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Strategies for the Application of Quantum Computers in Computational Fluid Dynamics

Stefan Görtz[a,*], Stefan Langer[a]

[a]German Aerospace Center (DLR), Institute of Aerodynamics and Flow Technology, Lilienthalplatz 7, 38108 Braunschweig, Germany

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ABSTRACT

A three-year DLR project entitled "Machine Learning and Quantum Computing – Digitalization of Aircraft Development 2.0", was established in spring 2021 with the goal to investigate whether and how high-fidelity aerodynamic simulations can be carried out using innovative methods from the field of machine learning and in which way these methods can also be implemented on quantum computers.

1. Introduction

The aviation industry faces the challenge of having to make significant contributions to achieving the ambitious global climate and environmental targets. To achieve this, future aircraft must consume significantly less fuel than today's or use more environmentally friendly engines, and also need to be quieter, especially during take-off and landing. In order to be able to assess these properties as early as possible in the development of a new aircraft, a very large number of computer simulations are required, which are barely feasible even on today's high-performance computers.

Accelerating these simulations, thanks to the use of quantum computers, promises to close this gap in the future. Unexpected characteristics of an aircraft that would only become evident later in flight testing can be uncovered in advance through a large number of scale-resolving simulations and remedied during the design process. As a vision, a complete flight from take-off to landing could be simulated on a quantum computer long before the real first flight, thus creating an accurate image of the aircraft and its environmental effects in advance. At DLR, these topics are addressed by the virtual product which has a central and important meaning in the context of the digitalization of aviation. The virtual product aims to comprehensively simulate and design aircraft in the computer. Its realization requires further development of modern methods and algorithms, which also have the potential to be implemented efficiently on hardware of the future, for example on quantum computers.

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*Corresponding author
stefan.goertz@dlr.de (S. Görtz); stefan.langer@dlr.de (S. Langer)
ORCID(s): 0009-0007-5379-785X (S. Görtz); - (S. Langer)

2. Content of the talk

Within this context, a three-year DLR project entitled "Machine Learning and Quantum Computing – Digitalization of Aircraft Development 2.0", was established in spring 2021 with the goal to investigate whether and how high-fidelity aerodynamic simulations can be carried out using innovative methods from the field of machine learning and in which way these methods can also be implemented on quantum computers.

2.1. PINNs and PIQCs

Among other things, novel simulation algorithms based on neural networks were being developed and applied to compressible fluid mechanics equations, such as the Euler equations [1, 2]. These so-called physics-informed neural networks (PINNs) can also be transferred to quantum computers, with certain adjustments, using physics-informed quantum circuits [3]. In contrast to established, classic methods, in which generally only a given, specific simulation can be carried out, this novel approach even opens up the possibility of integrating various parameters such as object shape or flow conditions as variables into the simulation. If a parameter-dependent solution is calculated, many different simulations can be carried out very efficiently by varying the parameters, demonstrated in Fig. 1. Physics-informed quantum circuits have so far only been applied to comparably simple differential equations, due to the computational effort required to simulate quantum computers. Nevertheless, these initial results look promising.

2.2. Correction of coarse grid results

Another research area of the project group dealt with the question of how machine learning can be used to improve the resolution of relatively imprecise simulation results that are based on relatively coarse discretizations, that is, a limited number of degrees of freedom corresponding to relatively

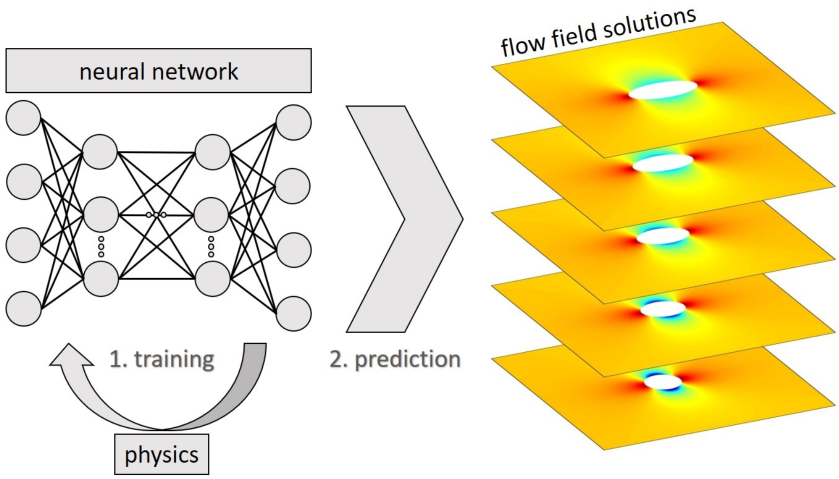

Figure 1: Physics-informed neural network for parametric prediction of compressible flow around a parameterized ellipse.

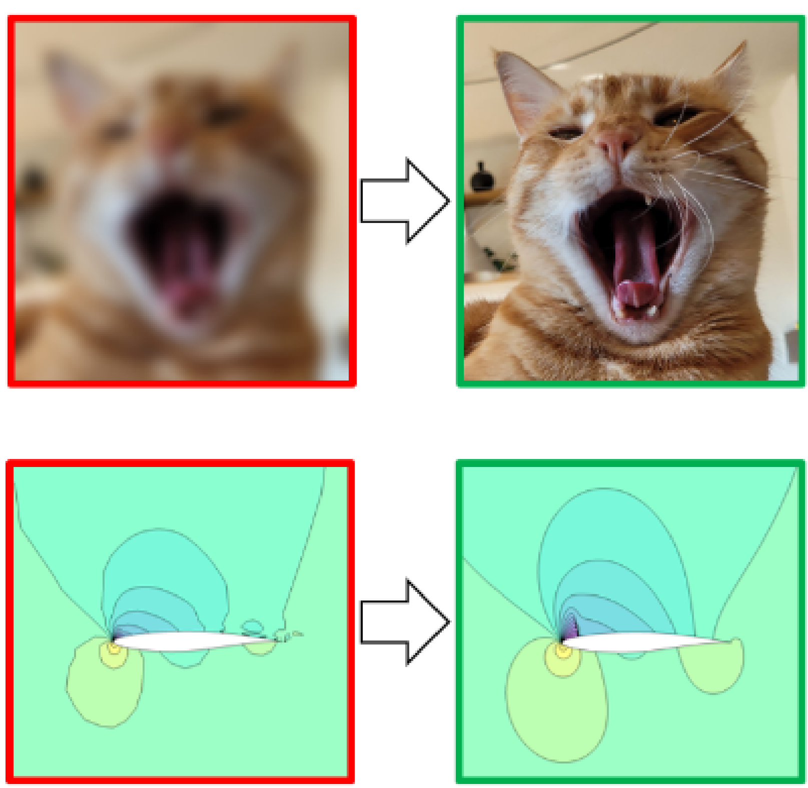

Figure 2: So-called "super-resolution problem" known from image processing (top), which inspires the correction of coarsely discretized flow simulations (bottom).

coarse grids. Well-known methods from image processing were used and adapted to enable corrections to flow simulations, as shown in Fig. 2. These methods open up the possibility of accelerating the still computationally very complex method for solving the Reynolds averaged Navier-Stokes equations. A reduction of this complex step, namely solving with a high number of degrees of freedom, is realized by carrying out a relatively inexpensive correction to a solution obtained by a reduced number of degrees of freedom, as a post-processing step [4, 5].

3. Conclusion

The work done in the project demonstrated that machine learning methods and in particular the use of neural networks can be applied to aerodynamically motivated problems. It was also possible to demonstrate ideas on how these methods can be used to apply novel technologies, such as quantum computers, for the simulation of compressible flows at high REYNOLDS numbers. Further investments and future work in this direction seem worthwhile to leverage the synergy effects of quantum computers and AI methods to make them accessible for industrial requirements.

The talk will give an overview of the key result of the project group, with a focus on topics that will be further investigated in the recently launched DLR Quantum-Computing Initiative project "Towards Quantum Fluid Dynamics" (ToQuaFlics), in particular quantum-inspired topics.

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