High-Performance Computing, Quantum Computing, and AI in Chemistry and Materials Science

Taha Selim & Alain Chancé
MolKet SAS

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MolKet's Github repository: `https://github.com/molket-io/molket.jl`

Contents

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1 Bios

Alain Chancé, Président MolKet SAS

Alain Chancé is the Président of MolKet SAS and founder of Quantalain SASU and Alainquant LLC, bringing over 30 years of expertise in enterprise transformation, data management, and governance. A Qiskit® Advocate and IEEE Senior Member, he is a recognized leader in Quantum Computing and AI, with speaking engagements at prestigious events like JuliaCon 2024, WAICF 2024. He participated in the IBM Quantum Developer Conference. Alain co-authored Quantum Chemistry and Computing for the Curious, and holds an Ingénieur Civil des Mines (ICM) degree from École des Mines de Saint-Étienne, France.

Taha Selim, General Manager MolKet SAS

Taha Selim is the General Manager of MolKet SAS and a Lecturer and Quantum Education Officer at Amsterdam University of Applied Sciences. With a PhD in Theoretical and Computational Chemistry from Radboud University Nijmegen, his research spans quantum machine learning, physics-inspired AI for chemistry and materials, and quantum dynamics. A co-founder of iQafé, he organizes the Quantum AI Monthly Series with Bibliotheca Alexandrina and has delivered talks at events like JuliaCon 2024, APS March Meeting, and the Washington DC Quantum Computing Meetup. Taha's work has been featured in high-impact journals, and he holds advanced degrees in quantum physics, materials science, and business administration.

2 Introduction

Workflows integrating high-performance computing (HPC), today's quantum processing units (QPUs), and AI are used for real-world applications in the fields of quantum chemistry, quantum molecular dynamics, material sciences, machine learning, generative AI, high energy physics and more, before the emergence of large scale quantum computing (QC).

"AI's biggest breakthroughs won't come from chatbots—they will come from AI that models the physical world, not just language." — Jack Hidary, CEO of SandboxAQ [6].

"Software 2.0 is the future of AI. It is the new way of programming computers. Instead of writing code, you build a model. Instead of debugging code, you tune the model. Instead of testing code, you validate the model. This is the new way of programming computers.", — Jensen Huang, CEO of NVIDIA [4].

"As quantum technology advances, we can begin to consider quantum agents/machines that retrieve/store/process quantum information from experiment to learn about the world (using quantum sensors, quantum memory & quantum computers)." - Hsin-Yuan Huang (Robert) [13].

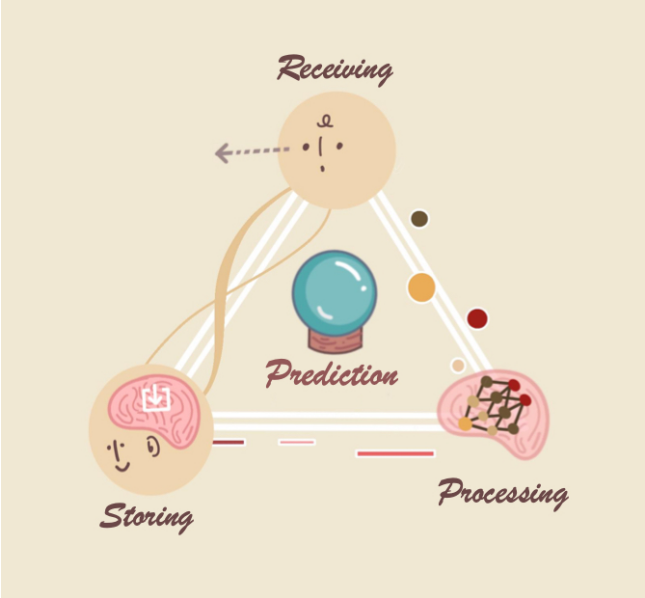

Figure 1: Quantum agents that retrieve/store/process quantum information to learn about the world. [12, 13].

Current state-of-the-art:

- **AI is able to invent new quantum computing algorithms**: for instance, a new protocol to create entanglement [14].
- **AI solves superbug mystery** in 48 hours – after it took scientists 10 years to crack [2, 3].
- **IBM quantum supercentric computing:** With IBM's Heron QPU and RIKEN's Fugaku supercomputer running Sample-based quantum diagonalization (SQD), an iron-sulfur cluster [4Fe-4S] can be modeled in just two hours compared to 3 million years on today's QPU alone. [5]
- **End-to-end simulations for chemistry:** A team from Microsoft Azure Quantum has demonstrated the first end-to-end integration of high-performance computing (HPC), reliable quantum computing, and AI in a case study on catalytic reactions producing chiral molecules. [7]

- **AI and AI Agents** in Quantum Chemistry Simulations [1].
- **Dynamic simulations of quantum processors**: NVIDIA's CUDA-Q, enhanced through collaboration with Google, enables rapid quantum processor simulations, cutting down computation times from weeks to minutes [10].
- **NVIDIA advances quantum algorithm design with GPTs**: The fusion of machine learning techniques with quantum computation to develop next-generation quantum algorithms [8, 9, 11]

3 Quantum chemistry and quantum molecular dynamics

Selim's PhD work provided ingredients to model CO_2 spectra coming from the James Webb Space Telescope (JWST).

Accurate simulations are performed with quantum chemistry and quantum molecular dynamics. It is quite challenging to simulate the spectra of large molecules, and the computational resources required HPC resources.

Simulating molecular collisions in a quantum molecular dynamics problem is a typical use case. Such simulation involves solving extensive number of coupled equations.

Typical quantum chemistry simulations workflow

- First, derive the theoretical model for the system of interest:
  - Match the size, symmetry, and complexity of the system to the theoretical model.
- Second, translate the theoretical model into a computational model:
  - Choose the appropriate basis set and method for the system of interest.
- Third, compute the molecular properties of interest:
  - choose the proper basis set,
  - rotational-vibrational wavefunctions,
  - potential energy surfaces,
  - energy levels,
  - the choice of the kernel in which the wavefunctions are computed and the solutions are performed.
- Fourth, analyze the results, and compare them to experimental data.

Computational complexity: scaling up the calculations to large systems is challenging and computationally expensive, and requires more resources.

Typical solutions: Using approximations, also may require extra theoretical work to validate the approximation, and certain administration of the code and the computations. Key points:

- It saves time,
- demanding less computational resources,

- and drawbacks:
  - the approximations may not be accurate,
  - no guarantee accurate or high quality results all the time,
  - may not be applicable to all systems.

Check out the following papers for more information: Selim et al.[16], [17], and Selim et al. [15].

4 Quantum AI in chemistry and materials:

Quantum simulations in chemistry and material design involves multi-step, complex calculations, and requires a lot of computational resources.

To optimize the simulation, typically, distributing the computations among CPUs, GPUs, and QPUs gives the best results. Hence, each part of the computation is done on the most suitable hardware. This is known now as hybrid quantum-classical computing.

5 Glossary

HPC: High-performance computing
QPUs: Quantum processing units
GPUs: Graphics processing units
JWST: James Webb Space Telescope
QML: Quantum machine learning
QMC: Quantum Monte Carlo
GPT: Generative Pre-trained Transformer
VQE: Variational Quantum Eigensolver
GQE: Generative Quantum Eigensolver

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