A Quantum Annealing Approach to Fluid Dynamics Problems Solving Navier-Stokes Equations

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***Abstract*—Partial differential equations (PDEs) present important computational challenges in several scientific disciplines. Classical numerical methods, while effective, often encounter scalability issues and high computational costs, particularly for complex problems. Quantum computing seems to address these challenges, offering a potential exponential speedup over classical methods. The presented work studies the application of quantum computing, specifically Quantum Annealing, to the computational complexities inherent in solving the Navier-Stokes equations within Computational Fluid Dynamics (CFD). Our study examines the quantum annealing methodology, conducting two different experiments and analyzing the error between the simulation and the analytical solution. The results obtained demonstrate that quantum annealing paradigm can solve this problems and the errors obtained are acceptable in comparison with other methods in the state of the art. By combining theoretical insights with practical implementation, this research clarifies the potential of quantum annealing, providing a comprehensive overview of the simulation framework, analyzing the obtained results, and suggesting future research avenues.**

***Index Terms*—quantum annealing, computational fluid dynamics, Navier-Stokes equations, partial differential equations, numerical techniques**

I. Introduction

Partial Differential Equations (PDEs) are ubiquitous in various fields of science, such as: physics, engineering or even economy and finance. In many cases, finding a solution to these problems is challenging and requires advanced numerical techniques and high computational cost. The classical numerical methods for solving PDEs can be divided into local and global methods. Local approaches rely on discretization of the space of variables, with derivatives being approximated with numerical differentiation techniques [1]. Often a fine grid for multivariable functions is required to represent a solution qualitatively and quantitatively, leading to an increasing computational cost. Global methods represent the solution in terms of a suitable basis set [2]. This recasts the problem to finding optimal coefficients for a polynomial approximation of the sought function. Finding spectral solutions for complex problems may require large basis sets to achieve high accuracy, introducing difficulties when dealing deterministically with boundary conditions and leading again with an increasing computational cost.

Quantum computing is expected to produce a significant advantage with respect to these computational cost issues. In one of the earliest papers motivating the development of quantum computers [3], Feynman pointed out that such computers are better suited to simulate the dynamics of a quantum system than existing classical computers. Few years later, other works by Shor [4] and Grover [5] presented quantum algorithms that provide an exponential speedup over classical computers in general purpose tasks, setting a starting point to this relatively new discipline. After that, several quantum algorithms have been developed with the key feature of a theoretical exponential speedup, some of them proved and tested in the actual Noisy Intermediate-Scale Quantum (NISQ) [6] hardware.

Many important classical systems exist whose dynamics strongly couple many degrees of freedom over multiple length scales, making their simulation with classical computers hard. An example is a viscous fluid whose flows satisfy the Navier–Stokes (NS) nonlinear PDEs [7]. Solving these PDEs is the primary task for computational fluid dynamics (CFD) problems as in weather forecasting, aircraft design and determining the magneto-hydrodynamics of plasmas in space and in nuclear fusion reactors. In spite of its importance, little work has been done on finding quantum algorithms for the Navier–Stokes equations. The first known work is based on a quantum lattice-gas model [8]. Recently, new works on the topic have appeared based on different methods like variational quantum algorithms [9], quantum annealing [10] or the lattice Boltzman method [11].

In addition to CFD, the scope of several recent studies are the solution of general differential equations using several quantum computing techniques, such as differentiable quantum circuits [12], quantum annealing [13], variational quantum algorithms [14] or the HHL algorithm [15] and continuous versions of it [16]. We hypothesize that the current quantum algorithms are able to solve at least part of the Navier-Stokes equations, fitting well the exact solution and proving that this methodology can be used to solve CFD problems. Therefore, a corresponding set of studies testing their implementation

This research work is funded by Fundación Séneca and co-funded by Libelium LAB S.L. Región de Murcia (Spain), grant Nº 21681/EFPI/21, and the EIT Digital Predictive Analytics Development for Smart Cities and Business, grant 23368

in practical and concrete problems should follow. In this work, we aim to test the feasibility of using one of the current paradigms in quantum computing, known as Quantum Annealing, in solving the NS equations in some concrete scenarios, using the general method for differential equations presented by Criado and Spannowsky [13]. Unlike previous related work in this topic [10], based on local methods using finite differencing and time stepping, the approach used in this study is based on spectral methods, which avoid some potential issues like the need of repeated communications between a classical and a quantum computer.

This paper is organised as follows: in *Section* II, the methods to understand and replicate the work done are presented, reviewing the theoretical and experimental framework of quantum annealing and describing the followed process. Then, *Section* III shows the results of our concrete calculations, with their corresponding discussion in *Section* IV. Finally, *Section* V presents the conclusion of the paper and points possible future work.

II. Methodology

The computation of the problem was carried out using the quantum annealing paradigm in quantum computing. By the means of that, the set of Navier-Stokes equations need to be encoded as an optimization problem. The set of equations, which describe the dynamics of a viscous fluid, has the following expression:

$$\partial_t \rho + \nabla (\rho \vec{v}) = 0 \tag{1}$$

$$\partial_t (\rho \vec{v}) + \nabla \left(\rho v^2 + P - \tau\right) = 0 \tag{2}$$

$$\begin{aligned} &\partial_t \left[\rho \left(e + \frac{v^2}{2}\right)\right] \\ &+ \nabla \left[\rho \left(e + \frac{v^2}{2}\right) \vec{v} + P\vec{v} - \tau\vec{v} + \kappa \nabla T\right] = 0 \end{aligned} \tag{3}$$

where the unknown functions ρ, $\vec{v}$, P, e and T are the density, velocity, pressure, local internal energy and temperature of the fluid respectively. In addition, τ and κ are the viscous stress tensor and the thermal conductivity.

Once the encoding procedure is known, is time to use a quantum annealer to run the problem and obtain a solution. In the following subsections, a brief review om how a quantum annealer works is done, showing how to encode the system of PDEs in an understandable way for the device and explaining how to generate the solution in the practice.

A. Quantum Annealing

In the quantum annealing paradigm, firstly introduced by Benioff [17], the problem relies on finding the ground state of an Ising model Hamiltonian, exploiting pure quantum phenomena such as superposition of states, quantum entanglement and quantum tunneling [18]. Internally, the quantum annealing device has access to a quantum system that it partially controls. The system is described by a Hilbert space of N qubit spaces $\mathbb{C}^2$ and a Hamiltonian

$$\begin{aligned} H_{\text{Annealing}}(s) = A(s) \sum_i \sigma_x^{(i)} \\ + B(s) \left[\sum_{ij} J_{ij} \sigma_z^{(i)} \sigma_z^{(j)} + \sum_i h_i \sigma_z^{(i)}\right], \end{aligned} \tag{4}$$

with $\sigma_x^{(i)}$ being the x-Pauli matrix applied to the i^{th} qubit, and $A(s)$, $B(s)$ being the scheduled functions governing the annealing process satisfying $A(1) = B(0) = 0$. The J_{ij} and h_i factors are the interaction strengths between qubits and their on-site energy respectively. The annealer can set the values of J_{ij} and h_i, prepare the system in the ground state of $H_{\text{Annealing}}$ at $s = 0$, change the value of s continuously, and measure the observable $\bigotimes_{i=1}^{N} \sigma_z^{(i)}$ at the end of the annealing process, when $s = 1$.

The dependence $s(t)$ of the parameter s with time t is known as the schedule. A typical schedule is a monotonically increasing function from $s = 0$ at initial time to $s = 1$ at the final time, which can vary from few μs to about 1 ms. When an appropriate schedule is selected, the final measurement of the annealer is expected to return a sufficient low energy state of H. The annealing process is usually run several times, and the final state with the minimal solution is selected to reduce noise error.

B. Problem Encoding

In this subsection, the method described by Criado and Spannowsky [13] that allows to embed a set of differential equations in $H_{\text{Annealing}}$ is revisited for the better understanding of the reader. They start writing each equation of the NS system as a functional

$$\mathcal{F}_i(\vec{x}, t)\,[f_j]\,\Big|_{\mathcal{D}} = 0. \tag{5}$$

Where $\mathcal{F}_i$ (i = 1, ..., 5) are the corresponding functional of each equation acting on $f : \mathcal{D} \in \mathbb{R}^4 \to \mathbb{R}^7$, which is a vector function that contains the system functions (ρ, $\vec{v}$, P, e, T), while the domain of the variables where the solution of the equations is considered is $\mathcal{D}$. The reader should note that there are two more unknown functions than equations in the NS set, leading to and undetermined system. This can be easily fixed by two procedures, one is adding an Equation of State to the set, which would establish the relations $P(\rho, T)$ and $e(\rho, T)$, and the other is simply setting two of the functions to a fixed distribution, directly increasing the number of equations or reducing the number of unknowns in each case.

Imposing that the functionals are linear in f_j and its derivatives, it is possible to write them as

$$\mathcal{F}_i(\vec{x}, t)[f_j] = \sum_{jk} A_{ij}^{(k)}(\vec{x}, t) \cdot \partial^k f_j(\vec{x}, t) + B_i(\vec{x}, t)\,, \tag{6}$$

where $\partial^k f_j(\vec{x}, t)$ is a vector containing all the partial derivatives of order k of f_j, $A_{ij}^{(k)}(\vec{x}, t)$ are its corresponding coefficients and $B_i(\vec{x}, t)$ are the inhomogeneous terms.

As discussed before, the set of equation needs to be encoded as the ground state of an Ising Hamiltonian. To achieve that, it is necessary to formulate them as an optimization problem. For that, it is needed to discretize the variables domain into discrete subsets of points $\mathbf{D}_i \subset \mathcal{D}$ and define the following loss function:

$$\mathcal{L}[f] = \sum_i \sum_{\vec{x},t \in \mathbf{D}_i} \left(\mathcal{F}_i(\vec{x},t)[f] \right)^2 . \tag{7}$$

The global minimum $\mathcal{L}[f_{sol}]$ is only reached if all the equations are satisfied at all the sample points in the $\mathbf{D}_i$ sets.

Parametrizing now the functions f_n as a linear combination of a finite set of "basis" functions Φ_n, it is possible to write

$$f_j(\vec{x},t) = \sum_n w_{jn} \Phi_n(\vec{x},t) . \tag{8}$$

where w_{jn} are the weights of the basis functions for each initial function f_n. Then, expression (6) can be written as a linear function of the weights:

$$\mathcal{F}_i(\vec{x},t,w) = \sum_{jn} H_{ij}(\vec{x},t)[\Phi_n] \cdot w_{jn} + B_i(\vec{x},t) \tag{9}$$

$$H_{ij}(\vec{x},t)[\Phi_n] = \sum_k A_{ij}^{(k)}(\vec{x},t) \cdot \partial^k \Phi_n(\vec{x},t) , \tag{10}$$

and he loss function (7) becomes a quadratic function of them:

$$\mathcal{L}(w) = \sum_{jnpq} J_{jn,pq} w_{jn} w_{pq} + \sum_{jn} h_{jn} w_{jn} \tag{11}$$

where the new coefficients are

$$J_{jn,pq} = \sum_i \sum_{\vec{x},t \in \mathbf{D}_i} H_{ij}(\vec{x},t)[\Phi_n] H_{ip}(\vec{x},t)[\Phi_q] \tag{12}$$

$$h_{jn} = 2 \sum_i \sum_{\vec{x},t \in \mathbf{D}_i} H_{ij}(\vec{x},t)[\Phi_n] B_i(\vec{x},t) . \tag{13}$$

The last step remaining is the binary encoding of each weight in terms of the spin variables $\hat{w}_{jn}^{(\alpha)} = \pm 1$, as

$$w_{jn} = c_{jn} + s_{jn} \sum_{\alpha=1}^{n_{\text{spins}}} \frac{\hat{w}_{jn}^{(\alpha)}}{2^\alpha} , \tag{14}$$

with the free parameters c_{jn} and s_{jn} being the center and the scale values of each weight w_{jn}. Replacing this expression in (11), it is finally possible to get the form of the Ising Hamiltonian

$$H(\hat{w}) := \mathcal{L}(w) = \sum_{jnpq\alpha\beta} \hat{J}_{jn,pq}^{(\alpha\beta)} \hat{w}_{jn}^{(\alpha)} \hat{w}_{pq}^{(\beta)} + \sum_{jn\alpha} \hat{h}_{jn}^{(\alpha)} \hat{w}_{jn}^{(\alpha)} \tag{15}$$

where

$$\hat{J}_{jn,pq}^{(\alpha\beta)} = 2^{-(\alpha+\beta)} s_{jn} s_{pq} J_{jn,pq} \tag{16}$$

$$\hat{h}_{jn}^{(\alpha)} = 2^{-\alpha} s_{jn} (h_{jn} + 2 c_{pq} J_{jn,pq}) . \tag{17}$$

The original problem can then be solved by minimizing H (15) in a quantum annealing device. The solution is recovered by decoding the weights using (14) and substituting them in the linear decomposition (8) of the original functions.

C. Problem Description

For the simplicity of implementation, only the first equation of the NS set is considered (1), which is known as the continuity equation. Restricting us to that equation, it is needed to specify a velocity field $\vec{v}$ for being able to obtain a solution for the density ρ function.

Two different scenarios were selected to solve the equation, having two spatial coordinates and an additional one for time. In addition, the polar symmetry of the chosen velocity fields allowed to reduce the number of variables present in the PDE to the radius r and time t. For those cases, the proper form of the continuity equation is

$$\partial_t \rho + v_r \partial_r \rho + \frac{1}{r} \partial_r (r v_r) \rho = 0 , \tag{18}$$

where ∂_r is the partial derivative with respect the radius and v_r is the radial component of the velocity field. The domain of study used in both cases is $\mathcal{D} = \{(r,\theta,t) \in \mathbb{R}^3 : 0 \leq r \leq 1, 0 \leq \theta \leq 2\pi, 0 \leq t \leq 1\}$.

The first case considered was motivated by the work presented in [19], in which the authors used another quantum computing approach to solve a fluid dynamic problem related to submarine volcanic eruptions. In this scenario, a radial and constant function suits the velocity field

$$v_r = \lambda , \tag{19}$$

where λ is the constant value. Considering the medium surface density σ, satisfying $\rho(r,t) = \sigma(r,t) h(r)$ with the medium thickness being approximately $h(r) \simeq \frac{h_0}{r}$, and adding sink term $-w\sigma$, the authors arrived from (18) at the following PDE with its corresponding exact solution

$$\partial_t \sigma + \lambda \partial_r \sigma + \frac{w}{h_0} r \sigma = 0 \tag{20}$$

$$\sigma(r,t) = \sigma_0 \cdot e^{-kt} e^{-\frac{w}{2\lambda h_0} r^2 + \frac{k}{\lambda} r} . \tag{21}$$

where σ_0 and k are constants to be fixed by choosing some initial and boundary conditions. In our simulation, $\lambda = 5$, $w = 5$ and $h_0 = 0.1$ are set and conditions that impose $\sigma_0 = 1$ and $k = 2$ were chosen.

In the second case, a radial and linear velocity field was considered, which can be suited to any situation where a fluid is dragged in a circular motion with constant angular speed. The field for this case can be expressed as follows

$$v_r(r) = \omega r \tag{22}$$

where ω is the slope of the linear function. This choice, produces an exact solution from (18) given by

$$\rho(r,t) = \rho_0\, e^{-kt}\, r^{\frac{k-2\omega}{\omega}}\,, \tag{23}$$

where ρ_0 and k are again constants to be fixed by some conditions. In this simulation, $\omega = 1$ is set and conditions that impose $\rho_0 = 1$ and $k = 3$ were chosen, noting that $k - 2\omega \geq 0$ is needed to avoid divergences inside the domain of study.

It is worth mentioning that in both cases, the time interval was sliced in five equally spaced sub-intervals, in order to improve the tracking of the exponential behaviour. This procedure, allows to obtain better solutions for complex behaviours with a more simple set of basis functions.

D. Practical Computation

The results of our study, presented in the following section, were performed by a real quantum annealer. The problems were sent to a Quantum Processing Unit (QPU) provided by D-Wave Systems. Communication with their QPU is carried out via API through the D-Wave Leap environment [20]. The problems were formulated for the quantum annealing device using the *Qade* package in Python, presented also by Criado and Spannowsky in [13] and properly documented in [21]. To use this package to send the problem, one must only specify the space of variables, the differential equations with their corresponding initial or boundary conditions and some hyper-parameters related to the problem encoding and the quantum annealer execution. The values of the hyper-parameters need to be adjusted to suitable ones before application to a concrete problem, this can be achieved taking advantage of previous knowledge, such as which basis of functions is more suited or what are the expected size of the corresponding weights. When this knowledge is not available, the process involves some trial and error. In Table I, the values used that need to be specified and others which differs from default are collected.

III. Results

In this section, the results of the quantum simulations are presented. As explained in *Section* II-C, experiments in two different scenarios were conducted to validate our hypothesis: i) assuming a radial and constant velocity field and ii) assuming a radial and linear velocity field.

A. Radial and Constant Velocity Field

Fig. 1, shows the solution obtained using the quantum annealer compared to the analytical solution, while Fig. 2a displays a contour plot for the obtained radial profile for different times. Two different error metrics for the computed simulations are collected in Table II, the Mean Absolute Error (MAE) and the Root Mean Square Error (RMSE) for a given value of time. The full time evolution values were computed as the mean of MAE for all time steps and the root mean square of RMSE of all time steps respectively. The errors decrease over time as the value of the density does, since they are proportional to it. One should notice that the error committed in each run of the problem vary from one to another, since it is partially originated by the quantum nature of the annealer.

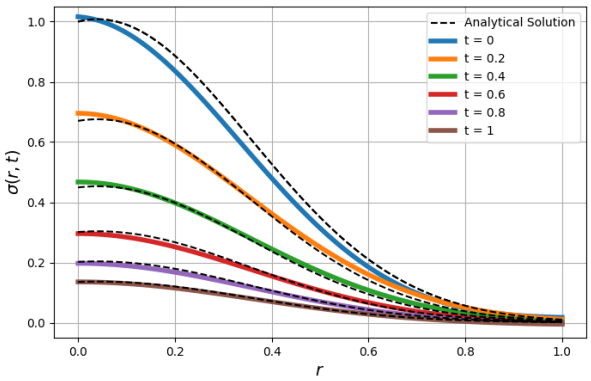


Fig. 1: Radial profile of the surface density for the case of a radial and constant velocity field for different times. Solutions obtained by the annealer are in color while exact are dashed.

B. Radial and Linear Velocity Field

For this case, Fig. 3 shows the solution obtained by the quantum annealer compared to the exact solution in a similar way as before, while Fig. 2b displays the corresponding contour plot. In Table III the same error metrics as in the previous case are collected. As in the previous experiment, the error values shows the same trend.

IV. Discussion

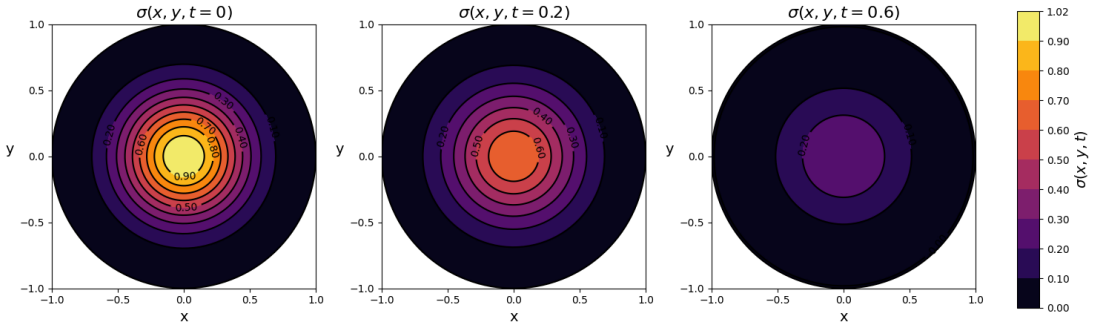
This papers aims to demonstrate that quantum algorithms could be suitable for solving CFD problems, opening a new research area with a wide range of applications in engineering, meteorology, air quality and smart cities. For this purpose, two

TABLE I: Problem Hyper-Parameters

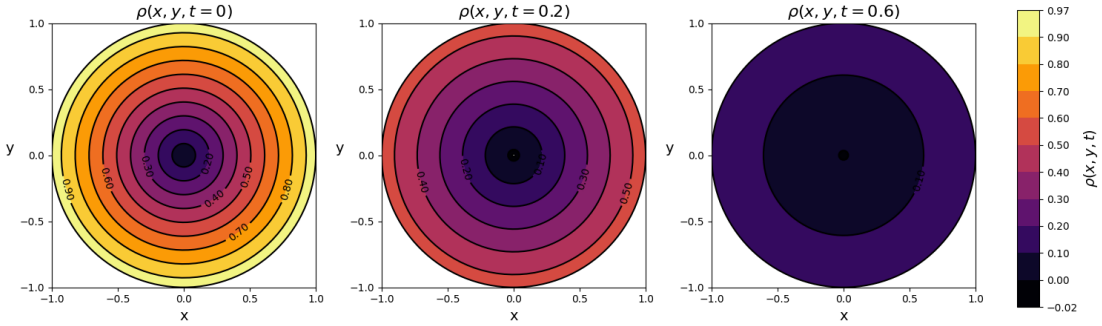
Symbol	Value	Description
Φ_n	gaussian, monomial	Function basis used in sections III-A and III-B, explained in [21]
$size\_per\_dim$	3, 2	Number of functions per input variable
num_reads	300	Number of runs performed by the quantum annealer
n_{spins}	5, 4	Number of spins used per weight (14)

TABLE II: Error Analysis Simulation I

Time Value	Mean Absolute Error	Root Mean Square Error
0	0.0269	0.0326
0.2	0.0104	0.0122
0.4	0.0082	0.0102
0.6	0.0060	0.0079
0.8	0.0049	0.0063
1	0.0030	0.0036
Full Time Solution	0.0099	0.0154



(a) Surface density distribution for the constant velocity field.



(b) Density distribution for the linear velocity field.

Fig. 2: Contour plots of the density distribution obtained by quantum annealing in Cartesian coordinates. Each row corresponds to the described scenarios while each column corresponds to a concrete value of time.

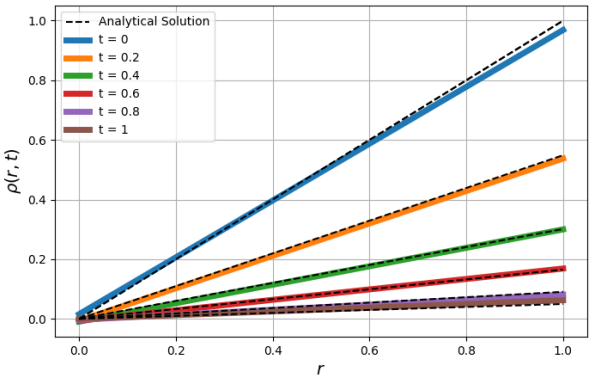


Fig. 3: Radial profile of the density function for the case of a radial and linear velocity field for different times. Solutions obtained by the annealer are in color while exact ones are dashed.

experiments were conducted to find out if quantum annealing can solve the Navier-Stokes equation.

Regarding the presented results, in which the proposed experiments are solved, it is possible to state that quantum annealing can be actually used to solve fluid dynamics problems in some concrete scenarios and conclude that the hypothesis

TABLE III: Error Analysis Simulation II

Time Value	Mean Absolute Error	Root Mean Square Error
0	0.0131	0.0157
0.2	0.0088	0.0089
0.4	0.0053	0.0058
0.6	0.0026	0.0032
0.8	0.0063	0.0066
1	0.0064	0.0074
Full Time Solution	0.0071	0.0088

formulated has been validated. This can be observed in detail in Fig. 1 and Fig. 3, where it is shown that the computed solution fits the analytical one, highlighting that our approach is an acceptable approximation.

In addition, it is important to note that error values confirm this analysis, as shown in Table II and III. Regarding this point, previous works treating similar problems using other quantum computing approaches [19], reach MAE values ranging between $0.0070 - 0.0087$ while our approach based on quantum annealing obtain MAE values between $0.0030 - 0.0269$, highlighting that our approach has lower error values in some cases but with a higher variability. Moreover, a quantum exponential speed up is only achieved in problems with certain specific features in other quantum approaches.

While it is true that this work does not include any study on computational speed, it is important to point out that the quantum annealing approach is expected to eventually provide the desired quantum exponential speed up for any given general problem [22]. Therefore, all the advances with their usage are of interest.

The contribution proposed in this paper it is important because it opens a new research area in quantum computing applied to CFD problems. It is important to note that the resolution of CFD problems are key in cutting edge digital technologies. One important use case is Smart Cities, in which it is important to combine meteorological and air quality models with urban data to compute sustainability indicators [23]. In this sense, chemistry transport models are a key element in smart cities architectures. This models has different components based on partial differential equations that are difficult to solve with traditional methods. In the last years, machine learning approaches has been explored but, to our knowledge, works regarding quantum computing [24] are sometimes limited. For this reason, the approach proposed in this paper could be a first step in this direction.

However, there are some limitations that are important to be concern before scaling up our solution to more complex scenarios. First, the method used presents a similar problem as found in global methods in classical computing. To achieve good accuracy for complex solutions, an everincreasing basis of functions is needed, leading to the use of a large number of qubits, which introduces significant errors in NISQ era computers [6]. In practical application, an important limitation is the difficulty in selecting appropriate hyper-parameters. Prior knowledge can help a lot to overcome this obstacle in order to arrive at a good enough solution [13].

V. Conclusion And Future Work

This paper has contributed to the state of the art in using the first spectral method for solving the Navies-Stokes equation using the quantum annealing paradigm, demonstrating that it is possible to solve CFD problems thanks to quantum computing. In addition, our results confirm that our method has similar error levels that other approaches in the state of the art, and present the advantage of the exponential speed up of quantum methods. However, next research should deal with the following challenges: i) improve the accuracy of the methods and reduce errors inherent to current quantum hardware, ii) assess the effect of hyper-parameters in the solution by sensitivity analysis and iii) deal with the difficulty of adding more equations of the NS set, leading to a coupled system of several variables. In this context, quantum algorithms could be the next step for solving CFD problems in real scenarios with applications in engineering, meteorology, air quality and smart cities.

Authors' contribution: J. Rodríguez, A. Pujante and E. Illueca wrote the manuscript. J. Rodríguez designed and carried out the experiments and A. J. Jara supervised the project and carried out the funding acquisition.

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