Qubit PHARMACEUTICALS

How Short-Term Hybrid HPC-QC Can Accelerate Computational Chemistry

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We pioneer quantum-aided drug design to design novel molecules for complex targets

Started operations in Q2 - 2021

50+ team members in Paris & Boston

A portfolio of 6 drug discovery programs

A HPC-QC supercomputer 50pFlops AI & 30+ qubits

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QUANTONATION XAnge OMNES bpifrance i-Lab

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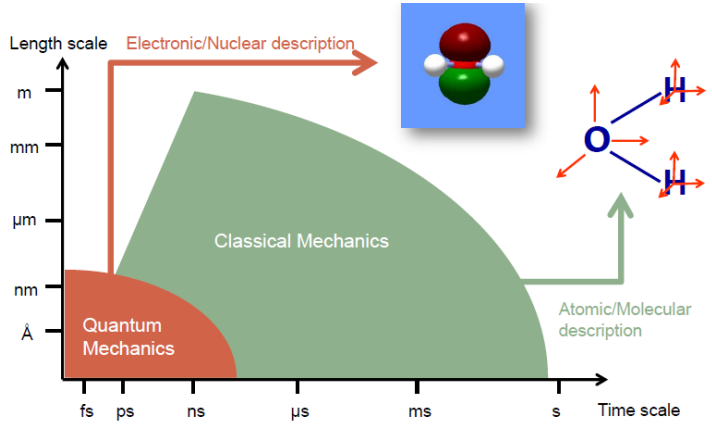
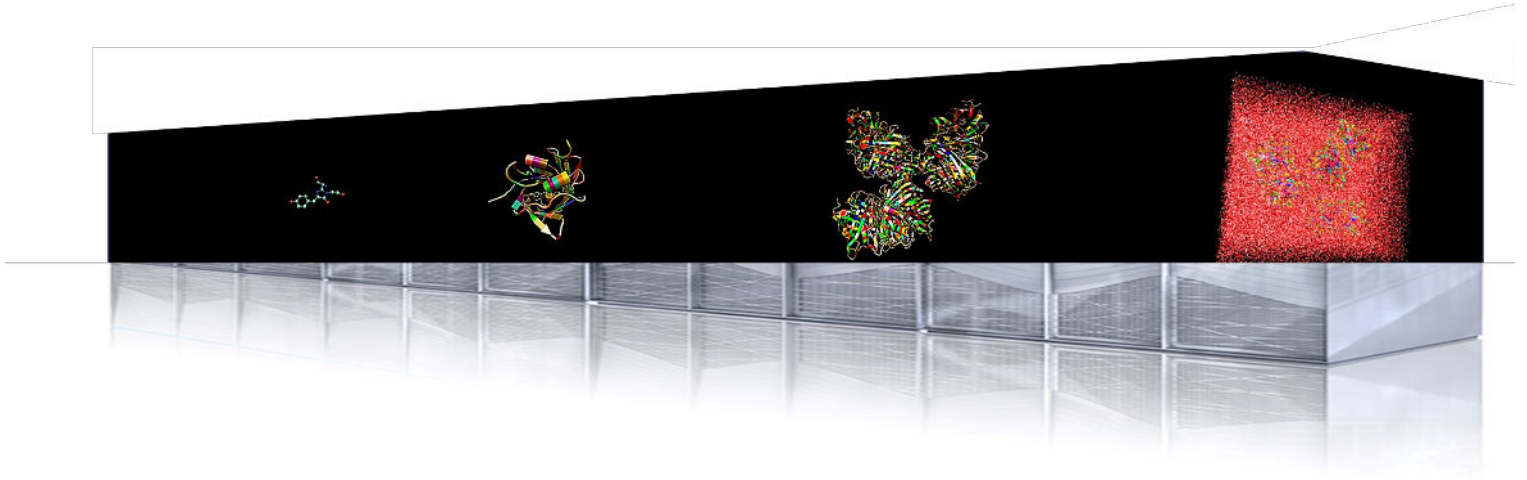
LA FRENCH TECH 2030

Computational Chemistry

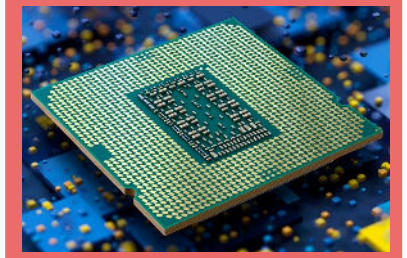
Computational chemistry (first pen and paper computation by London in 1927) is a branch of chemistry that uses computer simulation to assist in solving complex chemical problems. It exploits methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures, the interactions, and the properties of molecules.



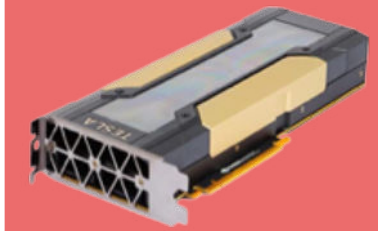


It requires to solve equations originating from quantum mechanics and statistical physics.

Computational Chemistry: the importance of hardware evolutions

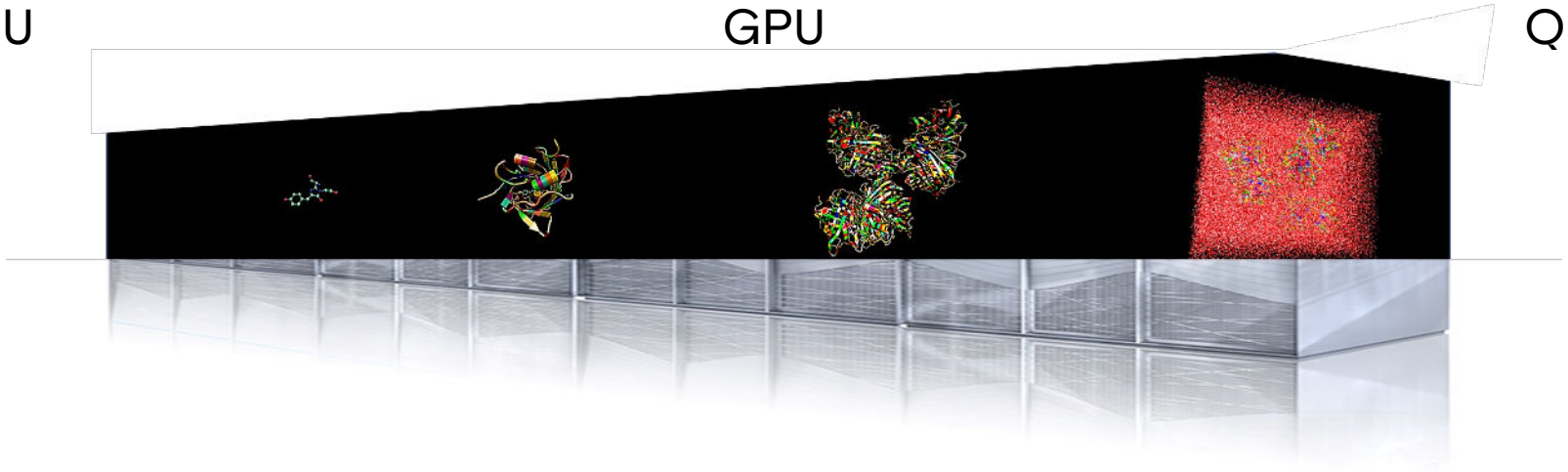


CPU



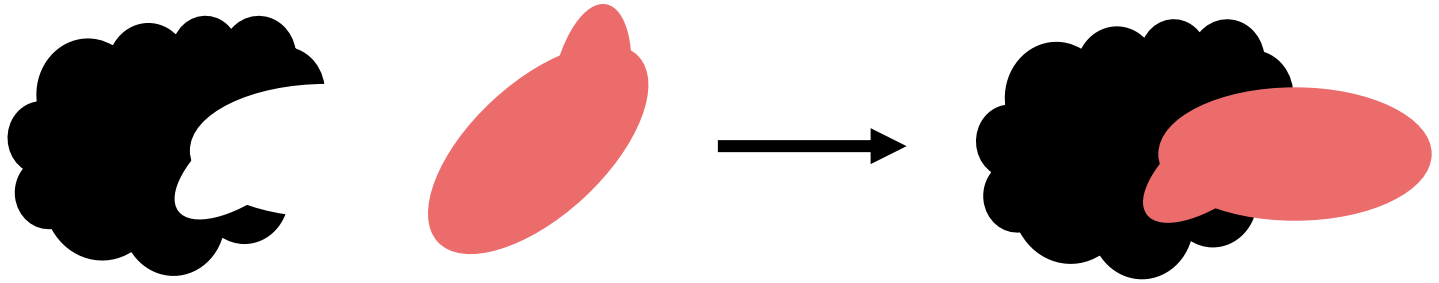
GPU

QPU

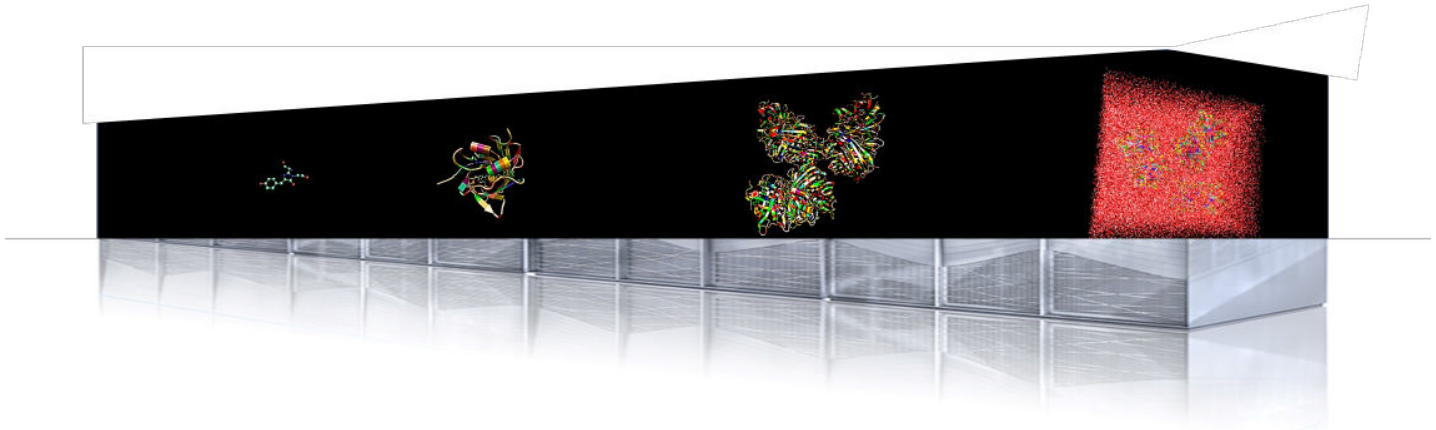


Computational Chemistry

Modeling drug-target interactions requires high precision



Chemical accuracy = 1kcal/mol (10^{-3} Hartree)



Computational Chemistry & Quantum Computing

- Quantum Chemistry: approximation of the time-independent Schrödinger equation (for small molecules)

$$-i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi \Rightarrow H\Psi = E\Psi$$

$$H = \sum_{i=1}^{n}\left[-\frac{h^2}{2m}\nabla_i^2 - \sum_{\alpha=1}^{N}\frac{Z_\alpha}{r_{i\alpha}}\right] + \sum_{j>i}\sum_{i=1}^{n}\frac{1}{r_{ij}}$$

$$H = \sum_{i=1}^{n} h(i) + \sum_{j>i}\sum_{i=1}^{n}\frac{1}{r_{ij}}$$

Computational Chemistry & Quantum Computing

- Quantum Chemistry: Hamiltonian of a molecule

$$\hat{\mathbf{H}} = \sum_{i}^{electrons} \frac{-\hbar^2}{2m_e}\nabla_i^2 + \sum_{A}^{nuclei} \frac{-\hbar^2}{2m_A}\nabla_A^2 + \sum_{i}^{electrons}\sum_{A}^{nuclei} \frac{-e^2 Z_A}{r_{iA}} + \sum_{i>j}^{electrons} \frac{e^2}{r_{ij}} + \sum_{A>B}^{nuclei} \frac{e^2 Z_A Z_B}{R_{AB}}$$

- kinetic energy of the electrons
- kinetic energy of the nuclei
- electrostatic interaction between the electrons and the nuclei
- electrostatic interaction between the electrons
- electrostatic interaction between the nuclei

Choice of the Ansatz & of the methodology

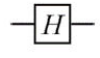
- Variational Quantum Eigensolver

  Heuristics. NISQ Friendly + FTQC.

- Quantum Phase Estimation (QPE)

  Proven quantum advantage. Requires FTQC.

Quantum Computing for Chemists

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

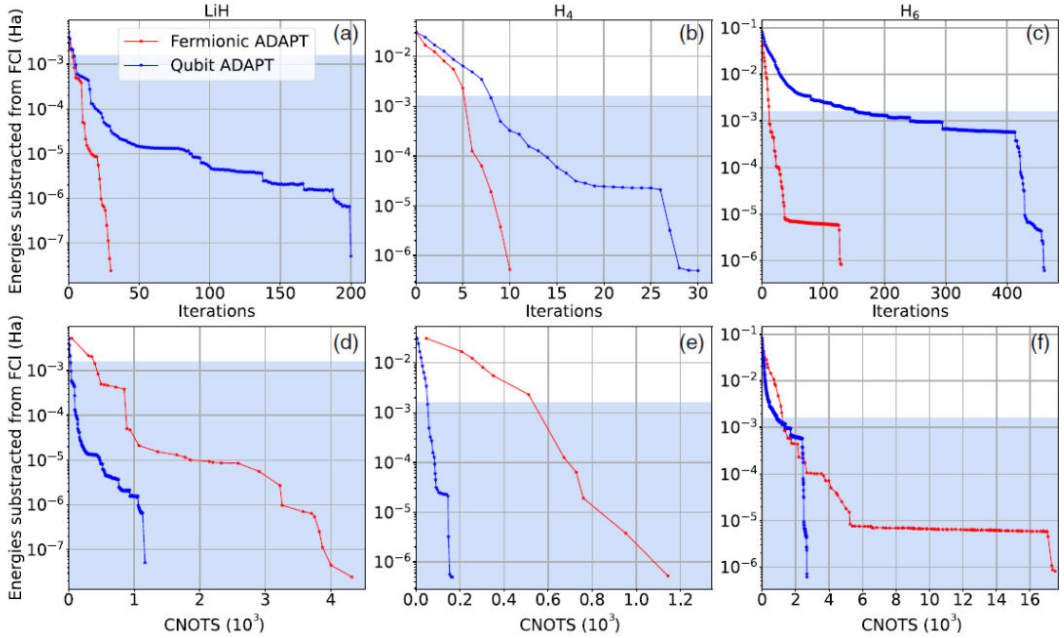
- Quantum computers do exist but limited availability (for now);
- Present applications on NISQ systems; FTQC yet to come;
- Quantum Gates programming on NISQ: number of physical qubits up to a few thousands but in practice…no practical (chemical) use beyond a certain limit due to noise;
- Analog machines (Pasqal) can deliver some useful algorithms;
- Quantum emulators (state vectors) available (Qiskit, QLM/Captiva, Hyperion-1..) are mandatory to test new algorithmics: they can simulate logical qubits.

- Quantum chemistry: 1(logical) qubit per spin-orbital is required

$$\hat{\mathbf{H}} = \sum_{i}^{electrons} \frac{-\hbar^2}{2m_e}\nabla_i^2 + \sum_{A}^{nuclei} \frac{-\hbar^2}{2m_A}\nabla_A^2 + \sum_{i}^{electrons}\sum_{A}^{nuclei} \frac{-e^2 Z_A}{r_{iA}} + \sum_{i>j}^{electrons} \frac{e^2}{r_{ij}} + \sum_{A>B}^{nuclei} \frac{e^2 Z_A Z_B}{R_{AB}}$$

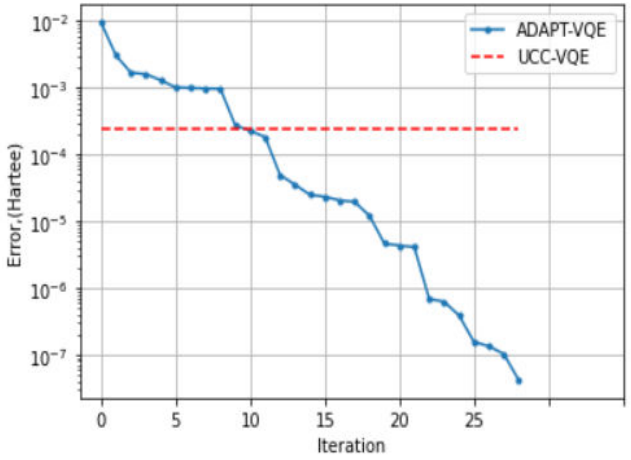
Present best in class method: ADAPT-VQE

- Goal: deal with strongly correlated systems with guaranteed « chemical » accuracy (1kcal/mol)



- Less C-NOT gates
- Less parameters
- Less iterations

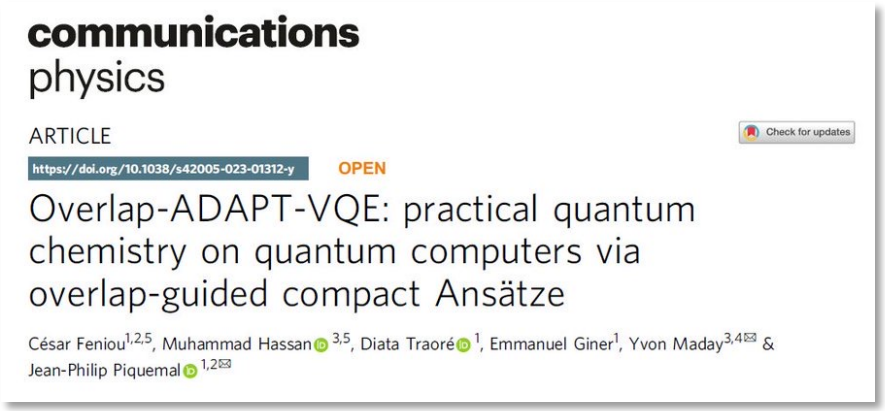
- Reduced circuit Depth

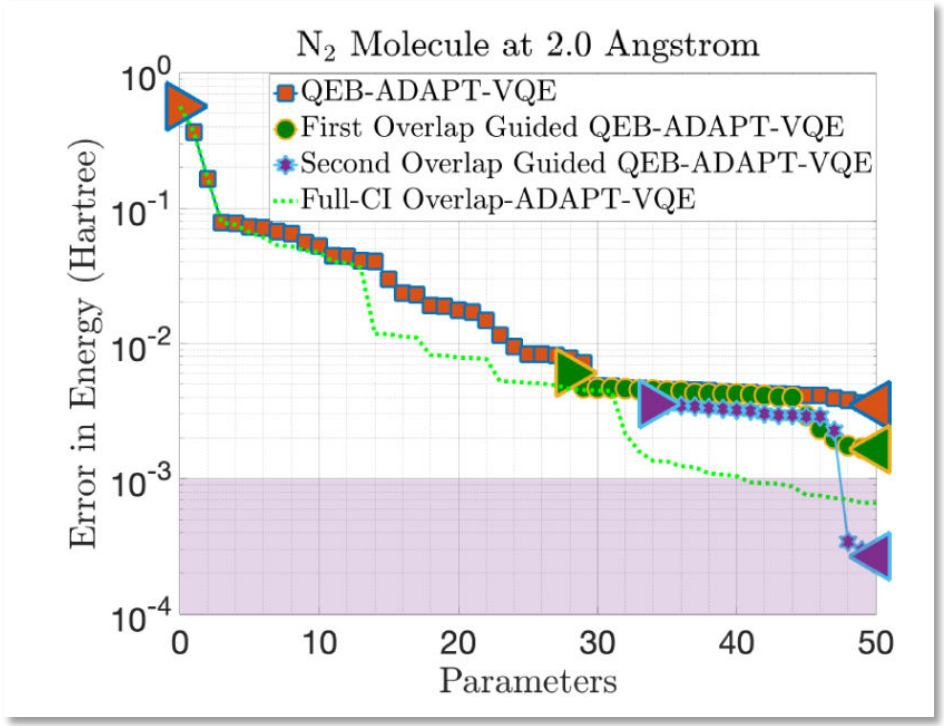


R. Grimsley, S. E. Economou, E. Barnes, and N. J.Mayhall, Nature Communications 10, 1 (2019).

Overcoming the ADAPT limitations going more hybrid: Overlap-ADAPT

- We can grow wave-functions by maximizing their **overlap** with any intermediate target **classical wave-function** that already captures some electronic correlation.
- By avoiding building the ansatz in the energy landscape strewn with local minima, the Overlap-ADAPT-VQE produces ultra-compact ansätze suitable for high-accuracy initializations of a new ADAPT procedure: **compression strategy suitable for barren plateaus.**





Hybrid Adaptive simulations on a Quantum Computer ?

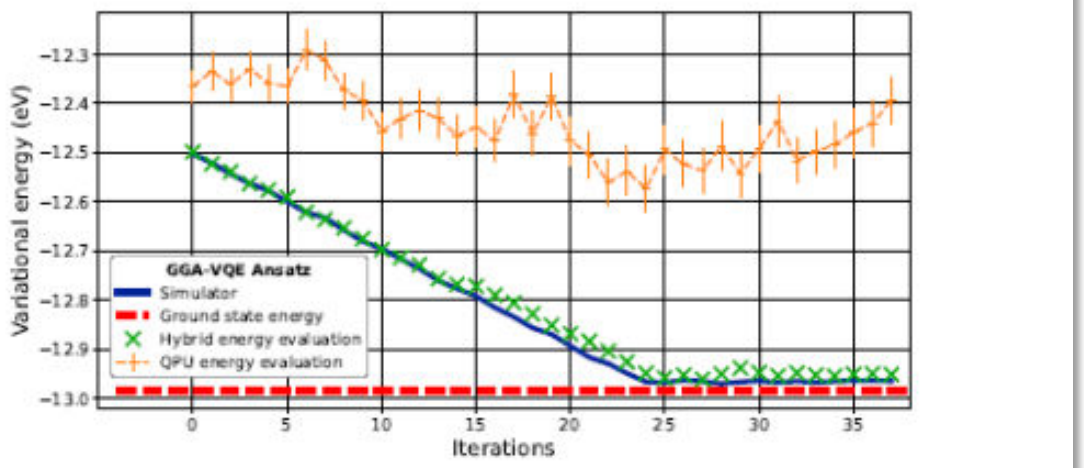
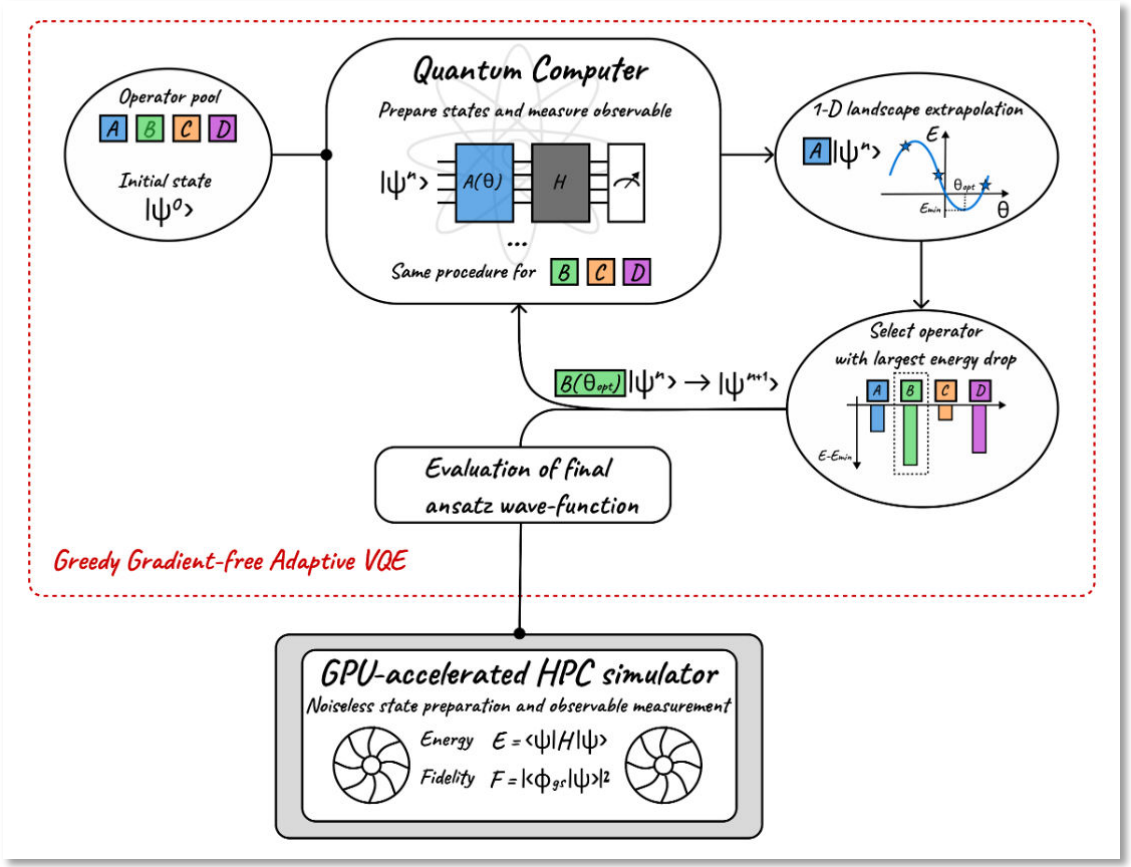


Figure 4. Energy convergence of the GGA-VQE algorithm with respect to the number of iterations. The blue reference curve denotes the energy of a classically simulated ansatz. The green and orange curves denote the hybrid and QPU energy evaluations of the GGA-VQE ansatz wave-function respectively. Note that the hybrid evaluation is carried out by retrieving the GGA-VQE ansatz wave-function generated by the QPU, re-implementing it on the Hyperion HPC simulator, and then evaluating the variational energy.



Greedy Gradient-free Adaptive Variational Quantum Algorithms on a Noisy Intermediate Scale Quantum Computer.
C. Feniou, B. Claudon, M. Hassan, A. Courtat, O. Adjoua, Y. Maday, J.-P. Piquemal, **2024**, in revision
DOI: 10.48550/arXiv.2306.17159

Is it a problem of machine or a problem of algorithms – or both?

ARTICLE OPEN

Check for updates

Quantifying the effect of gate errors on variational quantum eigensolvers for quantum chemistry

Kieran Dalton[1,2,3✉], Christopher K. Long[1,2], Yordan S. Yordanov[1,2], Charles G. Smith[1,2], Crispin H. W. Barnes[2], Normann Mertig[1] and David R. M. Arvidsson-Shukur[1]

Variational quantum eigensolvers (VQEs) are leading candidates to demonstrate near-term quantum advantage. Here, we conduct density-matrix simulations of leading gate-based VQEs for a range of molecules. We numerically quantify their level of tolerable depolarizing gate-errors. We find that: (i) The best-performing VQEs require gate-error probabilities between 10^{-6} and 10^{-4} (10^{-4} and 10^{-2} with error mitigation) to predict, within chemical accuracy, ground-state energies of small molecules with $4-14$ orbitals. (ii) ADAPT-VQEs that construct ansatz circuits iteratively outperform fixed-circuit VQEs. (iii) ADAPT-VQEs perform better with circuits constructed from gate-efficient rather than physically-motivated elements. (iv) The maximally-allowed gate-error probability, p_c, for any VQE to achieve chemical accuracy decreases with the number $N_{||}$ of noisy two-qubit gates as $p_c \propto N_{||}^{-1}$. Additionally, p_c decreases with system size, even with error mitigation, implying that larger molecules require even lower gate-errors. Thus, quantum advantage via gate-based VQEs is unlikely unless gate-error probabilities are decreased by orders of magnitude.

npj Quantum Information (2024)10:18 ; https://doi.org/10.1038/s41534-024-00808-x

Testing algorithms with high performance emulation

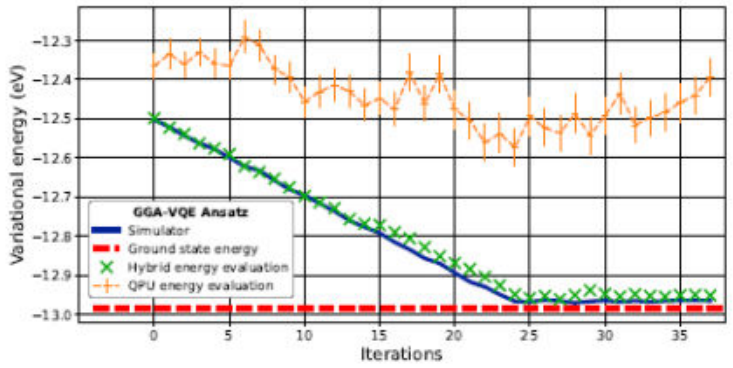
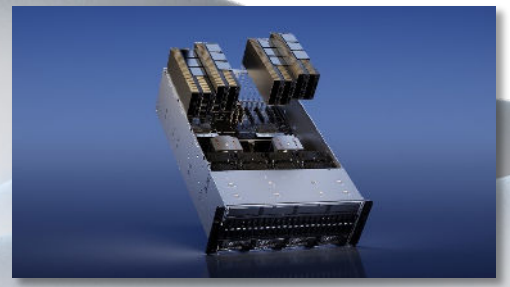


Figure 4. Energy convergence of the GGA-VQE algorithm with respect to the number of iterations. The blue reference curve denotes the energy of a classically simulated ansatz. The green and orange curves denote the hybrid and QPU energy evaluations of the GGA-VQE ansatz wave-function respectively. Note that the hybrid evaluation is carried out by retrieving the GGA-VQE ansatz wave-function generated by the QPU, re-implementing it on the Hyperion HPC simulator, and then evaluating the variational energy.



Exact simulations on Hyperion-1:

- Accelerated-state-vector emulator package
- multi-GPU (GPU=Graphics Processing Unit);
- fast custom CUDA/HIP-optimized sparse linear algebra libraries;
- Optimized to run fast using reasonable HPC ressources (< 16 nodes);
- A100/MI250X → H100/MI300X GPUs: time to solution divided by 2;
- Inclusion of noise.

High Performance Emulation: Hyperion-1

Exact simulations on Hyperion-1: exact means « equivalent » to N logical qubits.

What are the limits? Memory doubles at each qubits for state-vector

- 28-20 (exact) qubit per GPU compute node
- 40-42 (exact) in real life (128 nodes)

- 50 (exact) qubits on Jupiter/Jules Vernes exascale machine (not practical)
- 50-100 qubits (high fidelity) with tensor networks/MPS

- >200 « extrapolated » qubits with hybrid quantum schemes *: convergence to exact solutions for simple systems on a single GPU node: preparation of FTQC benchmarks

* D. Traore, O. Adjoua, C. Feniou, I.-M. Lygatsika, Y. Maday, E. Posenitskiy, J. Toulouse, E. Giner, J.-P. Piquemal, 2024

High Performance Emulation: Hyperion-1

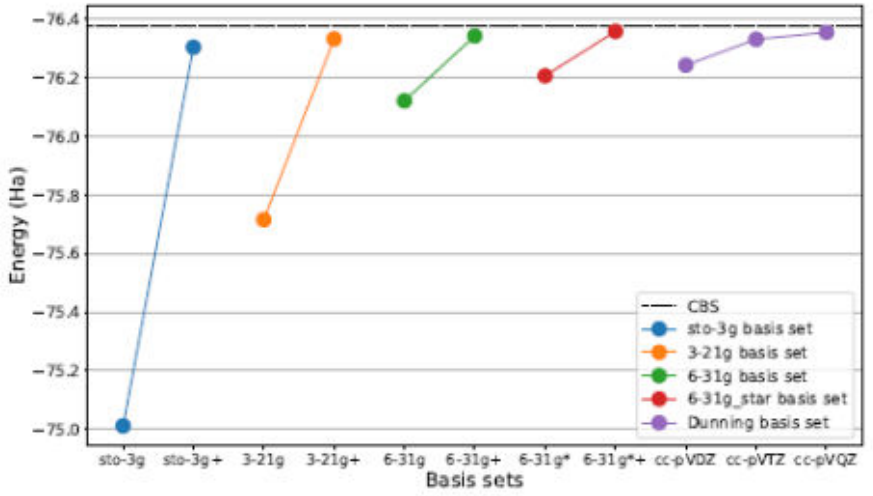


Figure 2: Ground-state energy of the H_2O molecule with different basis-sets. The $\mathcal{B}+$ indexes correspond to corrected energies with Equation (11) where $\mathcal{B}$ is STO-3G, 3-21G, 6-31g, or 6-31g*. The purple curve corresponds to the Dunning basis-set convergence curve to the CBS limit in dashed black line.

Exact simulations on Hyperion-1

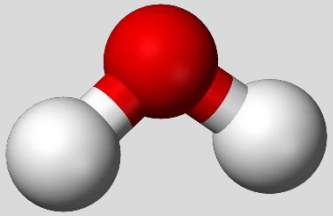
What are the limits?

- 40-42 (exact) in real life on pre-exascale machine
- 50 (exact) qubits of Jupiter/Jules Vernes exascale machine
- 50-100 qubits (high fidelity) with tensor networks/MPS

>200 « extrapolated » qubits with specific hybrid quantum schemes convergence to exact solutions for simple systems on a single node: preparation of FTQC benchmarks.

Applicable to real hardware: more qubits!

H_2O	n_{qubits}	FCI
STO-3G	12	-75.01250
pc-seg0	24	-75.90855
6-31G	24	-76.11995
cc-pVDZ	46	-76.24165
cc-pVTZ	114	-76.33250
cc-pVQZ	228	-76.35985
cc-pV5Z	400	-76.36877
CBS	-	-76.37812



More than 400 brut force logical qubits are required to model water!

* D. Traore, O. Adjoua, C. Feniou, I.-M. Lygatsika, Y. Maday, E. Posenitskiy, A. Peruzzo, J. Toulouse, E. Giner, J.-P. Piquemal, 2024

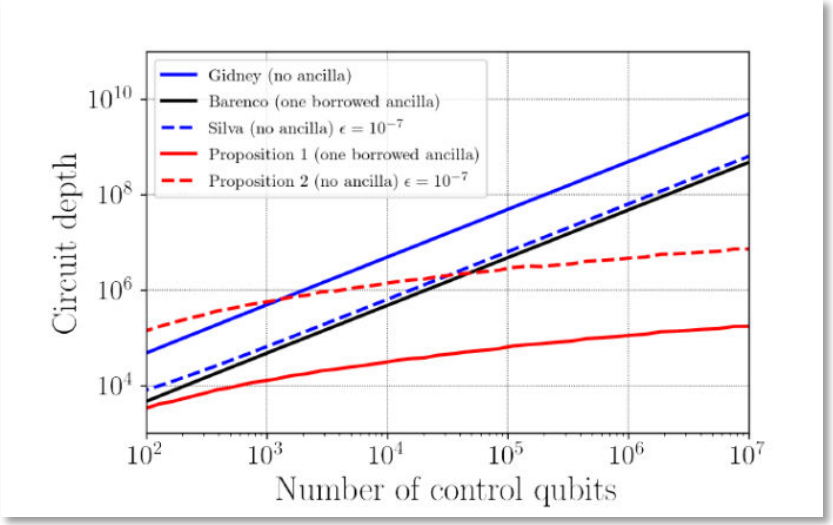
Algorithms and FTQC: Improvements

Polylogarithmic-depth controlled-NOT gates without ancilla qubits

Baptiste Claudon,[1] Julien Zylberman,[2] César Feniou,[1,3] Fabrice Debbasch,[4] Alberto Peruzzo,[1] and Jean-Philip Piquemal[1,3]

[1] *Qubit Pharmaceuticals, Advanced Research Department, 75014 Paris, France*
[2] *Sorbonne Université, Observatoire de Paris, Université PSL, CNRS, LERMA, 75005 Paris, France*
[3] *Sorbonne Université, LCT, UMR 7616 CNRS, 75005 Paris, France*
[4] *Sorbonne Université, Observatoire de Paris, Université PSL, CNRS, LERMA, 75005 Paris, France*

Controlled operations are fundamental building blocks of quantum algorithms. Decomposing n-control-NOT gates ($C^n(X)$) into arbitrary single-qubit and CNOT gates, is a crucial but non-trivial task. This study introduces $C^n(X)$ circuits outperforming previous methods in the asymptotic and non-asymptotic regimes. Three distinct decompositions are presented: an exact one using one borrowed ancilla with a circuit depth $\Theta\left(\log(n)^3\right)$, an approximating one without ancilla qubits with a circuit depth $\mathcal{O}\left(\log(n)^3 \log(1/\epsilon)\right)$ and an exact one with an adjustable-depth circuit which decreases with the number $m \leq n$ of ancilla qubits available as $\mathcal{O}\left(\log(n/\lfloor m/2 \rfloor)^3 + \log(\lfloor m/2 \rfloor)\right)$. The resulting exponential speedup is likely to have a substantial impact on fault-tolerant quantum computing by improving the complexities of countless quantum algorithms with applications ranging from quantum chemistry to physics, finance and quantum machine learning.



Improved QPE techniques for chemistry

arXiv:2312.13206 (2024), in review

Conclusion & Perspectives

Quantum Computing for Chemistry

- Better algorithms going beyond Adapt-VQE are required, emulators will help.
- More qubits required to get useful results in chemistry; Hyperion-1 is a first step in this direction with extrapolation schemes.
- Concerning the specific use case of quantum chemistry: concrete solutions using hybrid schemes that retain quantum features emerge and should pave the way to FTQC and possibly for improved NISQ platforms.
- **Quantum supremacy? Hundreds of real logical qubits for small systems are required but we have the benchmarks…**
- **Not all hardware are/will ve equivalent: algorithmic adaptations.**

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