Qiskit Nature: Quantum algorithms for applications on the natural sciences domain

Max Rossmannek[1], Dariusz Lasecki[1], Pauline Ollitrault[1], Ivano Tavernelli[1], Panagiotis Barkoutsos[1, *]

[1]*IBM Quantum, IBM Research Europe - Zurich*

Organisers

Max Rossmannek, Msc
Quantum Applications Researcher, PhD Candidate
IBM Quantum, IBM Research - Zurich

Dariusz Lasecki, Msc
Software Engineer
IBM Quantum, IBM Research - Zurich

Pauline J. Ollitrault, PhD
Quantum Applications Researcher
IBM Quantum, IBM Research - Zurich

Ivano Tavernelli, PhD
Quantum Applications Researcher, IBM Quantum global leader for advanced algorithms for quantum simulations
IBM Quantum, IBM Research – Zurich

Panagiotis Kl. Barkoutsos, PhD *
Quantum Applications Researcher
IBM Quantum, IBM Research – Zurich

Abstract

Natural sciences provide some of the most promising applications for near term quantum computers. Problems arising in domains like quantum chemistry and physics are best described using quantum mechanical principles and the classical calculation can be computationally costly. Quantum computers provide a new framework that is naturally suited for such simulations. In the last decades, extensive research in the field of applications of near term noisy quantum computers allowed scientists to start simulating chemical and physical systems using variational algorithms (e.g. Variational Quantum Eigensolver - VQE). The need to educate researchers and scientists from the respective domains on how these algorithms will impact their research is of great importance. In this tutorial, we are providing insights from our research and demonstrate the use of the open-source package Qiskit Nature for the simulation of natural science applications. We will introduce the respective algorithms and highlight how the end user can program such applications. This tutorial will serve as the basis for people to investigate the practical effects of near-term quantum computers on the performance of simulations of problems in natural sciences.

Goals of the Workshop

In the domain of natural sciences there are a lot of promising applications for near term quantum computers. In this tutorial we will try to demonstrate the use of noisy quantum processors for the simulation of such applications. Given that chemistry and physics are some of the most elaborate domains for quantum simulations we will focus on presenting the different aspects required to make such a simulation. The attendees of this tutorial will benefit from the better understanding of the developments in this space and will be exposed to concepts and materials which they may not be familiar with.

To this end, we plan half of the first session as an introductory lecture on applications of near term quantum computers on the natural sciences domain. We also give an overview of the classical approaches as well as their evolution over time. In the other half of the first session, we want to discuss the variational algorithms and their particular components in more depth. We provide insights for algorithms and methods used for quantum simulation of chemical models and molecular systems and dive into the details of methods to reduce the resource requirements and how to eventually prepare and map the classical Hamiltonian to a qubit operator.

In the second session of the proposed tutorial we want to focus more on the code that allows for the implementation of the points discussed in the first session. Some of the elaborate schemes may be difficult to implement and use, but most of them are directly accessible via using the newly released Qiskit Nature module. We want to demonstrate how the user can abstract the problem without the need to implement the full workflow required by the variational algorithms using this open-source framework. Furthermore, we want to highlight the fact that this workflow can be manually implemented and provide details of the relevant parts and show how a user can utilise the different steps of these methods.

Our goal is for the attendees to be able to get a feeling of the resource requirements and the methods used for the implementation of practical problems arising in the natural sciences domains and be able to tackle them using the open source Qiskit Nature module.

Schedule of the Tutorial

02:00 PM - 03:30 PM (90 min): Introduction to Quantum Simulation Algorithms for Natural Sciences problems

- Introductory Talk related to the methods and algorithms used for quantum simulations of problems arising in natural sciences
- Introduction to Quantum Algorithms for Natural Sciences
- Extension of VQE Algorithm
- Future Perspective on Hybrid Quantum/Classical schemes
- Q&A and Material Review

15 min break

03:45 PM – 05:00 PM (75 min): Setting up natural sciences problems using Qiskit Nature

- Introduction to Qiskit Nature and the software design
- Details on Qiskit Nature Submodules
- Coding Up an application example
- Final Remarks and Qiskit Nature Roadmap

Prerequisites from Participants

Participants should be familiar with Python. Some familiarity with qiskit would be helpful, but not required. Documentation and tutorials related to Qiskit Nature can be found in https://qiskit.org/documentation/nature/tutorials/index.html