Applied Quantum Methods in Computational Science and Engineering – AQMCSE 2025
October 8–10, 2025, Aachen, Germany

A roadmap to Quantum Computational Fluid Dynamics

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Key Words: *Computational fluid dynamics (CFD), Quantum machine learning (QML), Physics-informed neural network (PINN), Phyiscs-informed quantum circuit (PIQC), Lattice Boltzmann method (LBM)*

ABSTRACT

1. Problem description and relevance (100-300 words)

The accurate simulation of turbulent compressible fluids is a major computational challenge for the aviation industry and possibly a key technology for improving the efficiency of future aircraft so that the ambitious climate targets can be achieved. Even though great progress has been made in the field of CFD in recent decades, and simulation software is available to a wide range of users from both commercial providers and research institutes, it still has two major shortcomings:

a) The accuracy of the results is usually limited by the quality of the turbulence models. Even very advanced turbulence models such as Reynolds-Stress models are not able to accurately reproduce a wide range of flows, in particular at the border of the flight envelope. For unseen test cases involving complex physical phenomena or unconventional aircraft configurations, selecting an appropriate turbulence model is often challenging and not straightforward.

b) In order to overcome the shortcomings resulting from turbulence modeling, scale-resolving methods such as large eddy simulations or even direct numerical simulations are increasingly being carried out. However, the cost of these simulations for flight Reynolds numbers is so high that even under very optimistic assumptions about the development of future HPC resources and advances in algorithms, full-aircraft simulations seem unrealistic.

Even though the possibilities for the use of quantum computers in CFD are still limited due to their current stage of development, they may offer the potential to accelerate calculations in such a way that scale-resolving methods for complete aircraft seem possible. Since algorithms that can be efficiently implemented on quantum computers for solving compressible nonlinear transport equations are also largely not yet available, the time is now to deal with them.

2. Methodology (100-300 words)

Funded by the DLR Quantum Computing Initiative (QCI), a three year project called "Towards Quantum Fluid Dynamics" was set up to investigate a wide variety of algorithmic approaches to harness the potential of quantum computers for applications from CFD. Since it is not yet foreseeable which algorithms for

solving compressible transport equations can be successfully implemented on a quantum computer, so that they also promise a quantum advantage, various approaches are being pursued within the framework of the project. The algorithms and activities investigated in the project include, for example,

- Physics-Informed Neural Networks [3, 2] and Physics-Informed Quantum Circuits [1]
- Quantum-inspired algorithms
- Quantum Newton's method [5] using the HHL [4] algorithm
- Quantum Lattice-Boltzmann method
- Use of real and simulated quantum hardware
- Investigation of error propagation in quantum hardware

3. Practical demonstration (100-300 words)

Finding out which parts of the algorithms can be successfully implemented on a quantum computer, also with the aim of achieving a corresponding acceleration, i.e. gaining a quantum advantage, is a core task of the activity, as is the question what equations / PDEs lend themselves best to be solved on a QC and what requirements the hardware needs to fulfill in terms of, e.g., number of qbits. As an example of one of the topics mentioned above, we mention here the close connection between PINNs and PIQCs [1]. Figure 1 illustrates how the neural network in a PINN can be replaced by a quantum circuit to perform the training. Examples that this approach is indeed suitable for solving differential equations are also given in [1].

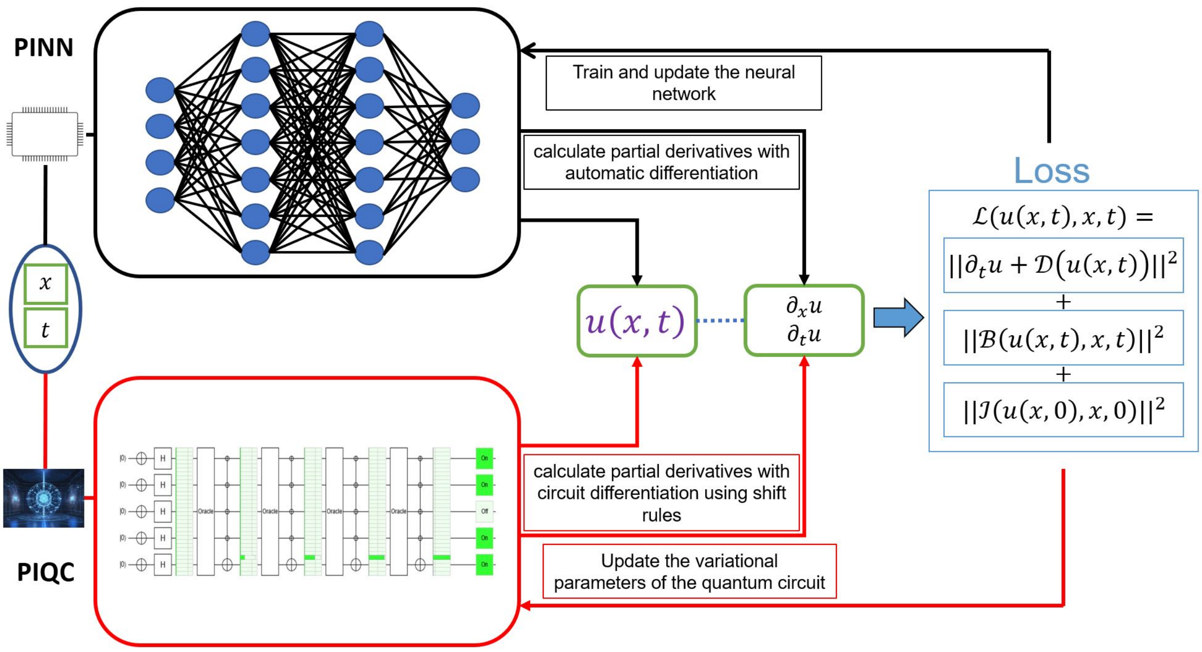

Figure 1. Schematic comparison of a PINN and a PIQC algorithm

4. Application potential (100-300 words)

The goal of the investigated methods is to show ways in which quantum computers can be used to solve nonlinear compressible transport equations, which are used to simulate viscous flows at high Reynolds numbers. In order to be able to assess whether a quantum advantage can actually be achieved compared to existing methods on classical hardware, the following questions will be discussed:

- Can we give a Classification if certain equations are better suited to solved on a quantum computer than others?
- Is it possible to efficiently implement time stepping methods on quantum computers?
- How does error propagation influence the results and is it possible to formulate requirements on the accuracy on the quantum hardware?
- How complex is the interaction between classical computers and quantum computers and how does the data transfer between them behave?
- Can we estimate the number of Qubits required for a complex 3-D industrial relevant simulation of an aircraft?

In order to use quantum computers profitably in the field of numerical simulation in future, the authors believe it will be important to identify the parts of the algorithms that promise a quantum advantage and combine them with the other parts as efficiently as possible.

Acknowledgment: This project was made possible by the DLR Quantum Computing Initiative and the Federal Ministry for Economic Affairs and Climate Action

We indicate our preference for a **poster** presentation.

For any further request, please contact the Conference Organizers:
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