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Opportunities for Quantum Computation in Computational Fluid Dynamics

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Abstract

The computational fluid dynamics is a modern study that utilize computational methods such as the direct numerical simulation, and analyze or simulate the interested fluid mechanical models such as air foils and the turbulence model. This paper reports the acquired knowledge of a literature research and introduces the computational fluid dynamics and algorithms of quantum computation as well as discusses examples of applications of the quantum computation algorithms. Quantum computation or quantum information is an area that utilizes the properties of quanta and try to build various quantum circuits or even quantum computers. On the one hand, it has an analogy to the classical computation; on the other hand, it also gains uniqueness and superiority at problem solving. Compared with the classical computing methods, the quantum algorithms can be quite faster at computing with higher accuracy as well as security. Due to the demand of improvement with respect to the computational methods in this area and the recent development in quantum computation field, there exists an opportunity to closely relate these two areas. By constructing new quantum algorithms, the computing methods can be expected to be exponentially faster than classical computing methods. A proposal is raised to consider the features of the quanta and try to apply the advantages towards the computational fluid dynamics.

Keywords-computational fluid dynamics, quantum computation, qubit, direct numerical simulation

1. Introduction

Computational fluid dynamics (CFD) is an area of study that intends to solve real-life problems with respect to fluid flows or find solutions to the major governing equations of fluid mechanics, such as the Navier-Stokes equation (N-S) or the Euler equation. Computational fluid dynamics implements various numerical methods and solvers on classical computers based on empirical results from experiments. It has many applications such as simulating the air foils and the turbine engines, or even the estimation of the turbulence model.

In addition, quantum computing is a major application of quantum mechanics (QM) to computers. It is broadly used in various areas such as machine learning, cryptography and laser optics. As an analogy to classical computing or binary computing, quantum computing employs the exclusive physical properties of quanta, such as superposition, interference or entanglement, to bring new concepts and possibilities to the computing logic of the classical computers.

The comparison between classical binary computers and quantum computers is always widely discussed. In terms of the speed, the accuracy, the security or even optimization, quantum computers are built to beat classical computers to some extent, but possibly fail in some other fields. This paper will introduce the mechanism of computational fluid dynamics and quantum computing, then discuss the possibility for quantum computing to step inside CFD and replace classical computers.

In addition, there has existed already numerous quantum computing methods with respect to CFD. Researchers from University of Science and Technology of China have developed a Quantum Finite Volume Method for CFD that can overcome classical algorithms, though some challenges such as the precision are still preserved [1].

2. Introduction to CFD and Evolution of CPU systems in CFD

Computational fluid dynamics requires computing power to carry out the analysis of the major governing equations and two of them take a significant place. The first equation is the continuity equation:

$$\nabla \cdot \boldsymbol{u} = 0 \qquad (1)$$

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where $\boldsymbol{u}$is the velocity field of the incompressible flow. The continuity dictates that the divergence of the fluid velocity is zero, which means there does not exist free import or export of fluid elements in the system. This agrees with the conservation of mass:

$$\frac{D\rho}{Dt} + \rho\left(\nabla \cdot \boldsymbol{u}\right) = 0 \quad (2)$$

where ρ is the density of the flow. If the density of a flow stays constant with respect to time, in other words, the flow is incompressible, then the mass of the flow is conserved, and hence the conservation of mass equation can be rewritten as the continuity equation, which is a crucial property for incompressible flows.

Another significant equation is the Navier-Stokes equation:

$$\rho\frac{D\boldsymbol{u}}{Dt} =- \nabla p + \mu\nabla^2\boldsymbol{u} \ + \rho\boldsymbol{g} \quad (3)$$

The N-S equation is a partial differential equation that there does not exist a general solution to it in three-dimensional space. It is an extremely complicated relation among the pressure field, the flow velocity and the body force, and here is what acquires a huge number of computations. There are more models in CFD such as the RANS turbulence models or the low Reynold's number model that need computations as well [2].

In retrospect of the evolution of computation, a single-core CPU was firstly used to carry out the computation. As the increasing number of computations along with the development of technology, the demand of faster computing was raised, then multi-core CPUs were invented to fulfill the requirement of speeding up. However, in nowadays scientific researches such as CFD, only one CPU may also not be abundant to carry out the computation, thus the systems of parallel CPUs are maneuvered to carry out various simulating and computing jobs as well as speed up. Even GPUs can be additionally supplementary to the computing systems [3]. In modern world or even the future, there should be an opportunity for quantum computers to enter the realms, such as CFD, as an innovational method to resolve the dilemma of speeding up the computations as well as security, accuracy and other merits.

3. Introduction to quantum computation

On the contrary to the classical bits, the quantum computers use the quantum bits, which are also known as the "qubits". The qubits seem not to obey the rules of classical physics, but gain exclusive quantum properties. Analogously, the quantum circuits and the quantum logic gates built up within the quantum computers also follow the own rules of quantum mechanics [4].

3.1. Single Qubit State

Classical binary bits can be only one state at the same time, 0 or 1, and it cannot become each other or interfere each other whatsoever. However, quantum bits, or qubits, obey the rules of superposition and measurement. Take an example of the wave-particle duality theory, a photon which is a typical quantum can act as a particle but remains the physical properties of a wave. Another example is a two level hydrogen atom. Which energy level does the two level hydrogen atom sit is unknown unless it is measured by the Hamiltonian operator which represents the energy of the atom. In Dirac notation, we write the wave function of a two level hydrogen atom as:

$$|\psi > \ = \ \alpha|g >+ \ \beta|e > \quad (4)$$

where $|\psi >$is the solution to the Time-Independent Schrödinger Equation (TISE)

$$H\psi = E\psi \quad (5)$$

|g> represents the ground state of energy and |g> represents the first excited state, and α and β are the time-independent probability amplitudes of the corresponding state such that $|\alpha|^2 + |\beta|^2 = 1$. The wavefunction $|\psi >$ is a linear combination of two basis states |g> and |e> of the Hilbert space and is called the superposition of the ground state and first excited state. Once a measurement is done, the superposition will collapse into the result of the measurement. For example, if the energy is measured to be E_0 as the ground state energy and the eigenvalue of the Hamiltonian operator, then the wavefunction will become $|\psi > \ = \ |g >$ with the probability amplitude being 1.

Similarly, a quantum qubit can also have such superposition of two basis states |0> and |1> as the eigenstates of the Pauli z matrix. We can write it as:

$$|\psi > \; = \; \alpha|0 >+ \; \beta|1 > \tag{6}$$

and α and β still obeys the normalization. In contrast with classical binary bits, the quantum bits can stay in such state of superposition until they are observed at the final output and the wave function collapse into a certain state. A number of quantum gate operations can then occur in the middle of the quantum process without the necessity of knowing what the input looks like. In this way various quantum algorithms can be invented by comprising a series of quantum gate operations.

3.2. Multiple Qubit State

Nevertheless, the information flowing within the quantum circuits may not always be so simple as single qubits. In fact, various information should be treated as a combined system of states, which interfere each other. For example, when we consider the combined state of a two-qubit system in a 4-dimensional Hilbert space, we may write the wave function as:

$$|\psi > \; = \; \alpha_1|00 >+ \; \alpha_2|01 >+ \; \alpha_3|10 >+ \; \alpha_4|11 > \tag{7}$$

where |00> represents the tensor product of the eigenstate of each qubit |0> ⊗|0> and so on. The probabilities of each state still add up to one. Moreover, in a n-qubit system, the combined state can represent n tensor products of each qubit's state. Since each qubit state corresponds to two basis states |0> and |1> of its Hilbert space, the n-qubit system then has N=2n dimension [5].

3.3. Quantum Gate and Quantum System

As an analogy to classical circuits in the computers, quantum systems also consist of quantum circuits, containing quantum gates as operators that act upon the quantum bits. Interestingly, the quantum gates not only can deal with one qubit but also multiple qubits or a sequence of qubits.

Let us take the quantum controlled-not gate, or CNOT gate as an example. The CNOT gate is analogous to the classical XOR gate, which is also known as the Exclusive OR gate. The XOR operation compares with both inputs, if they are the same it will output 0 and the output will be 1 if the inputs are different. The CNOT gate is defined in Dirac notation as:

$$CNOT = \; |0 >< 0| \otimes \mathrm{I} + |1 >< 1| \otimes \sigma_x \tag{8}$$

which utilizes the orthogonality of quantum states, but in short, changes a two-qubit state |x, y> to |x, x⊕y> so one can control the first qubit x and only operate upon the second qubit y when encountering the two-qubit scenario. [6] In this way, the quantum CNOT gate exhibits more efficiency by utilizing the properties of quanta. Similarly, such algorithm can apparently be generalized to n-qubit system and the advantages become more prominent.

In addition, a series of quantum gates, also known as a quantum circuit, is designed to apply a certain quantum algorithm to realize the desired operation upon qubits. Many existing operations can be realized using quantum algorithms. For example, the usual Fourier transform which changes the basis variable is performed by doing a specific integral over the original function, while in quantum computing, the quantum Fourier transform is done by a series of quantum gates. It is applicable for one-qubit system and many-qubit system, and eventually can even be generalized to n-qubit in an N=2n Hilbert space. Finally, such various quantum circuits consisting of quantum gates can make up the whole quantum system or the quantum computer.

3.4. Simple Assumption of Speeding Up

For single bit scenario, traditional computers can only cope with a single bit at a time to figure out whether the information appear as 0 or 1. As for quantum computers, a quantum bit represents two possible states |0> and |1> and will collapse to a definitive quantum signal when it is in need. To the simplest assumption, supposing that a quantum gate has same information processing rate of one signal as a classical gate, then for single-qubit scenario, a classical gate will take twice the time to process the workload compared with the quantum gate, and four times the processing time for double-qubits signal, and eight times more for triple-qubits signal. To conclude, for a n-qubits signal, a classical gate will take 2n times more processing time to deal with the information, i.e., it has O (2n) time complexity [7]. However, in reality, the advantage of quantum computers over classical computers in terms of speeding up the calculating is not as monotonous as this 2n times, it is much more complex but it is supposed to be at least an exponential superiority.

This intuition may seem to naïve but actually makes sense. The Quantum Finite Volume Method invented by the researchers from University of Science and Technology of China is capable to outperform classical methods when dealing with classical inputs and outputs, and it works well for solving CFD-related equations such as the Navier-Stokes equation. This method quantizes the classical inputs in a quantum RAM and sum over the entries, then sample the desired solution states as well as update the quantum RAM [1]. The result exhibits this method performs exponentially better than classical methods, despite the limitations.

4. Smallest scales and Direct Numerical Simulation

In reality, there are numerous computation methods in CFD to do the analysis for possible fluid dynamics models. Many models are too difficult to resolve by only physical assumptions, thus computational methods are applied to analyze the models experimentally instead. For example, the direct numerical simulation is one method to solve the fluid properties with respect to the turbulence model. The main idea is to break up the flow into grids, and resolve for the small scales or eddies hence make it possible to simulate for the larger eddies [8].

The grid size and the time step are closely related to the Reynold's number Re[9]:

$$Re = \frac{uL}{\nu} \tag{9}$$

where u is the flow velocity, L is the characteristic length of the fluid element and ν is the viscosity. The limitation for DNS is it is only effective for large Reynold's number before the viscous force take in charge[10], and for small eddies, because larger enough eddies are unstable and always break up. Simulating larger eddies will take a huge number of timesteps which favors good computing power, and the accuracy usually drops down. In other words, there are various chances for improving the methods and developing more efficient computing power as well as more accuracy. This suggests that there are opportunities for quantum computation to take over the stage, what's more, some extra merits such as security are also applicable.

5. Conclusion

In conclusion, quantum computation implements well the unique features of the quanta. The quantum gates are operators that act on the input qubits which are at superposition states before they are observed. Moreover, the quantum circuits are a series of quantum gates that implements certain quantum algorithms so that the whole quantum computer consisting numerous quantum circuits is able to realize the desired operation such as quantum sampling. The use of quantum computation can effectively speed up the computation processes.

Additionally, faster computing speed and more computing power are favored by modern technologies and sciences such as the computational fluid dynamics which requires frequent numerical computations and simulations. Researchers have invented relevant quantum methods for solving CFD-related problems, and shown the exponential computing speed advantage that the quantum methods perform. Therefore, the quantum computers can have an opportunity, because they have potentials to provide faster computing speed, more computing power and advantages like security. The application of quantum computing into actual modern researches is worth looking forward to.

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