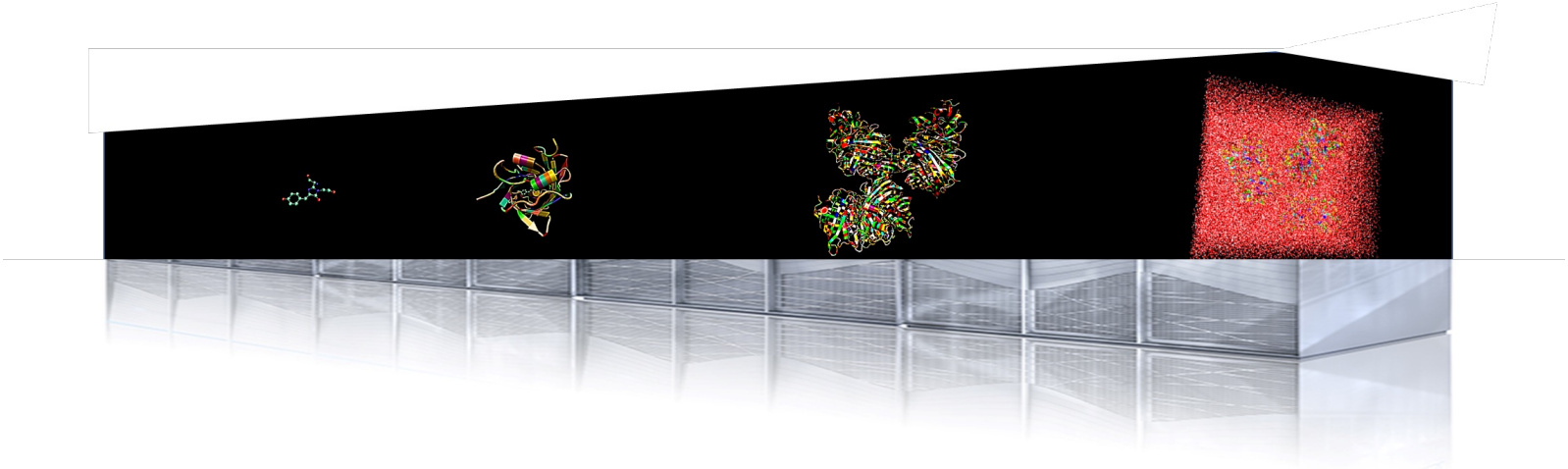
The importance of hardware evolutions



CPU

GPU

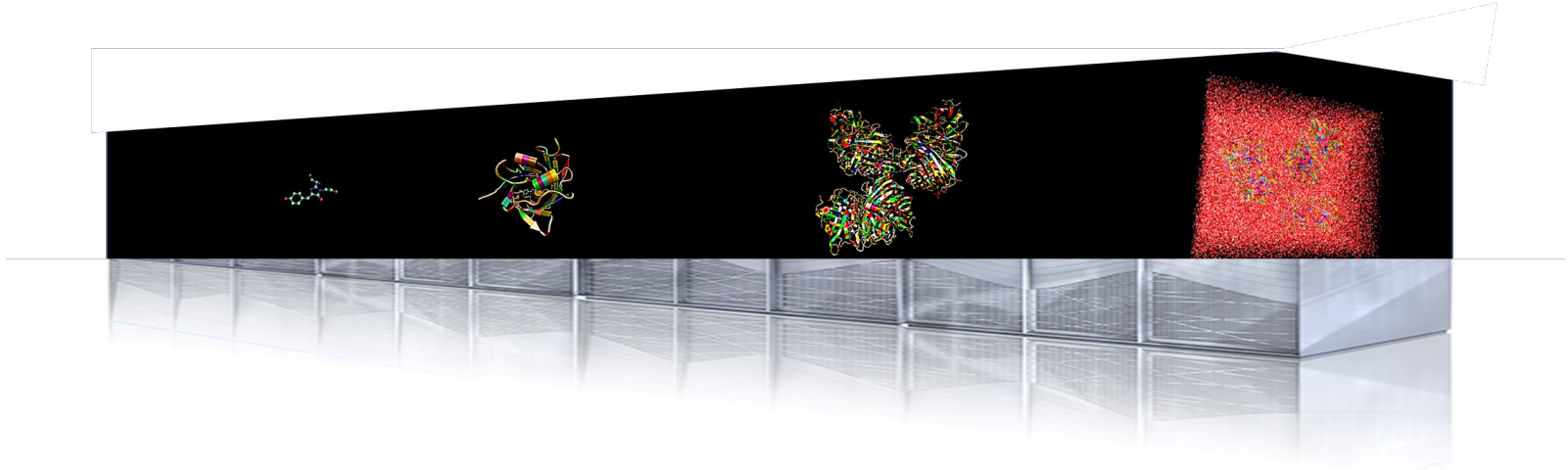
QPU



The importance of hardware evolutions

QPU

What's could be the next big thing?
Quantum Computing for Computational Chemistry



The importance of hardware evolutions

QPU

- Quantum computer do exist but limited availibility (for now).
- Present generation: NISQ (noisy intermediate scale quantum) systems
- Number of Qubits from 2 to a few hundreds but in practice…no practical use beyond a few dozen
- Analogic machines or/and Quantum Gates programming
- Quantum simulators available (QML, Qiskit..) and mandatory to test new algorithmics.
- Good to know: 1 Qubit per spin-orbital (basis sets!!!)

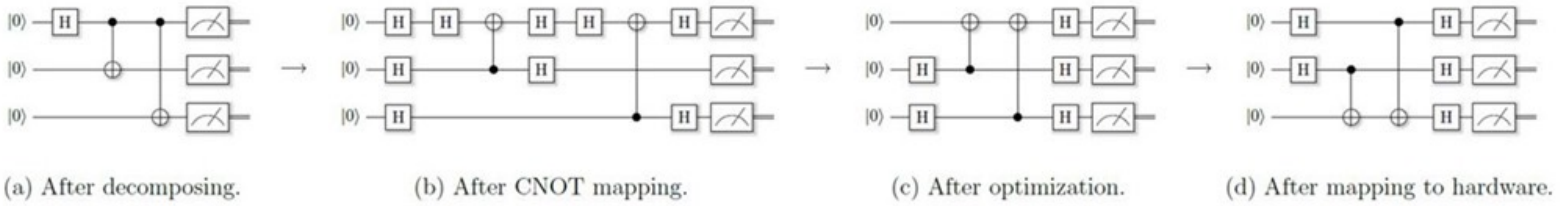


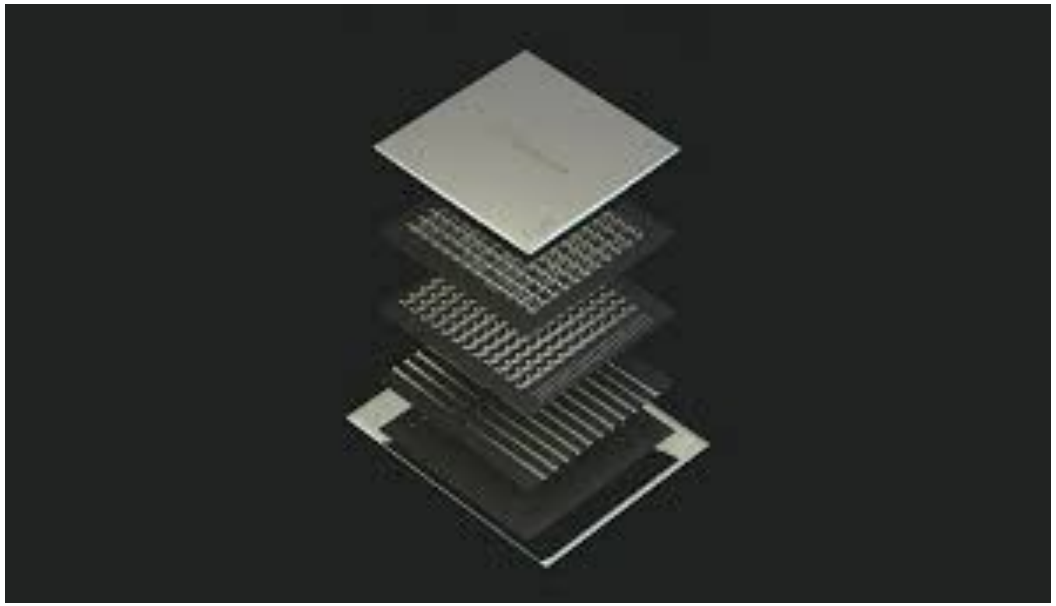
Figure 5: Individual stages of compiling an entangling operation for the IBM back-end. The high-level Entangle-gate is decomposed into its definition (Hadamard gate on the first qubit, followed by a sequence of controlled NOT gates on all other qubits). Then, the CNOT gates are remapped to satisfy the logical constraint that controlled NOT gates are allowed to act on one qubit only, followed by optimizing and mapping the circuit to the actual hardware.

Gate	Notation	Matrix
NOT (Pauli-X)	X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Z	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
CNOT (Controlled NOT)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

The importance of hardware evolutions

QPU

What can you expect? Testing IBM's Eagle (127 qubits)
On a real world chemical system: Benzene



CALCULATING THE GROUND STATE ENERGY OF BENZENE UNDER SPATIAL DEFORMATIONS WITH NOISY QUANTUM COMPUTING

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In this manuscript, we calculate the ground state energy of benzene under spatial deformations by using the variational quantum eigensolver (VQE). The primary goal of the study is estimating the feasibility of using quantum computing ansatze on near-term devices for solving problems with large number of orbitals in regions where classical methods are known to fail. Furthermore, by combining our advanced simulation platform with real quantum computers, we provided an analysis of how the noise, inherent to quantum computers, affects the results. The centers of our study are the hardware efficient and quantum unitary coupled cluster ansatze (qUCC). First, we find that the hardware efficient ansatz has the potential to outperform mean-field methods for extreme deformations of benzene. However, key problems remain at equilibrium, preventing real chemical application. Moreover, the hardware efficient ansatz yields results that strongly depend on the initial guess of parameters - both in the noisy and noiseless cases - and optimization issues have a higher impact on their convergence than noise. This is confirmed by comparison with real quantum computing experiments. On the other hand, the qUCC ansatz alternative exhibits deeper circuits. Therefore, noise effects increase and are so extreme that the method never outperform mean-field theories. Our dual simulator/8-16 qubits QPU computations of qUCC appears to be a lot more sensitive to hardware noise than shot noise, which give further indications about where the noise-reduction efforts should be directed towards. Finally, the study shows that qUCC method better captures the physics of the system as the qUCC method can be utilized together with the Hückel approximation. We discussed how going beyond this approximation sharply increases the optimization complexity of such a difficult problem.

TotalEnergies

Revised preprint available on ArXiv:arXiv:2203.05275
https://arxiv.org/abs/2203.05275

Simulating Benzene on a quantum computer

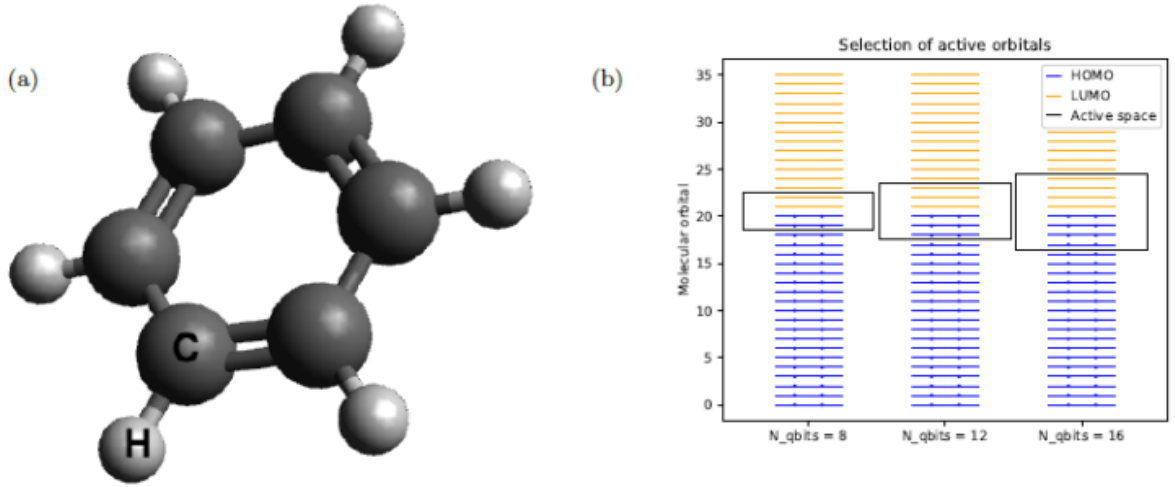


FIG. 1: (a) Molecular geometry of Benzene. (b) Selections of the active orbital space used throughout the manuscript.

System preparation using an in-house version of the QLM simulator.

3 test cases:

- 4 electrons in 4 orbitals (8 qubits)
- All active π orbitals= Huckel (12 qubits)
- Beyond Huckel (16 qubitss)

- All others lower orbitals are frozen and considered as full. QLM is able to generate two subsets of orbitals

Simulating Benzene on a quantum computer

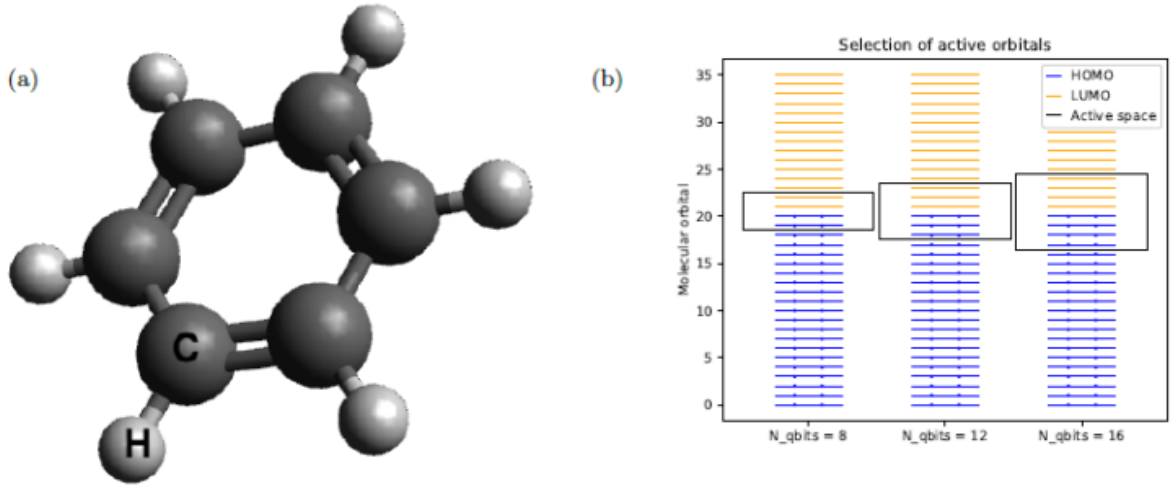


FIG. 1: (a) Molecular geometry of Benzene. (b) Selections of the active orbital space used throughout the manuscript.

Variational quantum eigensolver: choice of the ansatz

- UCCSD
- Hardware efficient ansatz

Variational quantum eigensolver (VQE): Unitary coupled cluster (UCC) with extensions- practices and results

P. K. Barkoutsos, J. F. Gonthier, I. Sokolov, N. Moll, G. Salis, A. Fuhrer, M. Ganzhorn, D. J. Egger, M. Troyer, A. Mezzacapo, S. Filipp, and I. Tavernelli, ***Phys. Rev. A 98, 022322 (2018).***

R. Grimsley, S. E. Economou, E. Barnes, and N. J.Mayhall, ***Nature communications 10, 1 (2019).***

UCC Method

- **Trial wavefunction**: $$|\Psi(\vec{\theta})\rangle = e^{\hat{T}(\vec{\theta})-\hat{T}^{\dagger}(\vec{\theta})}|\Phi_0\rangle$$

$$\begin{cases} |\Phi_0\rangle \text{ : Hartree Fock ground state} \\ \hat{T}(\vec{\theta}) = \hat{T}_1(\vec{\theta}) + \hat{T}_2(\vec{\theta}) + \cdots + \hat{T}_n(\vec{\theta}) \end{cases}$$

UCCSD: $\hat{T} = \hat{T}_1(\vec{\theta}) + \hat{T}_2(\vec{\theta})$

Unitary UCCSD operator: $$\hat{U}(\vec{\theta}) = e^{\hat{T}_{(1)}(\vec{\theta})+\hat{T}_{(2)}(\vec{\theta})-\hat{T}^{\dagger}_{(1)}(\vec{\theta})-\hat{T}^{\dagger}_{(2)}(\vec{\theta})}.$$

$$\begin{cases} \hat{T}_{(1)}(\vec{\theta}) = \sum_{ij} \theta_{ij}\hat{a}_i^{\dagger}\hat{a}_j \\ \hat{T}_{(2)}(\vec{\theta}) = \sum_{ijkl} \theta_{ijkl}\hat{a}_i^{\dagger}\hat{a}_j^{\dagger}\hat{a}_k\hat{a}_l \end{cases}$$

UCCSD within Trotter approximation

$$\hat{U}(\vec{\theta}) = \exp\left(\sum_{ij} \theta_{ij} \hat{a}_i^\dagger \hat{a}_j + \sum_{ijkl} \theta_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l - \sum_{ij} \theta_{ij} \hat{a}_j^\dagger \hat{a}_i - \sum_{ijkl} \hat{a}_l^\dagger \hat{a}_k^\dagger \hat{a}_j \hat{a}_i \right)$$

with $\vec{\theta} = (\{\theta_{ij}\}, \{\theta_{ijkl}\})$ and $\theta_{ij}, \theta_{ijkl} \in \mathbb{R}$.

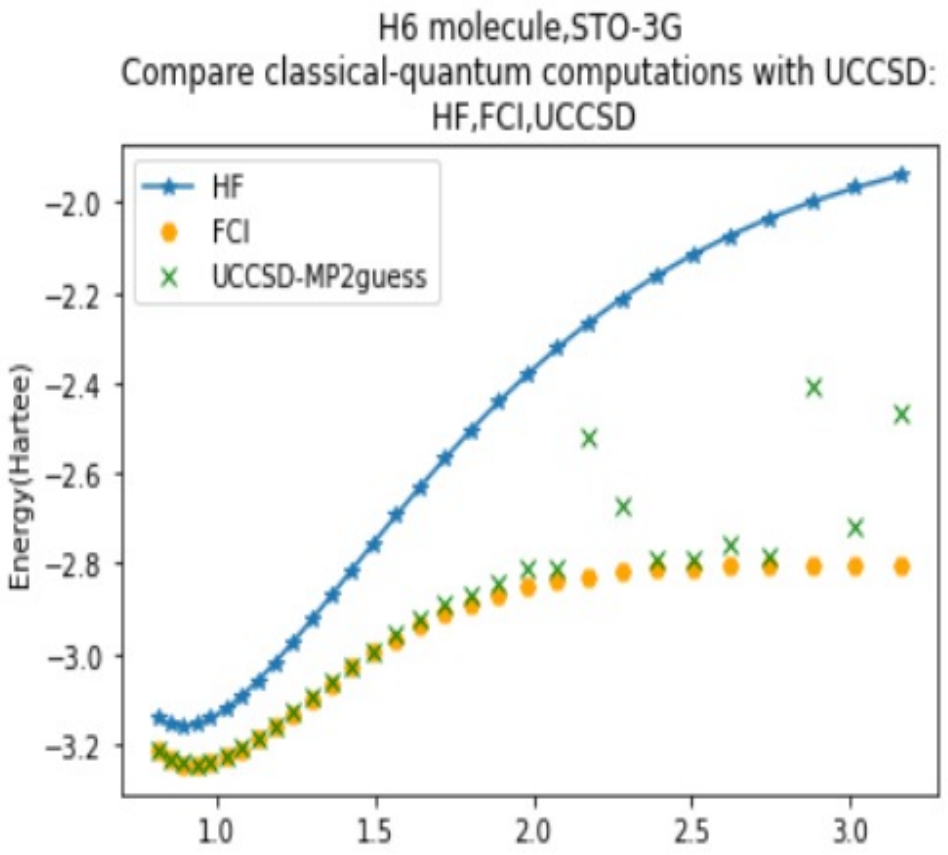
First-order Trotter approx: $e^{\hat{A}+\hat{B}} \approx e^{\hat{A}} e^{\hat{B}}$

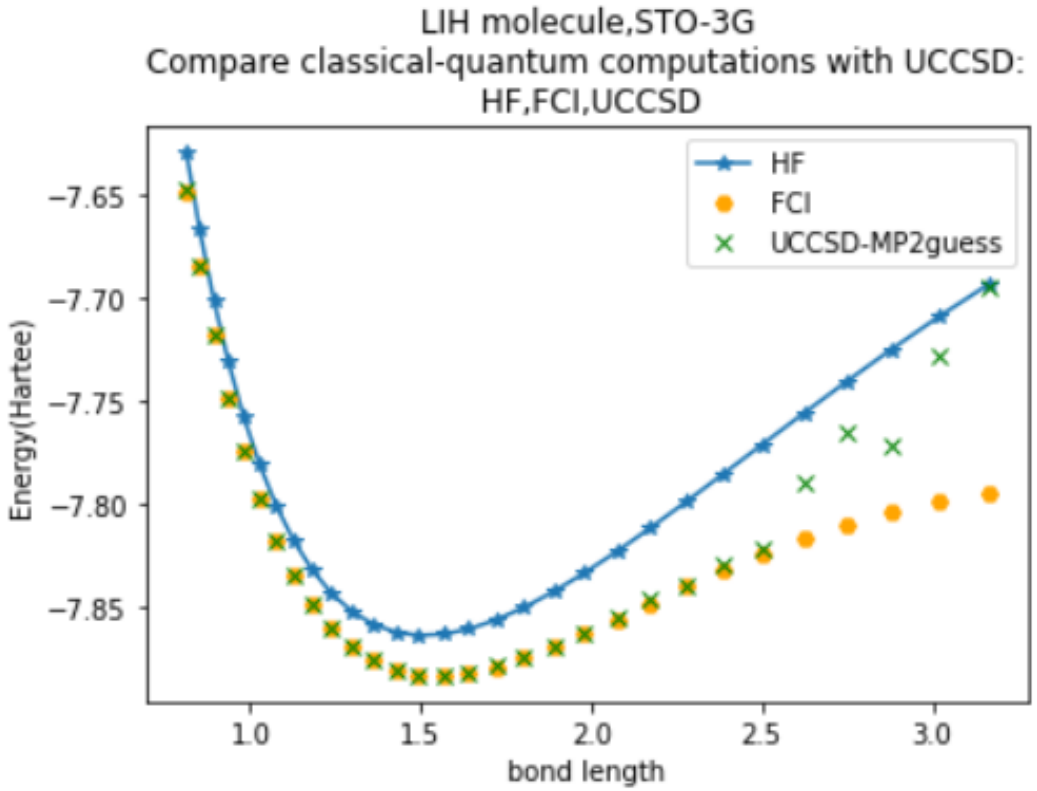
$$\hat{U}(\vec{\theta}) = \exp\left(\sum_{ij} \theta_{ij} (\hat{a}_i^\dagger \hat{a}_j - \hat{a}_j^\dagger \hat{a}_i) \right) \times \exp\left(\sum_{ijkl} \theta_{ijkl} (\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l - \hat{a}_l^\dagger \hat{a}_k^\dagger \hat{a}_j \hat{a}_i) \right)$$

Trotter expansion to first order:

$$\hat{U}(\vec{\theta}) = \prod_{ij} \exp\left(\theta_{ij} (\hat{a}_i^\dagger \hat{a}_j - \hat{a}_j^\dagger \hat{a}_i) \right) \times \prod_{ijkl} \exp\left(\theta_{ijkl} (\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l - \hat{a}_l^\dagger \hat{a}_k^\dagger \hat{a}_j \hat{a}_i) \right).$$

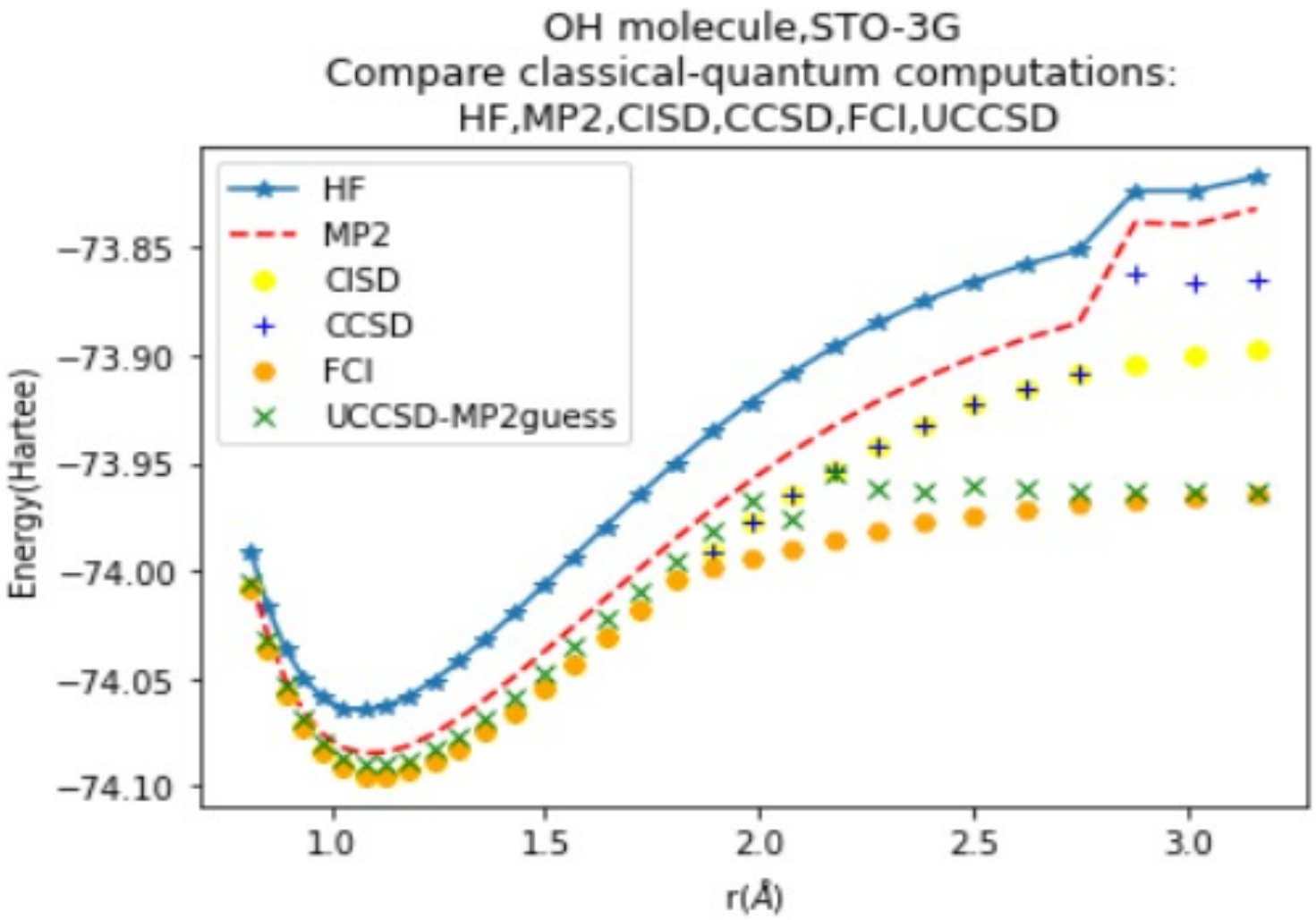
UCCSD simulations on QLM





- MP2 initial guess is very efficient around the equilibrium for weakly and strongly systems.

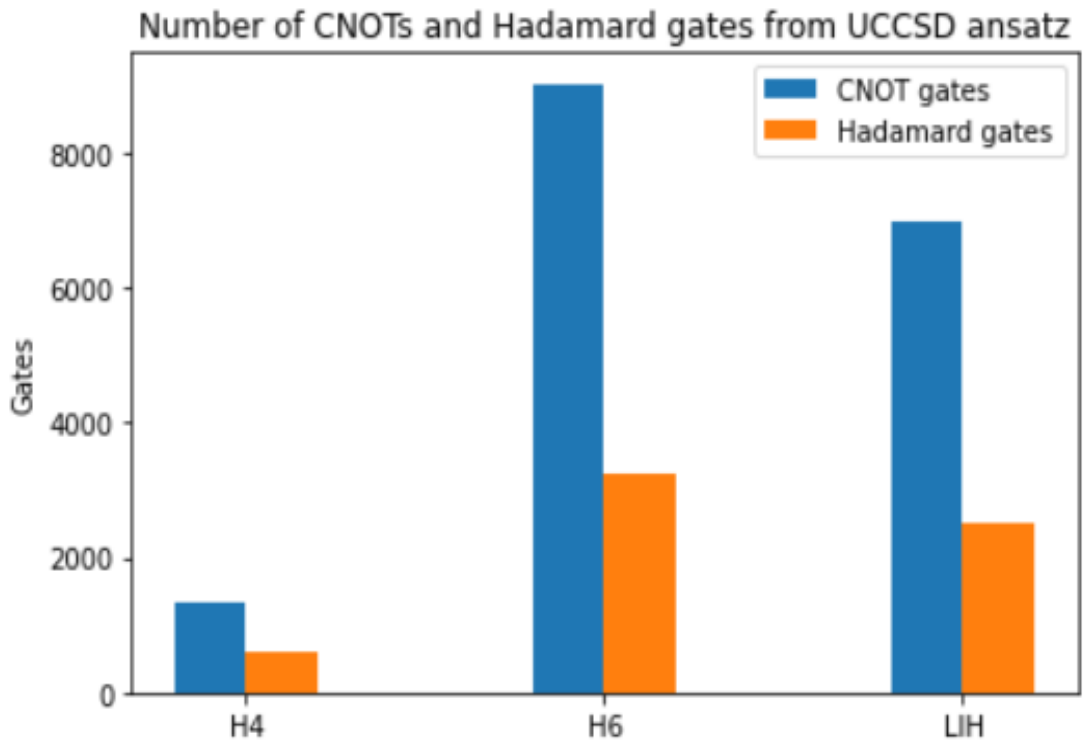
UCCSD: comparison with Classical computation methods

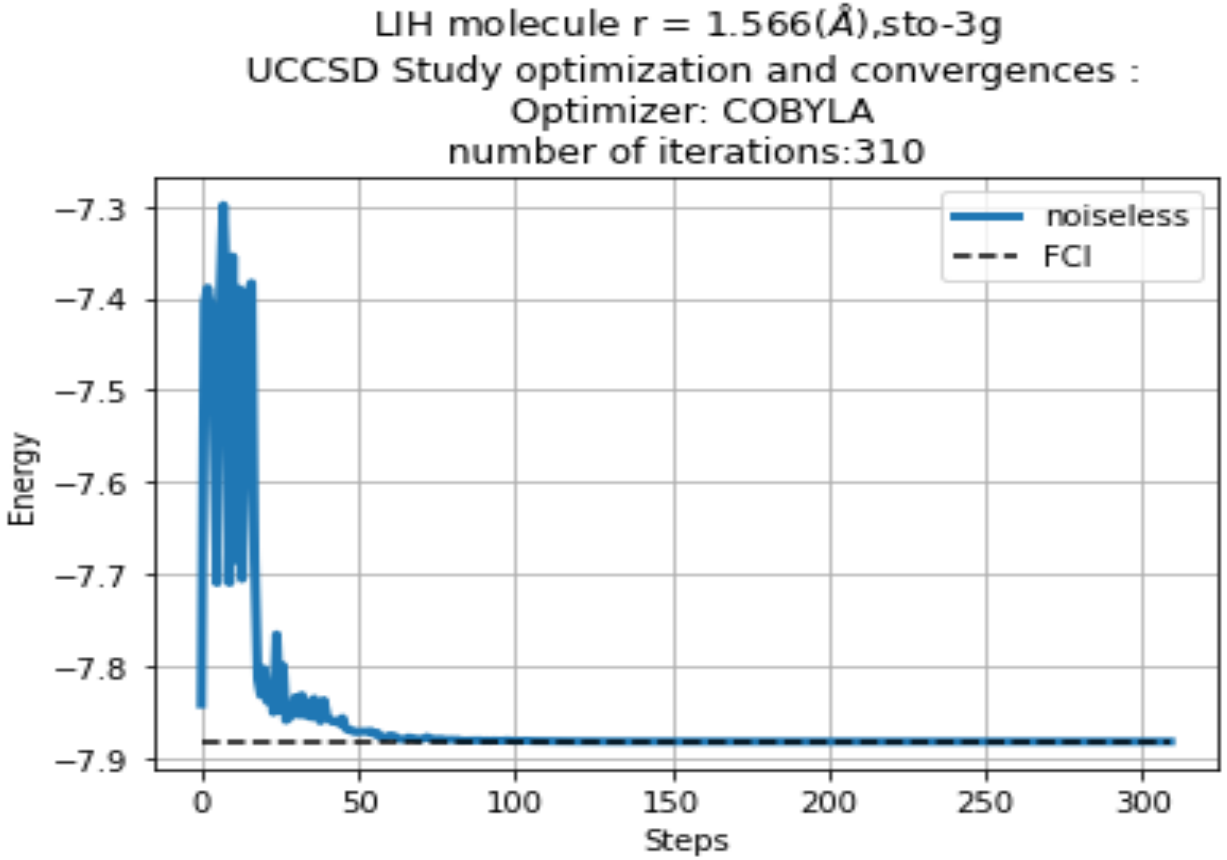


- **Fails for bond length beyond 2.0 (LIH, H_6, OH^-)**

Problems of UCCSD for strongly correlated systems

- Higher scale of parameters and gate counts (ex. CNOTs)
- Redundant excitation terms: unnecessary high numbers of parameters i.e long circuit depth.
- Parameters optimization procedure (initial guesses, MP2 Fails) test, consume high number of iterations to reach convergences (see example below)

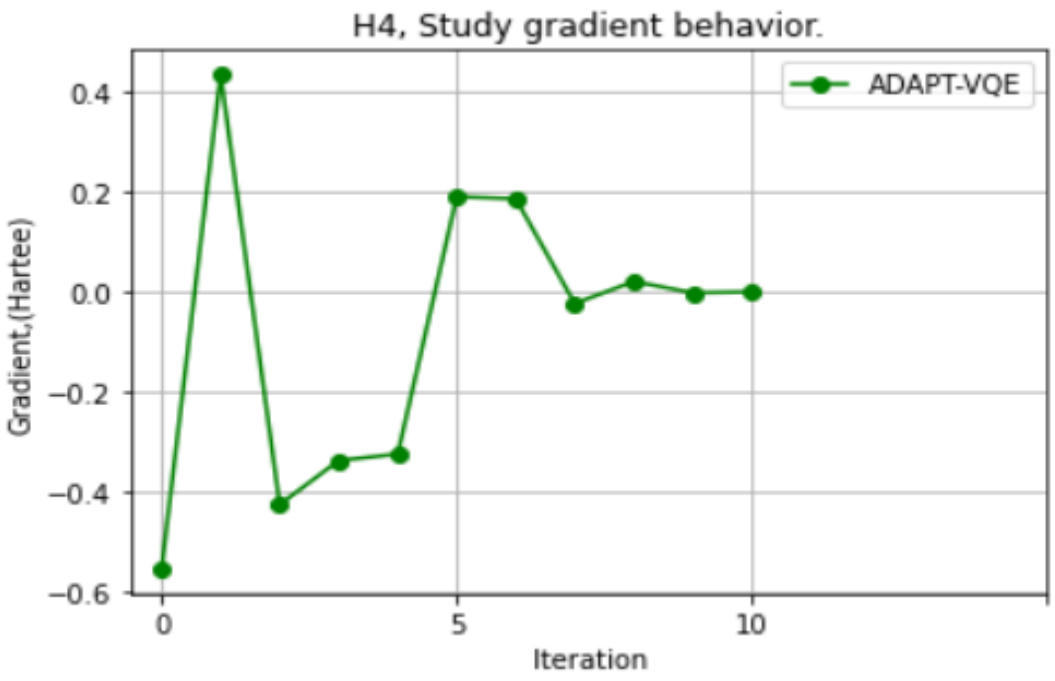


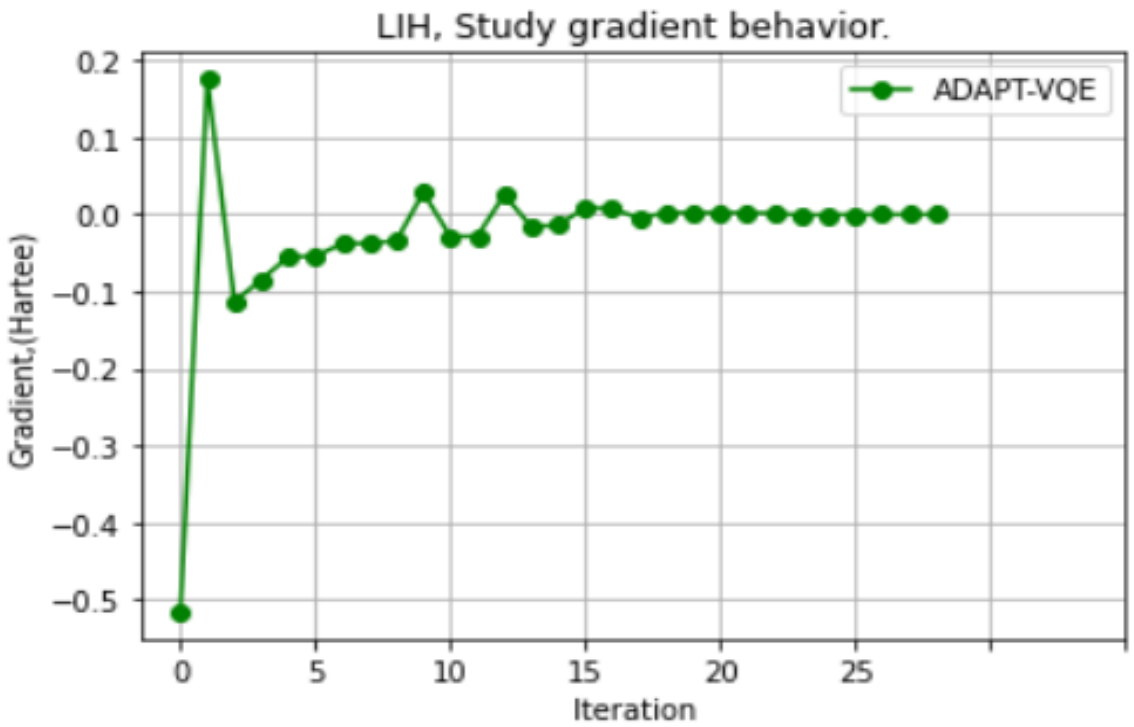


ADAPT-VQE:

- Goal to deal with Strongly correlated systems.

- ***Convergence: Norm of the gradients < threshold*** $\epsilon_m = 10^{-m}$ ***(m = 1,2,3).***

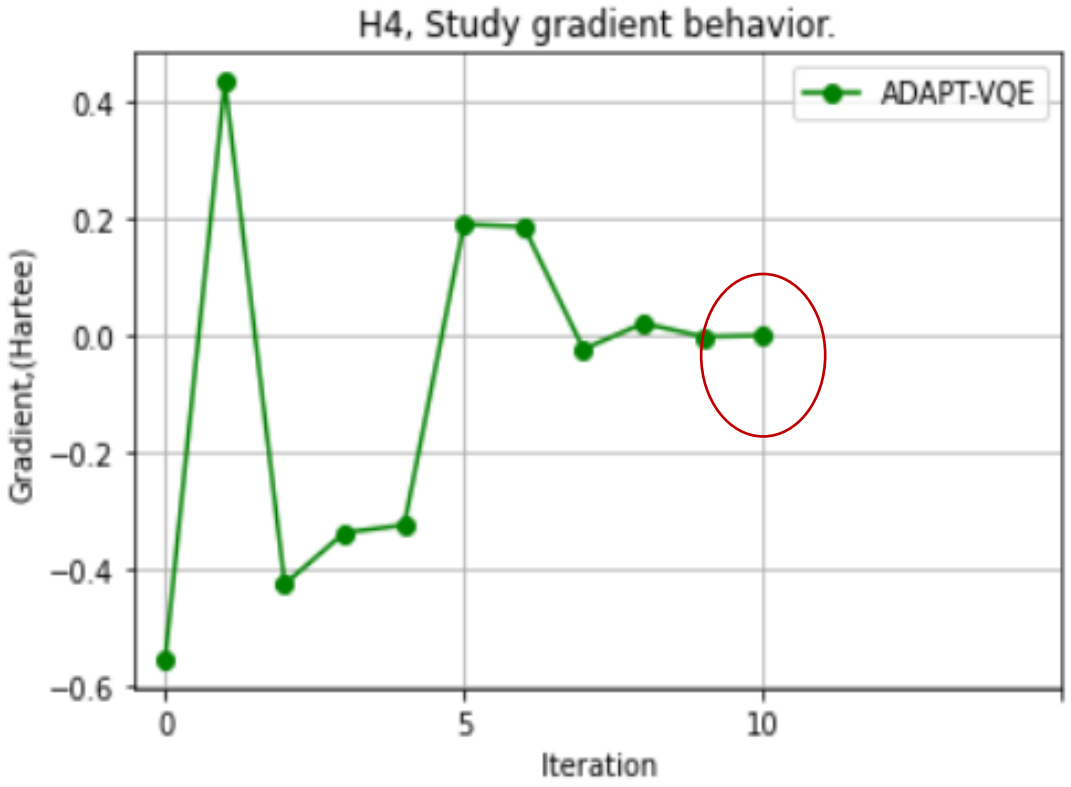


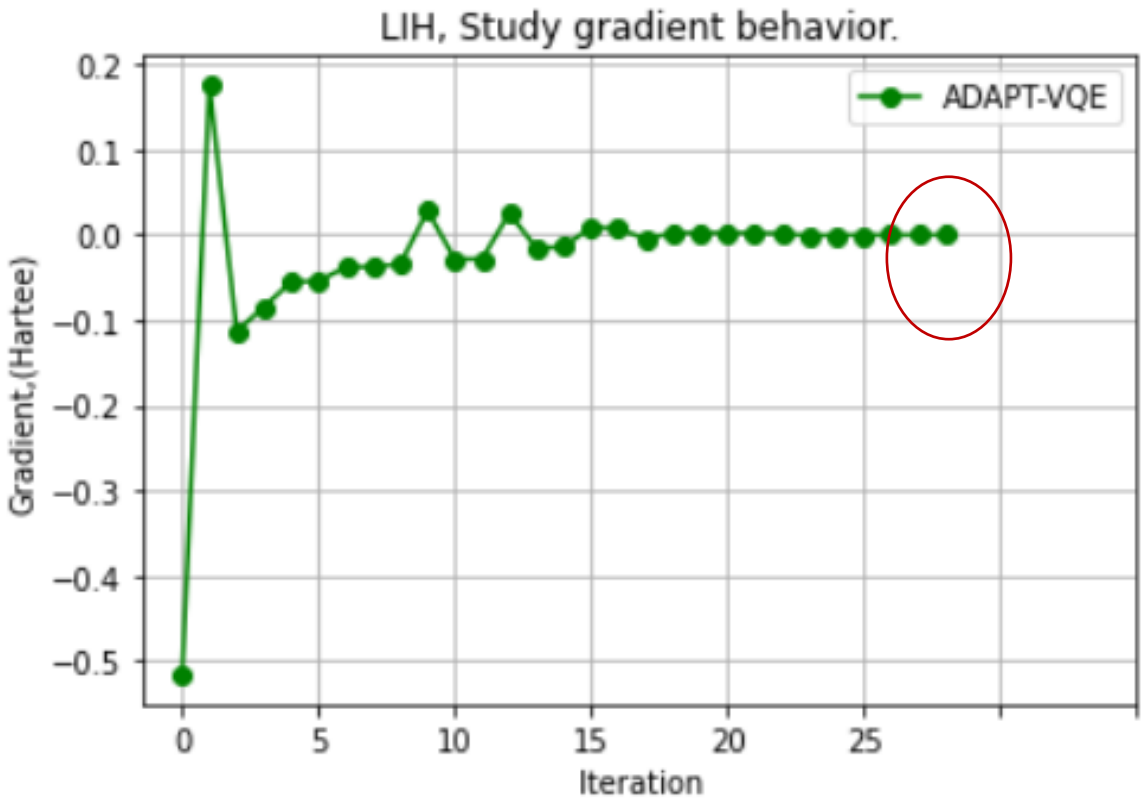


- R. *Grimsley, S. E. Economou, E. Barnes, and N. J.Mayhall,* ***Nature communications 10, 1 (2019).***

ADAPT-VQE

- ***Convergence: Norm of the gradients < threshold*** $\epsilon_m = 10^{-m}$ ***(m = 1,2,3).***

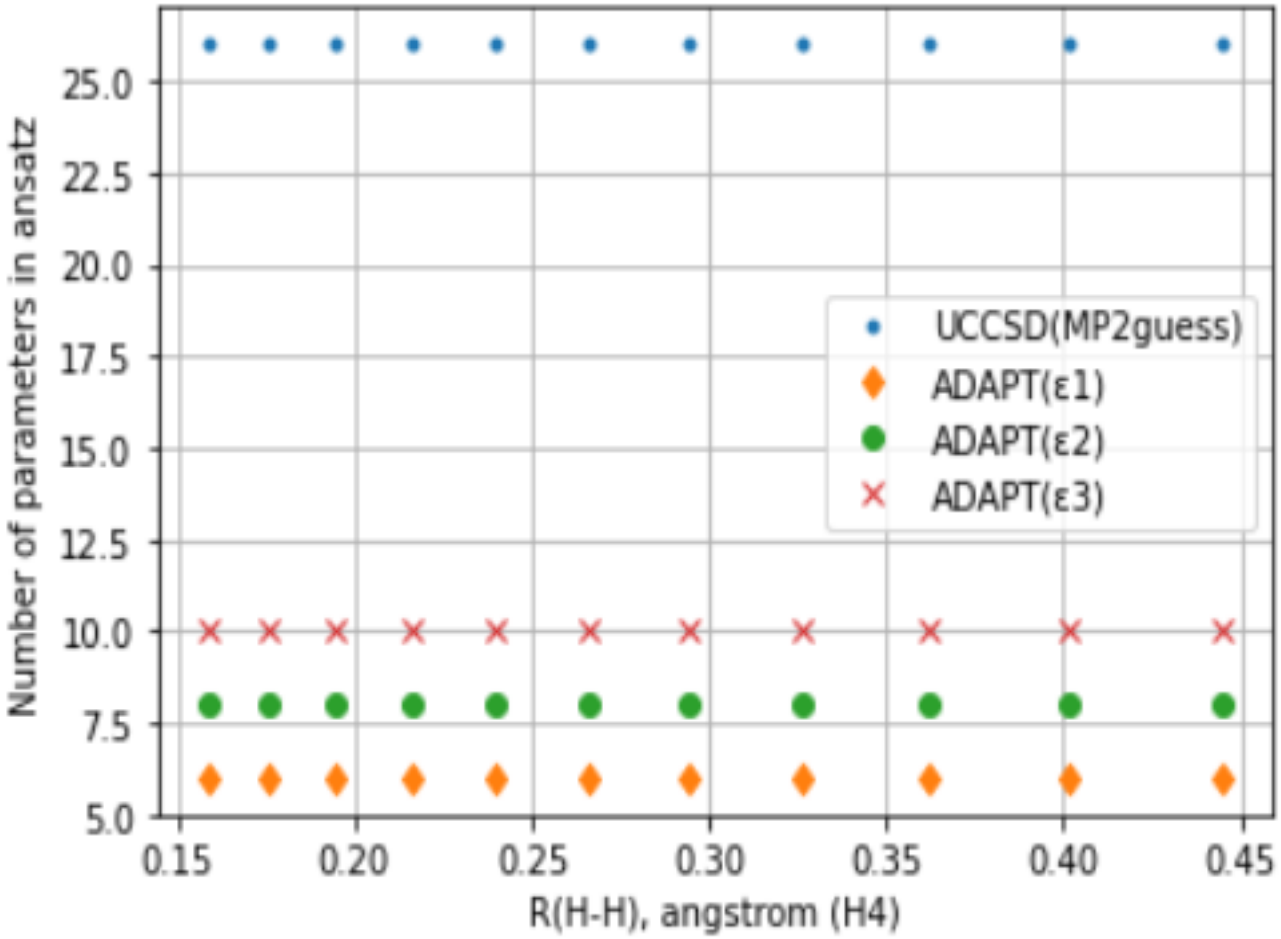


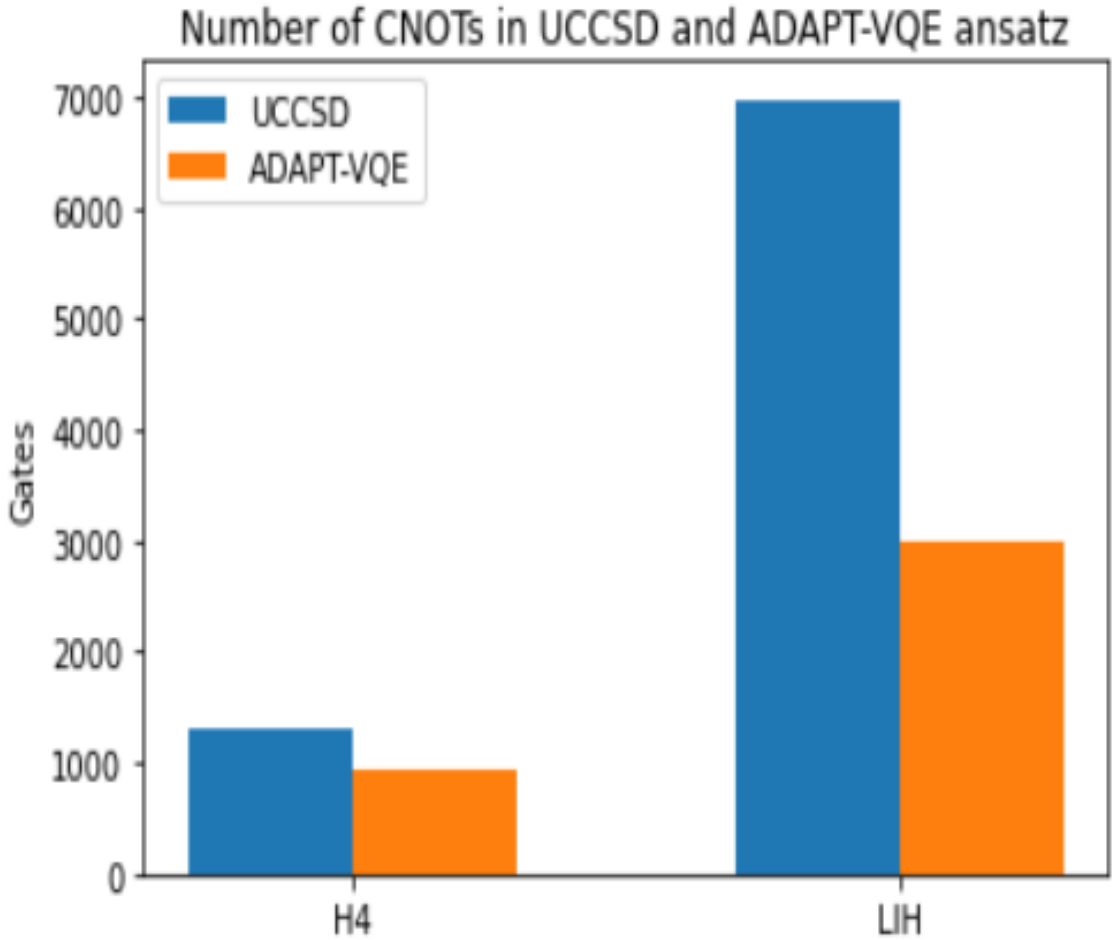


Less number of interation → **Reduced circuit Depth**

Compare UCCSD and ADAPT-VQE

- **Less number of Parameters in the circuit**
- **Less number of CNOT gates**





Back to Benzene: spatial distortion, UCCSD vs Hardware efficient ansatz

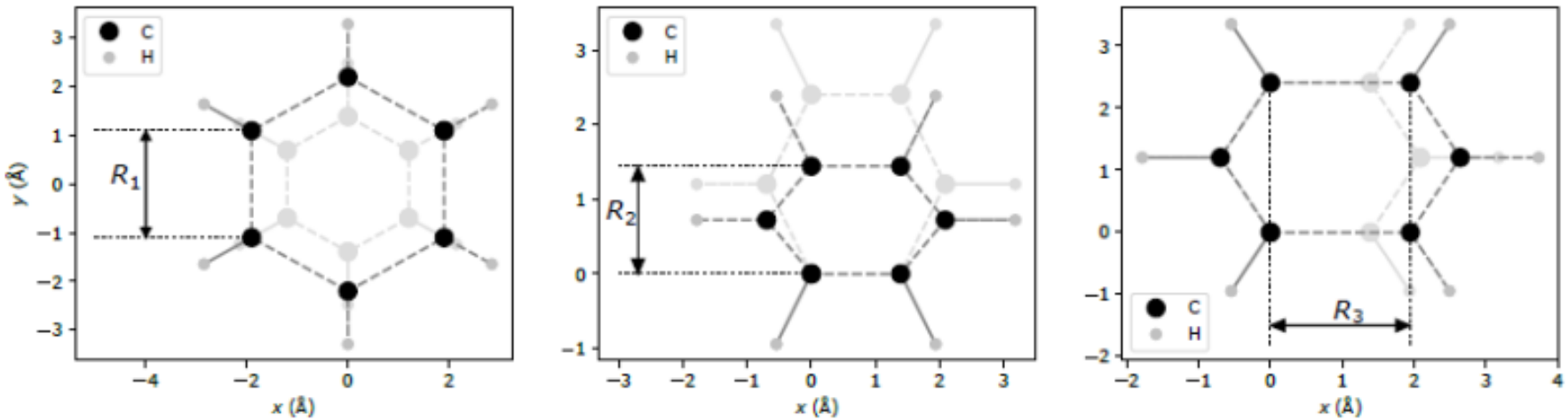


FIG. 2: The 3 types of distortions studied. In the remainder of the manuscript these distortions are refereed to as distortion 1, distortion 2 and distortion 3 respectively.

Back to Benzene: spatial distortion, UCCSD vs Hardware efficient ansatz

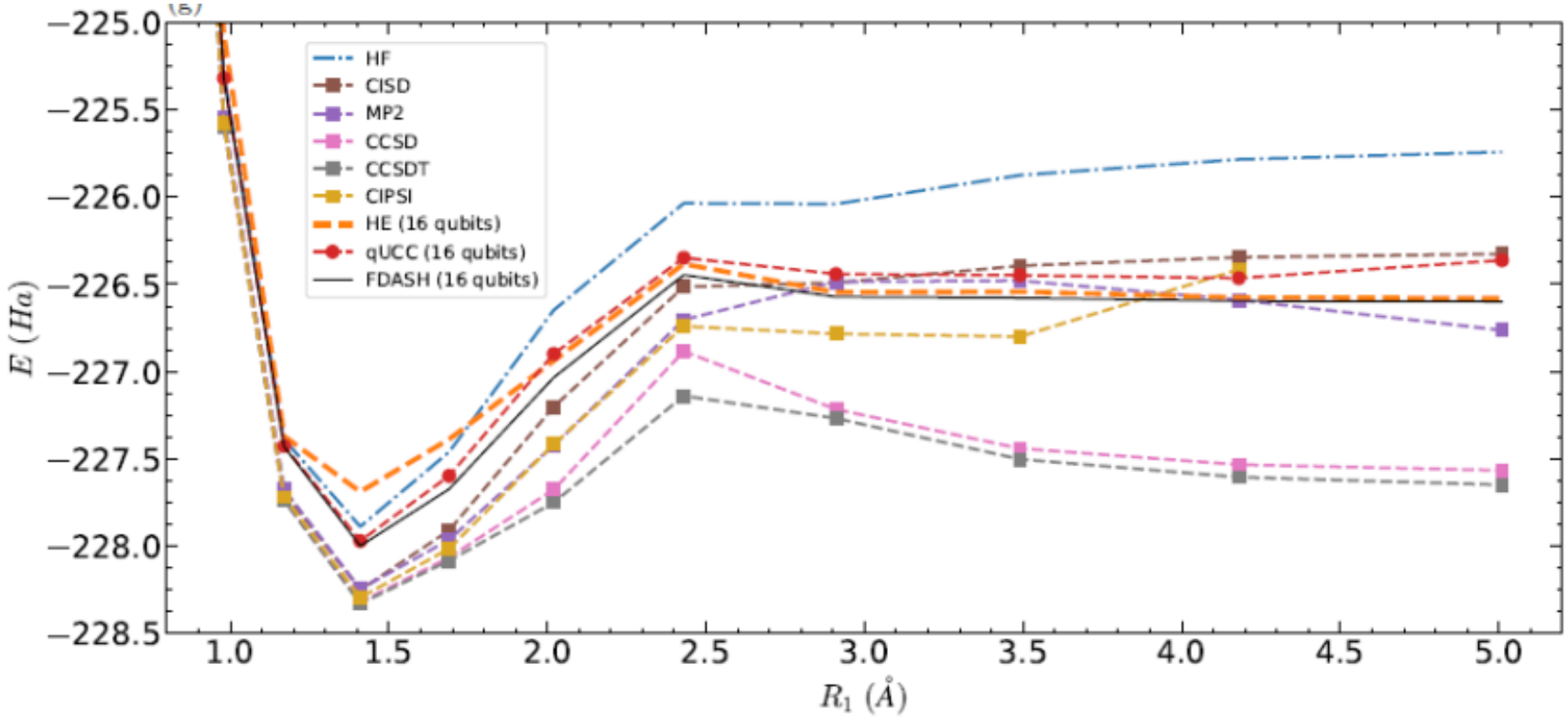


FIG. 8: NOONs obtained with (a) CISD, (b) CCSD, (c) MP2, (d) CASCI, (e) and (f) qUCC methods, for distortion 1. (a) (b) and (c) were obtained through a calculation on the whole benzene system while (d) (e) and (f) were obtained within different active-space selections. They all share the same axis, and the red-dashed vertical line indicates the equilibrium geometry. Finally (g) shows the ground state energy curves obtained with different methodologies. FDASH is an abreviation for "full diagonalization of the active-space Hamiltonian".

Noise issues.

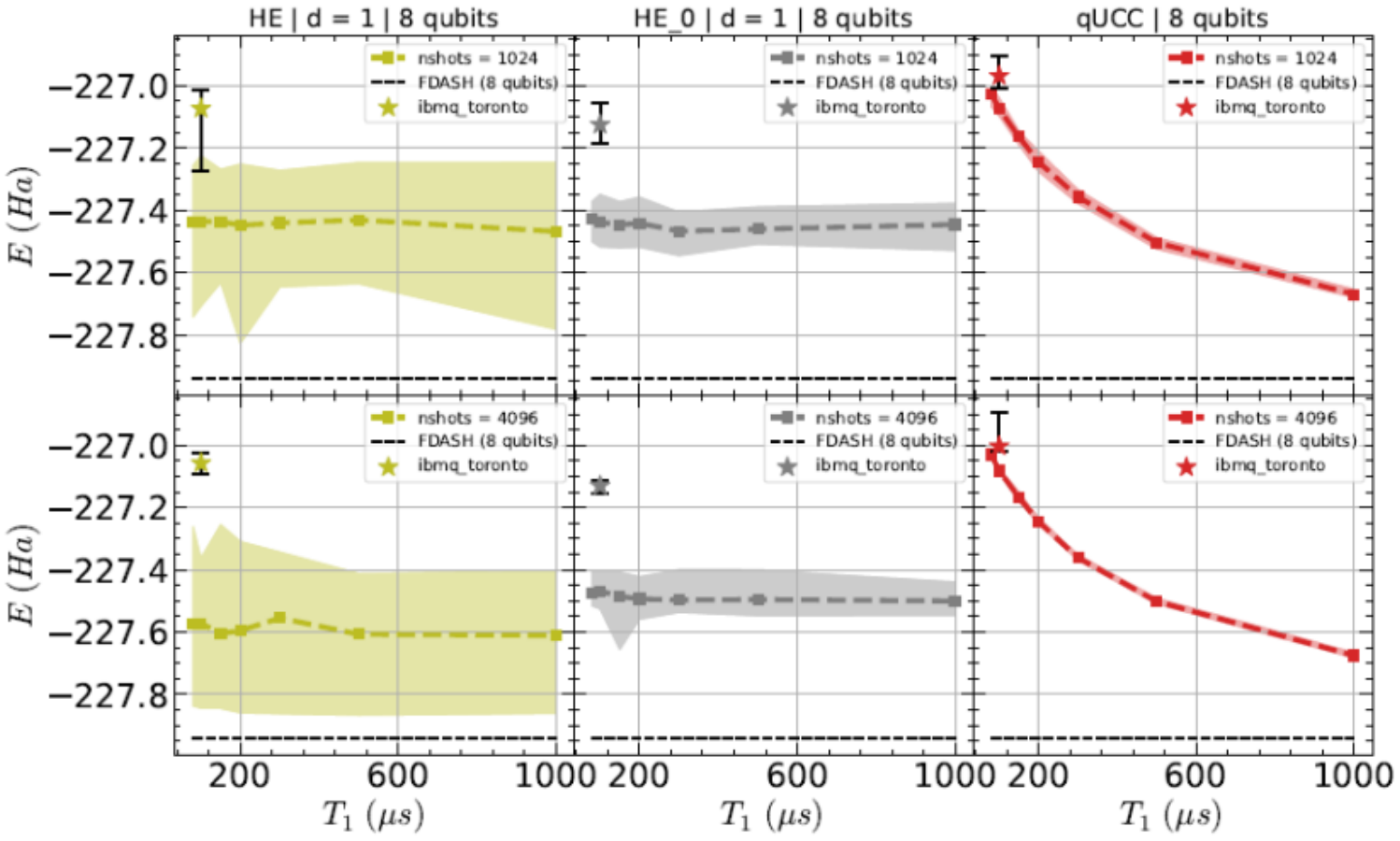


FIG. 9: Ground state energy of active-space Hamiltonian of 8 qubits of benzene at $R_1 = 1.41$ Å, as a function of T_1. The curves are noisy simulations while star markers were obtained with *IBMQ_Toronto*. The first row shows results with 1024 shots, the second one with 4096 shots. They share the same y axis. FDASH is an abreviation for "full diagonalization of the active-space Hamiltonian".

T1: qubit lifetime
T2: qubit phase coherence

In the IBM: T1=T2=100μs

- **UCC is more affected by decoherence noise than measurement noise.**
- **Opposite behavior fo HE: sensible to shot noise**
- **Depend on the landscape**

What should be T1 to reach:
- **10^{-2} precision: 36ms**
- **10^{-4} precision: 3.6s**

Noise issues.

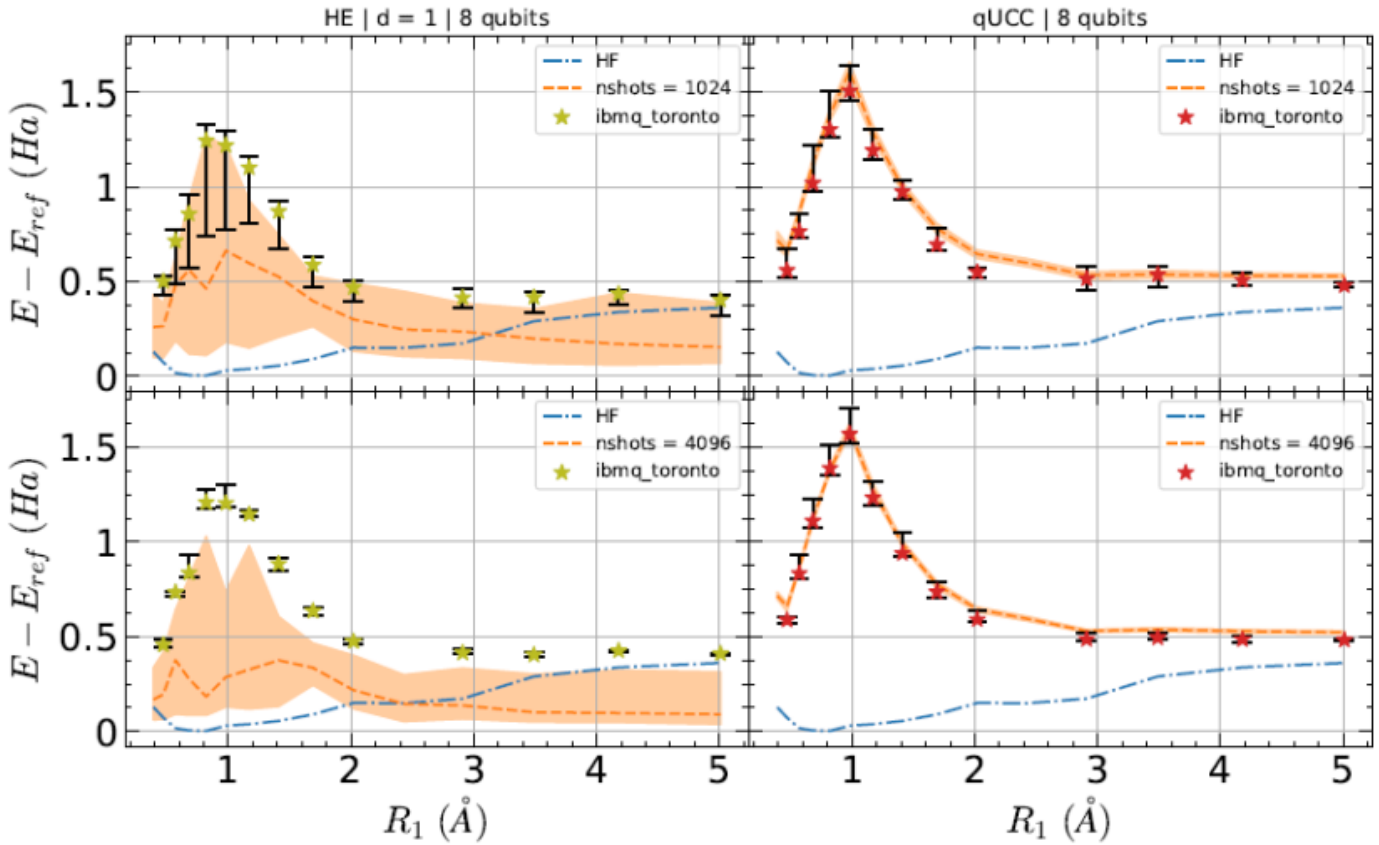


FIG. 10: Difference between the ground state energies of 8 qubits system obtained with HE and qUCC ansatz, either with our noise model or real *IBMQ_Toronto*, and the reference obtained with full diagonalization of 8 qubits system, for the first distortion. The first row shows results with 1024 shots, the second one with 4096 shots. All figures share the same y axis.

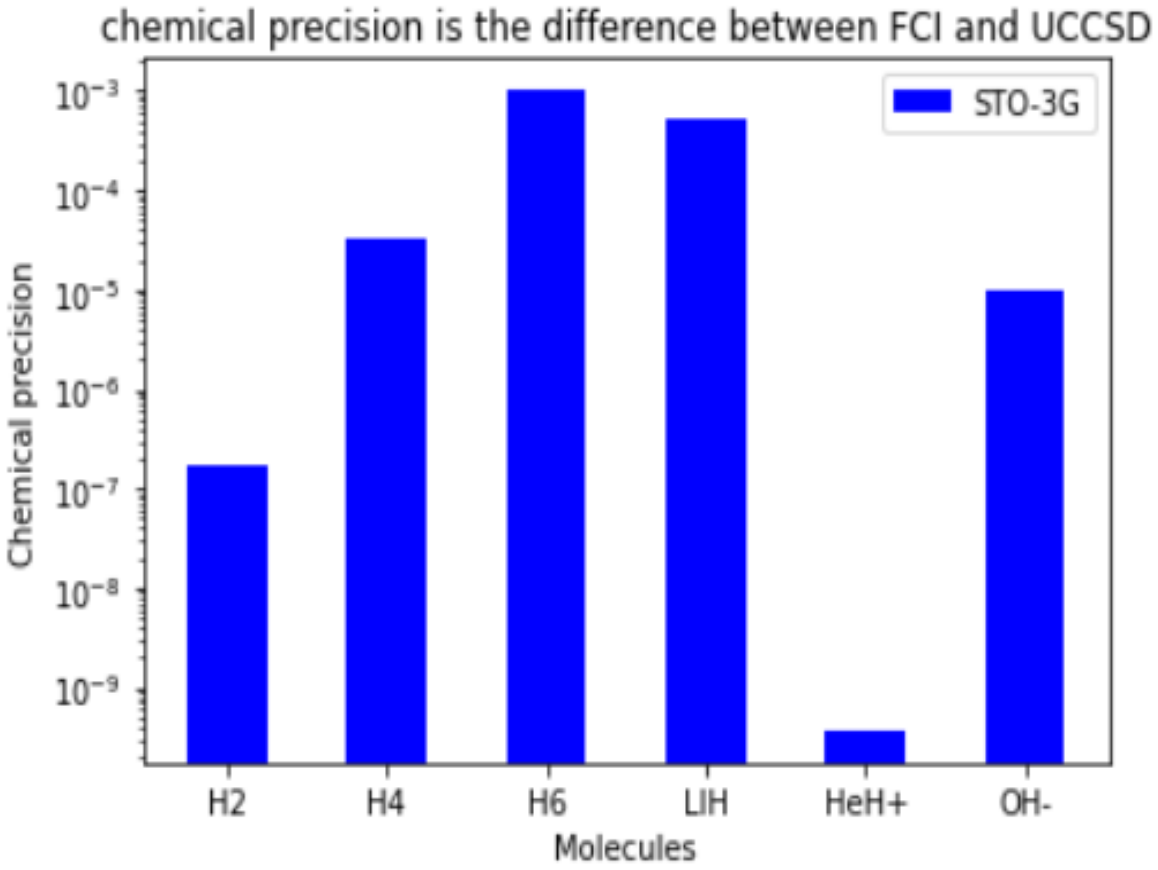
T1: qubit lifetime
T2: qubit phase coherence

In the IBM: T1=T2=100μs

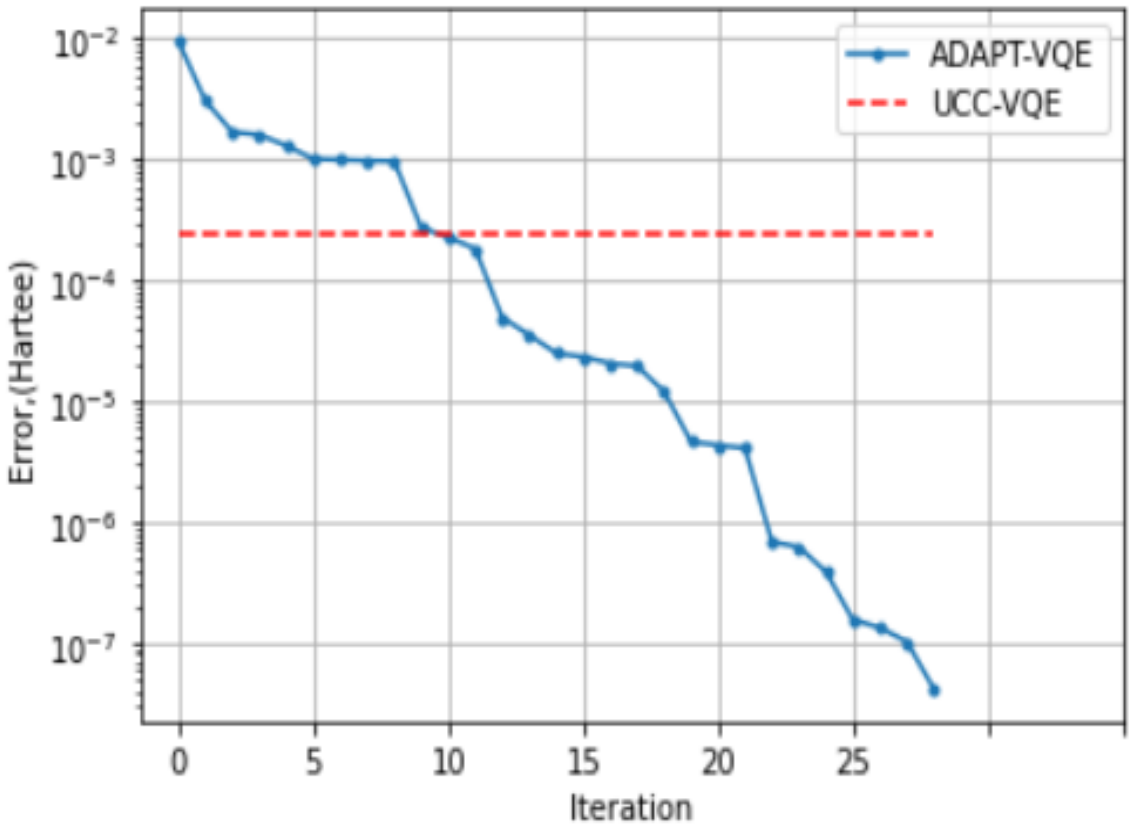
- **UCC is more affected by decoherence noise than measurement noise.**
- **Opposite behavior forHE**

- **QLM can be used to model noise: good noise model defined**

Chemical precision



LIH, STO-3G:
The difference between energy at each iteration and FCI



Chemical precision: we need better approaches

RESEARCH ARTICLE

Open Source Variational Quantum Eigensolver Extension of the Quantum Learning Machine (QLM) for Quantum Chemistry

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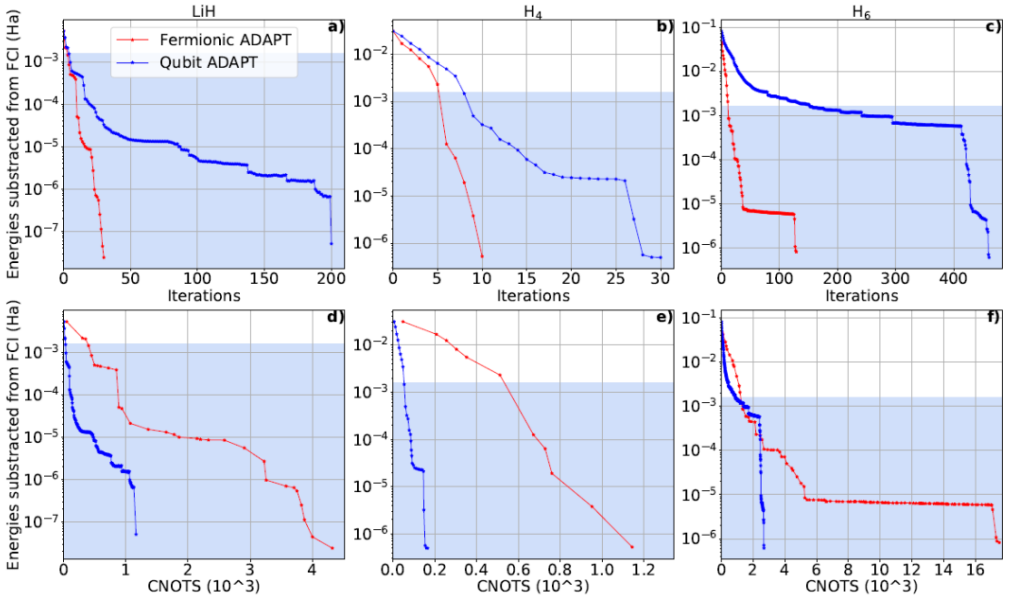
Abstract

Quantum Chemistry (QC) is one of the most promising applications of Quantum Computing. However, present quantum processing units (QPUs) are still subject to large errors. Therefore, noisy intermediate-scale quantum (NISQ) hardware is limited in terms of qubits counts and circuit depths. Specific algorithms such as Variational Quantum Eigensolvers (VQEs) can potentially overcome such issues. Here, we introduce a novel open-source QC package, denoted OpenVQE, providing tools for using and developing chemically-inspired adaptive methods derived from Unitary Coupled Cluster (UCC). It facilitates the development and testing of VQE algorithms. It is able to use the Atos Quantum Learning Machine (QLM), a general quantum programming framework enabling to write, optimize and simulate quantum computing programs. The QLM comes with a specific, freely available and open-source module, myQLM-fermion, that provides key tools to perform QC computations on a quantum computer (fermionic second quantization tools, UCC ansatz, etc). We give an extensive introduction to myQLM-fermion. Our package, OpenVQE, largely extends the QC capabilities of the QLM by providing: (i) the functions to generate the different types of excitations beyond the commonly used UCCSD ansatz; (ii) a new implementation of the "adaptive derivative assembled pseudo-Trotter method" (ADAPT-VQE), written in simple class structure python codes. Interoperability with other major quantum programming frameworks is ensured thanks to myQLM, which allows users to easily build their own code and execute it on existing QPUs such as IBM, Google, Rigetti or Microsoft, etc. The combined OpenVQE/myQLM-fermion libraries facilitate the implementation, testing and development of variational quantum algorithms, thus helping choose the best compromise to run QC computations on present quantum computers while offering the possibility to test large molecules. We provide extensive benchmarks for several molecules associated to qubit counts ranging from 4 up to 24 where we focus our work on reaching chemical accuracy, reducing the number of circuit gates and optimizing parameters and operators between "fixed-length" UCC and ADAPT-VQE ansatze.

Open-VQE: a new software coming on top of QLM
With nearly ALL available algorithms.

Associated to an open source version of QLM for Quantum chemistry: my-QLM fermion

https://arxiv.org/abs/2203.05275



Chemical precision: we need better approaches

RESEARCH ARTICLE

Open Source Variational Quantum Eigensolver Extension of the Quantum Learning Machine (QLM) for Quantum Chemistry

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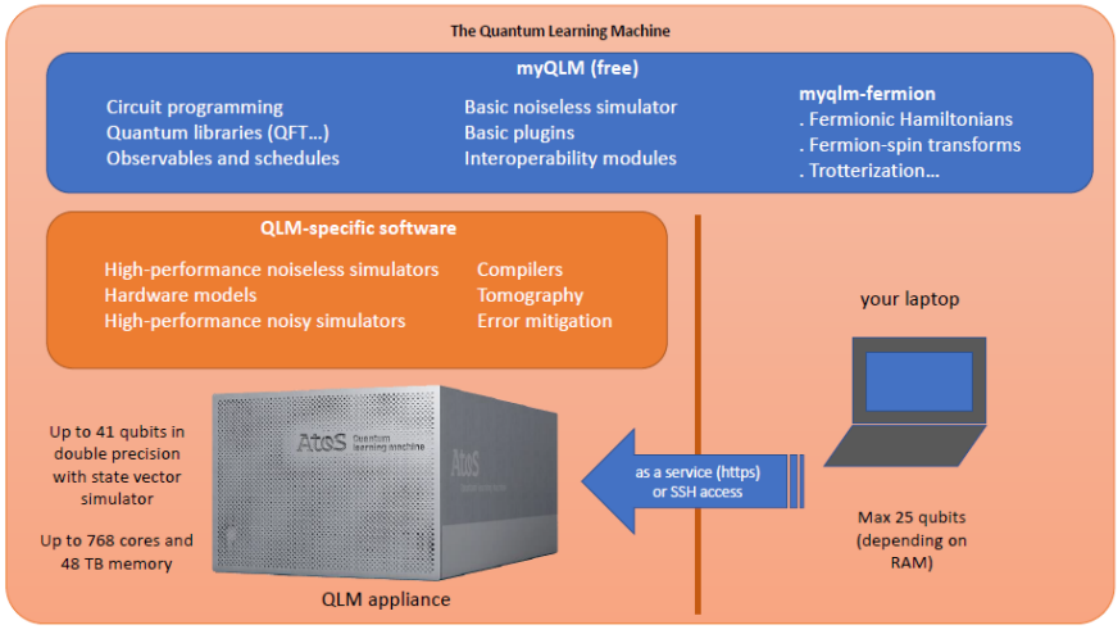
Abstract

Quantum Chemistry (QC) is one of the most promising applications of Quantum Computing. However, present quantum processing units (QPUs) are still subject to large errors. Therefore, noisy intermediate-scale quantum (NISQ) hardware is limited in terms of qubits counts and circuit depths. Specific algorithms such as Variational Quantum Eigensolvers (VQEs) can potentially overcome such issues. Here, we introduce a novel open-source QC package, denoted OpenVQE, providing tools for using and developing chemically-inspired adaptive methods derived from Unitary Coupled Cluster (UCC). It facilitates the development and testing of VQE algorithms. It is able to use the Atos Quantum Learning Machine (QLM), a general quantum programming framework enabling to write, optimize and simulate quantum computing programs. The QLM comes with a specific, freely available and open-source module, myQLM-fermion, that provides key tools to perform QC computations on a quantum computer (fermionic second quantization tools, UCC ansatz, etc). We give an extensive introduction to myQLM-fermion. Our package, OpenVQE, largely extends the QC capabilities of the QLM by providing: (i) the functions to generate the different types of excitations beyond the commonly used UCCSD ansatz; (ii) a new implementation of the "adaptive derivative assembled pseudo-Trotter method" (ADAPT-VQE), written in simple class structure python codes. Interoperability with other major quantum programming frameworks is ensured thanks to myQLM, which allows users to easily build their own code and execute it on existing QPUs such as IBM, Google, Rigetti or Microsoft, etc. The combined OpenVQE/myQLM-fermion libraries facilitate the implementation, testing and development of variational quantum algorithms, thus helping choose the best compromise to run QC computations on present quantum computers while offering the possibility to test large molecules. We provide extensive benchmarks for several molecules associated to qubit counts ranging from 4 up to 24 where we focus our work on reaching chemical accuracy, reducing the number of circuit gates and optimizing parameters and operators between "fixed-length" UCC and ADAPT-VQE ansatze.



Chemical precision: we need better approaches

RESEARCH ARTICLE

Open Source Variational Quantum Eigensolver Extension of the Quantum Learning Machine (QLM) for Quantum Chemistry

Mohammad Haidar*[1,2,3] | Marko J. Rančić[3] | Thomas Ayral[4] | Yvon Maday[2,5] | Jean-Philip Piquemal*[1]

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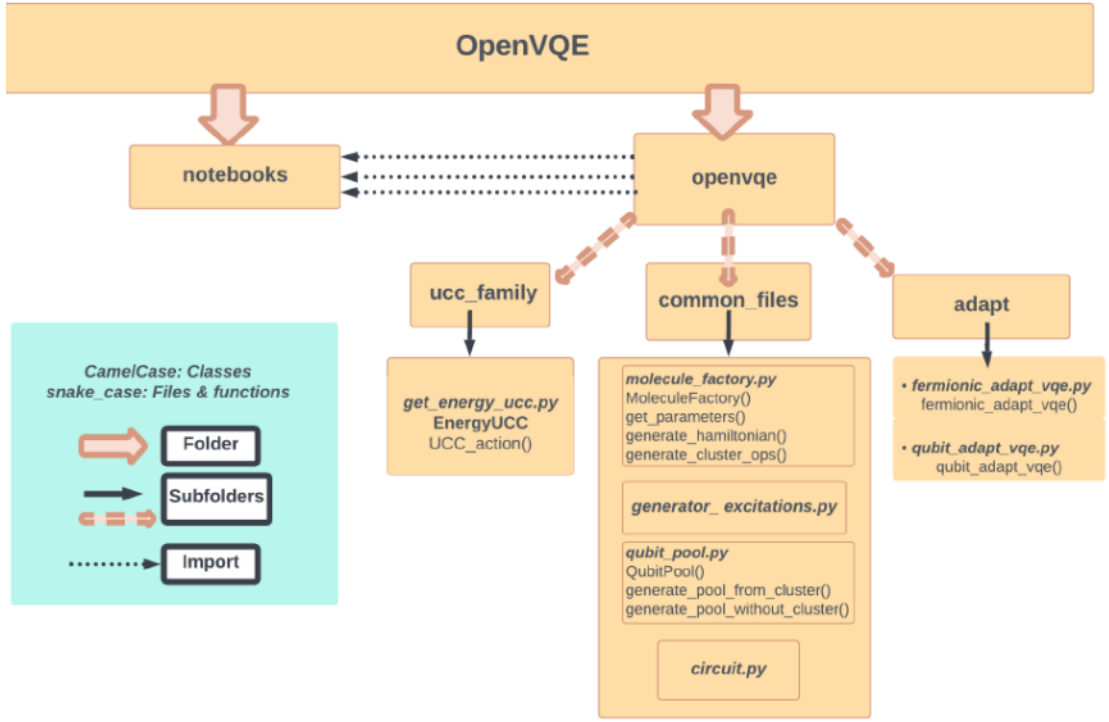

Flow chart of the OpenVQE package. The code is given in our Github repository and documentation[53]

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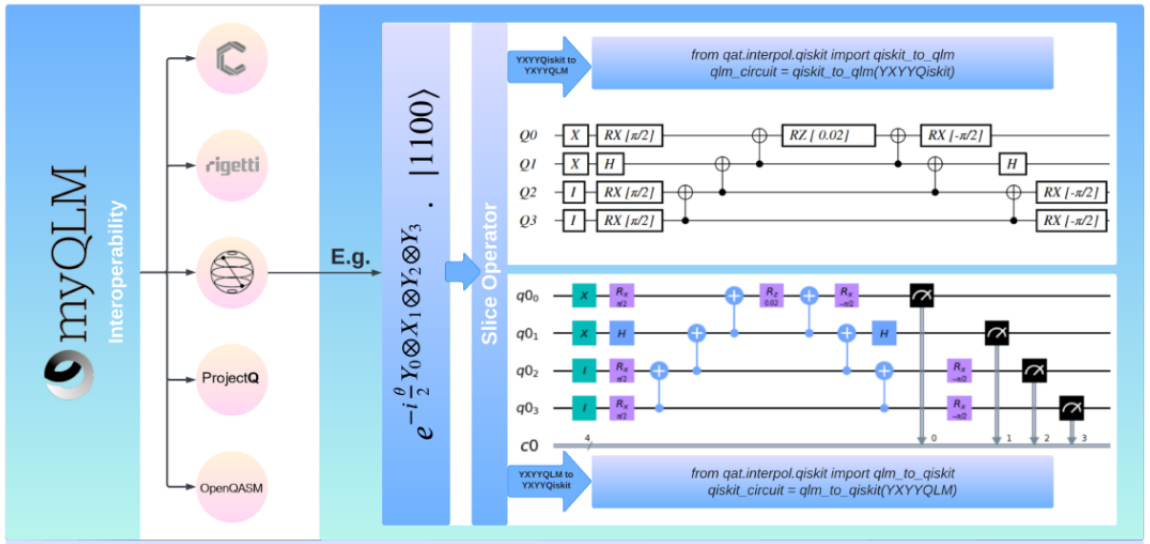

FrameWork		Qiskit	OpenQasm	PyQuit(no py 3.6)	Project Q	Cirq
Circuit translation	to QLM	Yes	Yes	Yes	Yes	Yes
	From QLM	Yes	No	Yes	No	Yes
QPU connection	to QLM	Yes	N/A	Yes	No	No
	From QLM	Yes		No	No	No

FIGURE B2 Interoperability packages with myQLM. YXYYQLM (top circuit) and YXYY (bottom circuit). These circuits consists of 4 qubits that represents $e^{Y_0\otimes X_1\otimes Y_2\otimes Y_3}|1100\rangle$ with θ is equal to 0.01.

Conclusion & Perspectives

Quantum Computing

- Better ansatze going beyong Adapt-VQE are required (essentially solved)
- More Qubit required to go to decent basis sets.
- Issues of noice on real machines (noise mitigations):

HARDWARE is overhyped and not OK for applications. Simulators Era.

- Overall, basics are there in term of theory. We should focus on software

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