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Hybrid Newton Method with Quantum Linear System Solver for nonlinear Partial Differential Equations in CFD

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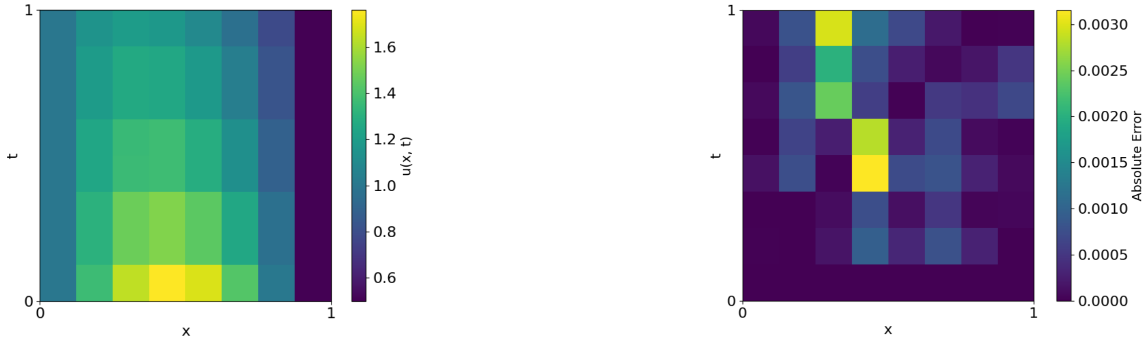
ABSTRACT

1. Problem description and relevance

Computational Fluid Dynamics (CFD) is an important, established tool in academia, research and industry for the simulation of flows. For high Reynolds number flows typically the Reynolds averaged Navier-Stokes (RANS) equations are solved in combination with a turbulence model. However, many years of experience in the use of this tool have shown that the accuracy of predictions decreases significantly, particularly at the borders of an aircraft's flight envelope, and that scale-resolving methods should be used. Unfortunately, even the most sophisticated algorithms coupled with powerful supercomputers cannot, in general, compute such a solution for a complete aircraft in an acceptable time. And, moreover, to further improve the aerodynamic performance of aircraft to reduce costs and fuel consumption, not just one, but a large number of such scale-resolving calculations would be necessary [1].
Most of the computational time comes from solving the high-dimensional, non-linear systems of the equations obtained after discretization. Typically, approaches closely related to Newton's method are used to approximate a solution [2, 3]. Then, the time required to solve the large-scale linear systems of equations, occurring in the iterative scheme, is a main contributor to the total runtime, exceeding classical capabilities [4].
To accelerate the procedure, we propose in which way a quantum linear system solver can support the classical Newton method to approximately solve the inner linear systems. The method and the obtained result show a potential use of Quantum Computers in the area of CFD, even when nonlinearities are present. This provides another promising application of Quantum Computers and presents a different approach of handling nonlinearities compared to Linearization methods, as for example the Carlemann Linearization [5]. The proposed method can be used in a wider context, to solve partial differential equations in a variety of areas.

2. Methodology

The proposed method combines a classical Newton method with a Quantum linear system solver to approximately solve partial differential equations. The combination of Newton's method or a variation of the method with a quantum linear solver was studied for machine learning [6, 7], electrical engineering [8] and even general sparse systems of nonlinear equations [9].
We implement a variant of the widely known HHL algorithm [10], based on [11], to handle a variety of linear systems with limited prior information regarding the system of equations. The implemented variant makes use of inverse-coefficient quantum state preparation [12] to approximate the conditional rotation in the original algorithm. The given circuit is using multiplication operators [13] and a routine



(a) Solution of the hybrid Quantum Newton Method

(b) Absolute Error of the hybrid Quantum Newton method compared to the classical method

Figure 1: First results of a practical demonstration of a hybrid quantum/classical approach to solve a nonlinear Diffusion equation with a Quantum Newton Method. The space and time are discretized into 8 grid points each.

to compare the size of two values saved in Quantum registers [14]. Different strategies to obtain the solution from the Quantum Computer for usage in the classical method are discussed with respect to loss of potential speed up, accuracy and scaling.

3. Practical demonstration

By applying the proposed method via a quantum simulator the hybrid methodology is showcased. For this we solve a nonlinear partial differential equation via an implicit Euler scheme, where each time step is solved via the hybrid Newton method. The problem is given by

$$\frac{\partial u}{\partial t} = \nabla(\alpha(u)\nabla u), \tag{1}$$

$$\text{where} \quad \alpha(u,x) = 0.4xu, \quad u(x,0) = 1 - \frac{1}{2}x + \sin(\pi x),$$

$$\text{and} \quad u(0,t) = 1,\, u(1,t) = 0.5.$$

Further, the implemented variation of the HHL algorithm is explained and tested on a variety of linear systems to present numerical evidence of its performance. First results indicate that the method performs as expected and errors introduced due to the quantum algorithm do not result in infeasible solutions. As can be seen in Figure 1, the algorithm is comparable to the purely classical Newton method with respect to the final solution. Further numerical tests will be performed to provide more analysis of the error influence. Such results from an application case will be further supplemented with a theoretical analysis of the Quantum algorithm and the estimated resource cost for industrial relevant use-cases.

4. Application potential

The proposed method is applicable to a wide range of engineering problems, surpassing the area of computational fluid dynamics since it is capable of solving problems with high nonlinear behavior, while theoretically yielding runtime improvements for certain sizes of problems. The current scaling of the method is mostly limited by access to hardware of sufficient size and limited error bounds. The communication of the classical system with a chosen quantum hardware is crucial for this method and is part of further studies. Current estimations imply that the number of logical qubits for industry relevant cases with acceptable error bounds does not exceed 400 qubits. Here, one should note that in order to make the Quantum Phase Estimation (QPE) more applicable in practice, one might need to add ancilla qubits to reduce the depth of the final Quantum Circuit. Still, this hardware requirements seem realistic within a mid- to long-term time-frame enabling the use of Quantum Computation for CFD.

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Hereby, we indicate a strong preference for an oral presentation over a poster presentation.

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