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Quantum computing CFD simulations: state of the art

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Abstract. This document is meant to review and discuss the possible applications of Quantum computing in the area of computational fluid dynamics (CFD). A review of the current state-of-the-art of quantum computing applied to computational fluid dynamics has been carried out, highlining how the technology is promising but still in an early stage of development. Furthermore, within the approaches developed to solve CFD problems with the use of quantum algorithms and / or quantum computers, this article discusses a quantum algorithm approach, based on the Lattice Boltzmann Method and developed to the study of 2D flow around a cylinder, a model which can be related to several industrial problems and, in the future, modified to simulate the refrigeration cycle used in aeronautical environmental control systems (ECS). This preliminary code helped to highlight the inherent difficulties to implement a quantum algorithm but helped also to demonstrate the applicability of quantum computing.

Introduction

Quantum computing is a type of computation that harnesses the collective properties of quantum states, such as superposition, interference, and entanglement, to perform calculations [1]. The devices that perform quantum computations are known as quantum computers.

Quantum Computing is currently a very active field of study and development, with expected applications in various fields ranging from the classical computer science problem, like cryptography and search problem, to engineering application, like structural optimization [2] and mechanical dynamics [3], but additional applications in different fields have been identified and developed [4], also for pure financial investments [5].

Indeed, several approaches have been proposed for the solutions of CFD problems with the use of quantum algorithms and / or quantum computers, as summarized in [6], being the rationale of the development the estimated scalability of quantum computing [7] and the analogy between Navier Stokes equations (NSE) with the Schrödinger equation through the Madelung transform, i.e., the Hydrodynamic Schrödinger equation (HSE) [8].

Known methodologies review and related works.

Basically, three approaches can be envisioned to solve fluid mechanics problems, namely the algorithmic approach, in which is focused on the development of numerical algorithms to be run on quantum computers, the analog approach, which can be described as the "design" of a quantum mechanical system able to "mimic" the fluid mechanic problem, and, last and not least, the development of machine learning codes for quantum computer.

An example of the "algorithmic" or "circuital" approach, implicitly demonstrating the applicability of quantum computing to the classical computational fluid dynamics equations despite the inherent complexity of these equations [7], is the resolution of classical Navier-Stokes equations for a typical De Laval nozzle, described by Gaitan [9].

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Another examples of the algorithmic approach are the solution of the vortex-in-the-cell method in a parallel environment by Steijl and Barakos [10] or the solution of Collisionless Boltzmann Equations by Steijl and Todorova [11], which highlights how the streaming operations can be effectively implemented in a quantum circuit by the use of one of elementary quantum gate, i.e., the controlled NOT (shortly CNOT) logic gates, under the assumed periodic boundaries conditions.

It is worth to noting that the problem associated with a (classical) lattice gas can be equivalently solved with a quantum computer implementing the "analog" approach, i.e., the use of a lattice gas quantum computer in which quantum bits replace classical bit and are arranged in a lattice-based array [12], whereas the "streaming" operations are carried out by the quantum system evolution.

Contributions of present work.

To verify the applicability of quantum computer to industrial problem, a relatively simple fluid dynamic problem has been considered, i.e., the flow around a cylinder in a 2D domain, solved with a quantum algorithm based on a two dimensional approach on nine variables (streaming/collision directions), or D2Q9, configuration of the Lattice Boltzmann Method (see the following figure for the calculation mesh), extending the previous works with a non-rarified fluid and consequently including collisions.

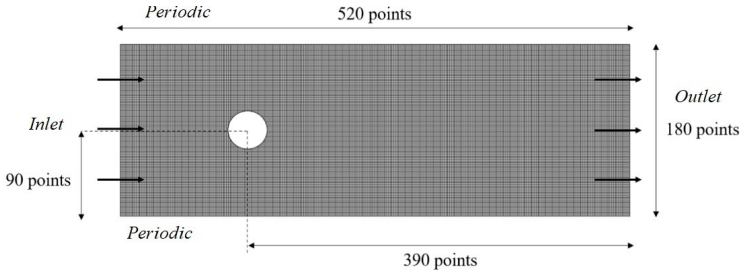

Figure 1 – Lattice mesh

The rationale of this selection is that flow around a cylinder is routinely used as benchmark problem for CFD algorithms because of the phenomena it exhibits but it is representative, in its simplicity, of many applications such as heat exchangers design or subsea pipeline assessment [13], as well as the modelling of porous media [14].

Indeed, the Lattice Boltzmann method has been considered due to the opportunity of extension of this study to porous media (as the filtering mesh used in aeronautical refrigerant system can be modelled) or to the refrigeration cycle itself (due to the presence of multiphase flow).

The flow is considered unsteady, incompressible, laminar, and with constant fluid properties. Inlet has been modelled imposing the flow velocity, whereas the outlet is a simple opening, with periodic boundary conditions on the upper and lower edge. The cylinder wall has been modeled with the bounce back technique to model the non-slip condition.

The equations regulating the flow can be summarized by the classical Lattice Boltzmann Equations with the BGK (Bhatnagar–Gross–Krook) approximation [15]:

$$f_k(\boldsymbol{x} + \Delta\boldsymbol{x}\,, t + \Delta t) = f_k(\boldsymbol{x}, t) \cdot (1 - \omega) + \omega \cdot f_k^{eq}(\boldsymbol{x}, t)$$

where **x** is the position vector, ω is the relaxation time, f_k is the particle distribution function, and f_k^{eq} is the local equilibrium distribution function defined as:

$$f_k^{eq}(x,t) \doteq w_k \cdot \rho(x,t) \cdot \left(1 + 3 \cdot \frac{\boldsymbol{c_k}\cdot\boldsymbol{u}}{c_s^2} + \frac{9}{2} \cdot \frac{(\boldsymbol{c_k}\cdot\boldsymbol{u})^2}{c_s^4} - \frac{3}{2} \cdot \frac{\boldsymbol{u}^2}{c_s^2}\right)$$

Where **u** is the particle velocity vector, w_k a weighting factor, while c_s is the isothermal speed of sound and $\mathbf{c_k}$ is the unitary velocity vector along the streamlines [15].

In the quantum algorithm, the equilibrium distribution function expression has been truncated to the first order terms respect the velocity to avoid non linearities for this first algorithm and rely only on linear operations, introducing an averaged expected velocity vector $\mathbf{u_0}$:

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$$f_k^{eq}(x,t) \simeq w_k \cdot \rho(x,t) \cdot \left(1 + 3 \cdot \frac{\boldsymbol{c_k} \cdot \boldsymbol{u}}{c_s^2} + \frac{9}{2} \cdot \frac{(\boldsymbol{c_k} \cdot \boldsymbol{u}) \cdot (\boldsymbol{c_k} \cdot \boldsymbol{u_0})}{c_s^4} - \frac{3}{2} \cdot \frac{\boldsymbol{u} \cdot \boldsymbol{u_0}}{c_s^2}\right)$$

The numerical expected error is quite small due to the range of velocity considered. Please note that the classical code has been implemented considering the full expression of the distribution function.

The full state of the quantum system is given by:

$$|\psi\rangle \equiv |a\rangle|F\rangle|y\rangle|x\rangle = |a_0 a_1 a_2\rangle|F_0 F_1 F_2 F_3 F_4\rangle|y_0 y_1 y_2\rangle|x_0 x_1 x_2 x_3\rangle$$

where $|a\rangle$, $|F\rangle$, $|y\rangle$, and $|x\rangle$ represent respectively the state vector relative to the ancilla qubits, the distribution function qubits, the macroscopic variables, and the spatial (*x,y*) coordinates.

The quantum algorithm has been developed and tested using the IBM's quantum computing software development framework *Qiskit* [16], and it can be generally discretized in five major steps [17]: initialization, collision, propagation, boundary condition implementation and, calculation of macroscopic quantities.

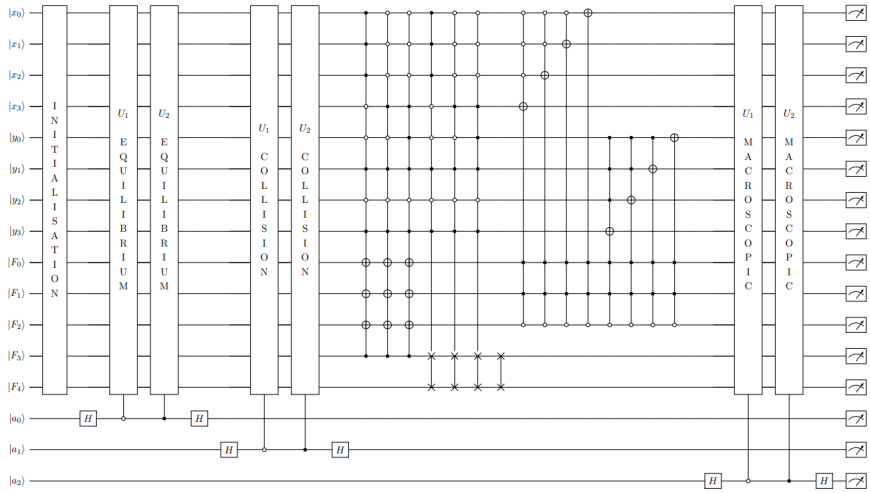

Figure 2 – Quantum algorithm scheme for the single iteration (simplified)

It is worth noting that, after one time step simulation is finished, it is necessary to re-initialize the quantum state for the next step. Indeed, classical programming tools like for-cycles or variables overwriting cannot be implemented into a quantum system.

Results, comparison, and validation

To assess the quantum algorithm, a verification of the implementation of the Lattice Boltzmann equations on classical computer has been carried for several Reynolds numbers, to verify the correctness of the underlying theoretical algorithm, retrieving not only the velocity and vorticity distribution but also evaluating the drag coefficient on the cylinder. Results are in accordance with available data from bibliography and results obtained through the solution of the classical Navier Stokes equations.

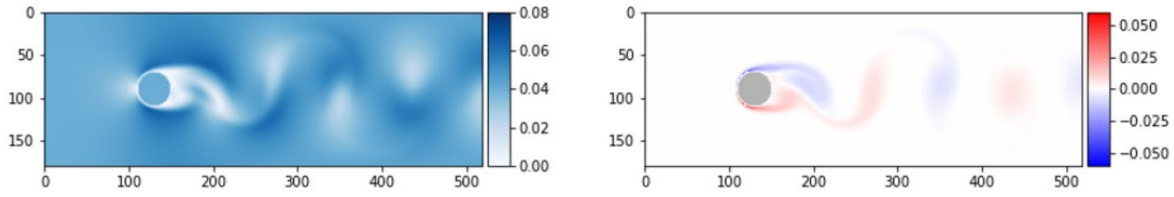

Figure 3 –Classical LBM algorithm results: velocity and vorticity profiles for R_E=1000

The quantum algorithm is still under investigation, but on-going preliminary results seem to be (at least qualitatively) in accordance with the results obtained at the previous step, even considering the strong simplification introduced by the linearization of equilibrium function.

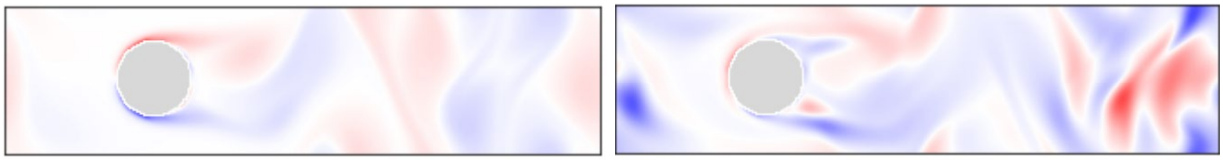

Figure 4 –Classical vs. quantum LBM algorithms results (vorticity)

Unfortunately, a significant drawback (beside the numerical error introduced by the linearization) is the time required to run the above-described algorithm, i.e., execute the algorithm on a quantum computer simulator, mainly due to the initialization and measurement process (roughly 2 minutes for iteration instead of few tenths of seconds for the classical algorithm) [18].

Conclusions

This paper summarized the three approaches that can be envisioned to solve fluid mechanics problems, namely the algorithmic o circuital approach, the analog or annealing approach and, finally, the machine learning applied to quantum computers.

A quantum algorithm for solving a classical two-dimensional fluid mechanic problem is introduced in the present work, based on the "translation" to a quantum computing framework of the numerical procedure known as Lattice Boltzmann method. The rationale of this choice is that the method shows similarities with the quantum operations themselves and it can be extended to multiphase flows and to complex geometrical domains, typical conditions of interesting industrial problems such as the modeling of aeronautical heat exchangers and in general, the refrigeration cycle of aircraft environmental control system.

Very preliminary results show that the quantum algorithm is able to achieve (even if under heavy mathematical simplifications) a result which is comparable with the results obtained with classically implemented Lattice Boltzmann codes, but the implementation shows the inherent difficulties to translate a classical code into a quantum framework (e.g., linearization, time required to simulate the quantum system on classical hardware) and the discrepancies due to the linearization.

Future steps include the implementation of nonlinear distribution function as well as the extension of algorithm to more sophisticated problem, including heat exchanges, also to confirm that the algorithm works fine even outside the range of unitary velocities. Furthermore, another aspect that requires a strong improvement is the numerical implementation in order to avoid the re-initialization of the code at each iteration, which is a major bottleneck in the current implementation.

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