Quantum Computing and Its Potential for Turbulence Simulations

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Abstract. A tutorial is provided of quantum computing (QC) and the way it has made significant speed-up in various simulations. A review will also be provided of the large eddy simulation (LES) of turbulent flows via the stochastic filtered density function (FDF) methodology. The potentials of the quantum speed-up in FDF simulation via QC appear to be significant. This can results to a revolutionary means by which turbulence simulations can be conducted in future.

1 Introduction

Quantum computation (QC) has undergone rapid development, both experimentally and theoretically, in recent years [1]. Used in appropriate ways, quantum mechanics can provide powerful resources for solving certain classes of problems, achieving speedups not available to classical computers. The best known examples are Shor's algorithm for factorization of integers [2], and Grover's algorithm for unstructured search problems [3]. The gain in efficiency can either be exponential (*i.e.*, a problem where the solution time on a classical computer scales exponentially in the size of the problem N can have a solution time that scales polynomially in that size on a quantum computer), or polynomial (*i.e.*, the problem scales polynomially with N on a classical computer, and with a smaller power of N on a quantum computer) [1]. In either case, for the solution of large-scale problems, quantum computers represent a potentially transformational new paradigm in computing.

Within the past decade much progress has also been made in experimental realizations of quantum computing hardware. Many architectures have been proposed based on a variety of physical hardware. On a small scale, quantum information has been stored and manipulated in superconducting quantum bits (qubits) [4,5], trapped ions [6,7], electron spins [8–11], nuclear spins in the liquid or solid state [12], and other systems. On the theoretical side, new quantum algorithms have recently been found, exhibiting significant polynomial speedups on quantum computers for solution of sparse linear equations or differential equations [13,14], quantum Monte Carlo problems [15], and classical simulated annealing problems [16].

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It is speculated that QC can be a very useful tool for simulation of turbulent reacting flows. These flows are of significant interest to many industries as well as several sectors of the government. A possible means of achieving this is to search for quantum algorithms which are capable of solving stochastic differential equations (SDEs) which are central to the classical large eddy simulation (LES) methods. The optimal means of capturing the detailed physics of such flows via LES utilizes the density function (FDF) methodology [17]. The FDF provides the most comprehensive form of accounting for the subgrid scale (SGS) quantities and it can be cast in the form of the Diffusion equation [17]:

$$\mathrm{d}\mathbf{X} = \mathbf{A}\mathrm{d}t + B\mathrm{d}\mathbf{W} \,, \tag{1}$$

where $\mathbf{X}$ is a vector specifying all of the fluid and thermodynamic variables associated with the flow, vector $\mathbf{A}$ and matrix B are the drift and diffusion coefficients, respectively, components of which are specific to a given FDF model, t is time and $\mathbf{W}$ is the set of independent Weiner processes. For LES to be practical it must be conducted in a computationally efficient manner, especially if it is employed for prediction of complex flows.

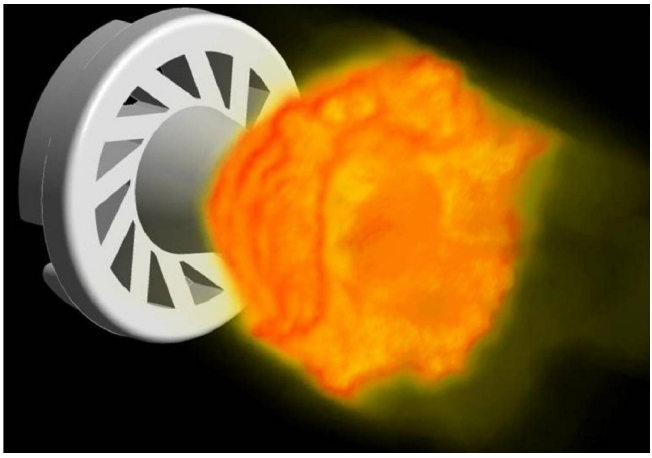

Fig. 1. Classical FDF Prediction of *CO* Mass Fraction in a Bluff-Body Reactor [21].

"Classical" computation of the FDF has experienced tremendous progress within the past decade; see *e.g.* Refs. [18,19]. As a results, it is now possible to conduct simulation of some of the most complex reacting flows. As an example, Fig. 1 shows LES/FDF prediction of a realistic chemical reactor [20]. The FDF simulated results as shown are within 95 % agreement with experimental measurements. However, some of these classical simulations can take of order of *several months* [21]!

2 QC for SDE Simulation

We speculate that quantum algorithms can be developed for efficient simulation of SDEs using two different methods. The first method is "algebraic" and computes arbitrary entries of the vector $\mathbf{X}$ in Eq. (1) using fast quantum algorithms for matrix multiplication. The second method prepares a quantum state such that, after a simple measurement, it samples from a probability distribution as determined by general Wiener processes. This method is "physical" in that the quantum states are prepared by quantum adiabatic evolutions of Hamiltonians that model the quantum harmonic oscillator and could be implemented by quantum simulators. In both methods, techniques from quantum walks developed in Ref. [16] to speedup conventional Monte-Carlo can be used. For that it is needed to investigate different reformulations of the FDF algorithm that are more amenable to implementation on a quantum computer.

Since the FDF is essentially modelled via a set of SDEs, it may be actually possible to employ QC for its simulations. This can be potentially achieved in two different ways. In the first case a simulation is aimed to output an arbitrary entry of the vector $\mathbf{X}(t)$, that satisfies a type of Eq. (1), with specified accuracy. This method works because $\mathbf{X}(t)$ can be sometimes written as a matrix product acting on some initial vector $\mathbf{X}(0)$, after discretization. Then, a fast quantum algorithm for matrix multiplication would provide the answer. The second method aims to prepare a quantum state that contains all the information about the evolved probability distribution as determined by a Fokker-Planck equation like Eq. (5) below. A simple measurement in such state allows to sample with exactly the desired probability. The quantum state is the lowest-energy (ground) state of a system of perturbed quantum oscillators. A generalization to the discrete case would provide quantum algorithms for this problem that could be readily implemented on a quantum simulator. Well-known tools for quantum speedups, such as the quantum Fourier transform (which is responsible for fast factoring as in Shor's algorithm) will play an important role here.

3 Turbulence Formulation via FDF

As indicated previously, the idea of employing QC for turbulence (including turbulent combustion) simulation appears promising because the essential means of enacting FDF is via modeled SDEs. These SDEs describe all of the basic transport variables and account for couplings of turbulence, exothermicity, variable density, and also differential diffusion. The primary transport variables in FDF formulation are the density $\rho(\mathbf{x}, t)$, the velocity vector $u_i(\mathbf{x}, t)$ $(i = 1, 2, 3)$, the pressure $p(\mathbf{x}, t)$, the internal energy $e(\mathbf{x}, t)$ and the species mass fractions ϕ_α $(\alpha = 1, \ldots N_s)$. The equations which govern the transport of these variables in space (x_i) $(i = 1, 2, 3)$ and time (t) are the continuity, momentum, energy and the scalar transport, all coupled through the equation of state [22].

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \tag{2a}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ji}}{\partial x_j} \tag{2b}$$

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_j e}{\partial x_j} = -\frac{\partial q_j}{\partial x_j} + \sigma_{ij}\frac{\partial u_i}{\partial x_j} \tag{2c}$$

$$\frac{\partial \rho \phi_\alpha}{\partial t} + \frac{\partial \rho u_j \phi_\alpha}{\partial x_j} = -\frac{\partial J_j^\alpha}{\partial x_j} + S(\Phi) \tag{2d}$$

$$p = \rho \frac{R^0}{W} T \tag{2e}$$

where R^0 denotes the universal gas constant and W is the mean molecular weight of the mixture. T denote the temperature, e is the internal energy $\gamma = \frac{c_p}{c_v}$ is the specific heat ratio, and $S(\Phi)$ denotes the chemical source term. The viscous stress tensor τ_{ij}, the energy flux q_j, the species α diffusive mass flux vector J_j^α and σ_{ij} tensor are represented by

$$\sigma_{ij} = \tau_{ij} - p\delta_{ij}, \quad \tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right),$$

$$q_j = -\lambda\frac{\partial T}{\partial x_j}, \quad J_j^\alpha = -\rho\Gamma\frac{\partial \phi_\alpha}{\partial x_j}, \tag{3}$$

where μ is the fluid dynamic viscosity, λ denotes the thermal conductivity and Γ is the mass diffusion coefficient. We assume calorically perfect gas in which the specific heats are constants. Large eddy simulation involves the spatial filtering operation: [23,24] $\langle Q(\mathbf{x},t)\rangle_\ell = \int_{-\infty}^{+\infty} Q(\mathbf{x}',t)G_{\Delta_l}(\mathbf{x}',\mathbf{x})d\mathbf{x}'$, where $G_{\Delta_{l_1}}(\mathbf{x}',\mathbf{x})$ denotes a filter function, and $\langle Q(\mathbf{x},t)\rangle_\ell$ denotes the filtered value of the transport variable $Q(\mathbf{x},t)$. The subscript l_1 indicates that $\langle Q(\mathbf{x},t)\rangle_\ell$ is the first level filter value of the variable $Q(\mathbf{x},t)$ [25]. In variable-density flows it is convenient to use the Favre-filtered quantity $\langle Q(\mathbf{x},t)\rangle_L = \langle \rho Q\rangle_\ell / \langle \rho\rangle_\ell$. We consider a filter function that is spatially and temporally invariant and localized, thus: $G_{\Delta_{l_1}}(\mathbf{x}',\mathbf{x}) \equiv G_{\Delta_{l_1}}(\mathbf{x}'-\mathbf{x})$ with the properties $G_{\Delta_{l_1}}(\mathbf{x}) \geq 0$, $\int_{-\infty}^{+\infty} G_{\Delta_{l_1}}(\mathbf{x})d\mathbf{x} = 1$.

The formal FDF is defined by $F_L(\boldsymbol{v},\boldsymbol{\psi},\boldsymbol{\Theta},\boldsymbol{\eta},\mathbf{x};t)$ where, $\boldsymbol{v}$, $\boldsymbol{\psi}$, $\boldsymbol{\Theta}$ and $\boldsymbol{\eta}$ are the velocity vector, the scalar array, the sensible internal energy and pressure in the sample space, respectively. The function F has all of the properties of a probability density function in that the filtered value of any function of the velocity and/or scalar variables is obtained by its integration over the sample spaces:

$$\langle \rho(\mathbf{x},t)\rangle_\ell \langle Q(\mathbf{x},t)\rangle_L = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} Q(\boldsymbol{v},\boldsymbol{\psi},\boldsymbol{\Theta},\boldsymbol{\eta})F_L(\boldsymbol{v},\boldsymbol{\psi},\boldsymbol{\Theta},\boldsymbol{\eta},\mathbf{x};t)d\boldsymbol{v}d\boldsymbol{\psi}d\boldsymbol{\Theta}d\boldsymbol{\eta}. \tag{4}$$

However, the transport equation for F_L is not in a closed form and must be modelled. For this, as indicted earlier, we consider the general diffusion process,[26,27] given by the system of SDEs. The modeling of the SDEs must be in such a way that is amenable to QC. The starting point will be our simplified Langevin model (SLM) and linear mean-square estimation (LMSE) [28] coupled with an equation of state and obeying the first law of thermodynamics. With construction of the SDEs, the corresponding Fokker-Planck equation [29] will essentially be the modelled FDF transport equation. Our proposed model is under construction and is of the form:

$$\begin{aligned}
&\frac{\partial F_L}{\partial t}+\frac{\partial v_i F_L}{\partial x_i}=\frac{1}{\langle\rho\rangle_\ell}\frac{\partial\langle p\rangle_\ell}{\partial x_i}\frac{\partial F_L}{\partial v_i}-\frac{2}{\langle\rho\rangle_\ell}\frac{\partial}{\partial x_j}\left(\mu\frac{\partial\langle u_i\rangle_L}{\partial x_j}\right)\frac{\partial F_L}{\partial v_i}-\frac{1}{\langle\rho\rangle_\ell}\frac{\partial}{\partial x_j}\left(\mu\frac{\partial\langle u_j\rangle_L}{\partial x_i}\right)\frac{\partial F_L}{\partial v_i}\\
&+\frac{2}{3}\frac{1}{\langle\rho\rangle_\ell}\frac{\partial}{\partial x_i}\left(\mu\frac{\partial\langle u_j\rangle_L}{\partial x_j}\right)\frac{\partial F_L}{\partial v_i}-\frac{\partial\left(G_{ij}\left(v_j-\langle u_j\rangle_L\right)F_L\right)}{\partial v_i}+\frac{\partial}{\partial x_i}\left(\mu\frac{\partial(F_L/\langle\rho\rangle_\ell)}{\partial x_i}\right)\\
&+\frac{\partial}{\partial x_i}\left(\frac{2\mu}{\langle\rho\rangle_\ell}\frac{\partial\langle u_j\rangle_L}{\partial x_i}\frac{\partial F_L}{\partial v_j}\right)+\frac{\mu}{\langle\rho\rangle_\ell}\frac{\partial\langle u_k\rangle_L}{\partial x_j}\frac{\partial\langle u_i\rangle_L}{\partial x_j}\frac{\partial^2 F_L}{\partial v_k\partial v_i}+\frac{1}{2}C_0\frac{\epsilon}{\langle\rho\rangle_\ell}\frac{\partial^2 F_L}{\partial v_i\partial v_i}\\
&+C_\phi\omega\frac{\partial\left(\left(\psi_\alpha-\langle\phi_\alpha\rangle_L\right)F_L\right)}{\partial\psi_\alpha}+\frac{C_e\omega}{\gamma}\frac{\partial\left(\left(\theta-\langle e\rangle_L\right)F_L\right)}{\partial\theta}\\
&-\epsilon\frac{\gamma-1}{\gamma}\frac{\partial}{\partial\theta}\left(\frac{\theta}{\eta}F_L\right)-\frac{\gamma-1}{\gamma}\frac{\partial\left(\theta A F_L\right)}{\partial\theta}+\frac{\gamma-1}{\gamma^2}\frac{\partial\left(\theta B^2 F_L\right)}{\partial\theta}-\frac{\partial\left(\eta A F_L\right)}{\partial\eta}\\
&+\frac{1}{2}\frac{(\gamma-1)^2}{\gamma^2}\frac{\partial^2\left(\theta^2 B^2 F_L\right)}{\partial\theta\partial\theta}+\frac{\gamma-1}{\gamma}\frac{\partial^2\left(\theta\eta B^2 F_L\right)}{\partial\theta\partial\eta}+\frac{1}{2}\frac{\partial^2\left(\eta^2 B^2 F_L\right)}{\partial\eta\partial\eta}.
\end{aligned}\tag{5}$$

In Eq. (5) k is the SGS kinetic energy, $\epsilon=\langle\rho\rangle_\ell C_\epsilon\frac{k^{3/2}}{\Delta_L}$ is the SGS dissipation, $\omega=\frac{1}{\langle\rho\rangle_\ell}\frac{\epsilon}{k}$ is the SGS frequency, A, B are the model parameters for the pressure SDE, and

$$G_{ij}=\left[\frac{\Pi_d}{2k\langle\rho\rangle_\ell}-\omega\left(\frac{1}{2}+\frac{3}{4}C_0\right)\right]\delta_{ij}.\tag{6}$$

The parameters C_0, C_ϕ, C_e, and C_ϵ are model constants and need to be specified [30,31]. The same goes for the pressure dilatation term Π_d [31,32]. The transport equations for all of the SGS moments are readily obtained by integration of this Fokker-Planck equation. This provides a complete statistical description of turbulence. The idea is to find methods that could take advantage of quantum resources in order to speed up these calculations, at least polynomially in the number of variables. Because of the size of the problem typically considered, such a speedup could transform the way these problems are treated in engineering; providing solutions to problems many orders of magnitude faster than are possible with classical computers.

Another challenge associated with FDF is its implementation in *complex* geometries. Structured multi-block grids lack the required flexibility and robustness for handling such geometries. The grid cells may also become too skewed

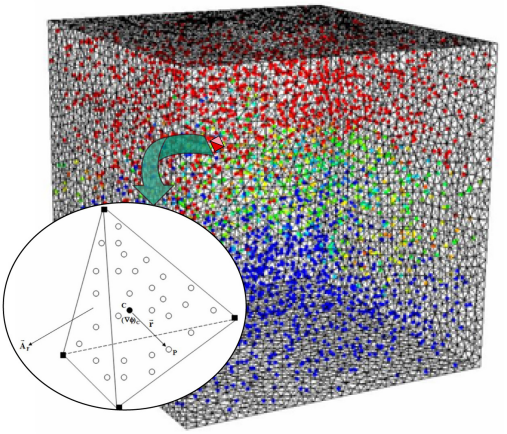

Fig. 2. Monte Carlo Particles on Unstructured Grids.

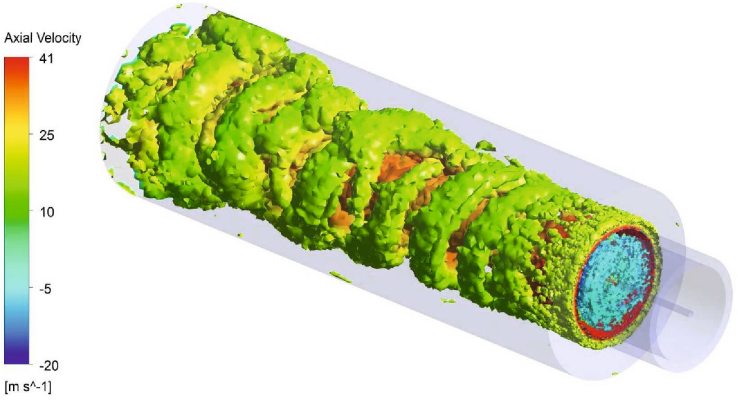

Fig. 3. Classical FDF Simulation of the Sandia/Sydney Burner [36].

and/or twisted, prohibiting efficient simulations. Unstructured grids provide a good solution for the problem of producing grids on complex shapes. Such grids have irregularly distributed nodes and their cells are not required to be of a specific shape. Furthermore, the connectivity of neighboring cells can vary spatially. The SDEs portraying the FDF will be primarily simulated via Monte Carlo methods [33,34], on a domain represented by unstructured grids. As an example, Fig. 2 shows a small fraction of the Monte Carlo particles used on unstructured meshes for the classical simulation results shown in Fig. 1. The essence of a quantum computing implementation would be to speed up these Monte Carlo simulations, either in direct solutions of the stochastic differential equations, or by solving equivalent problems (such as the Fokker-Planck equations).

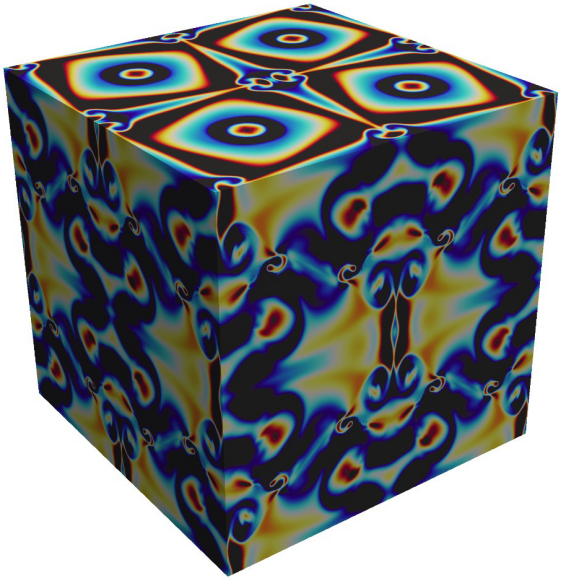

Fig. 4. Classical FDF Simulation of Taylor-Green Vortex Flow [37].

We expect to be able to conduct LES with over billions grid points and over tens of billions of Monte Carlo particles. These simulations are proposed to be conducted for prototype reactors with variable physical length and time scales. In this case, the effects of the flow residence time and the Damköhler number will be the primary subject of the investigations. In addition, the spatial and the compositional structures of the reacting flow field will be assessed.

At this end, to demonstrate superiority of our classical algorithms, we show some sample results of our most recent FDF simulation of the Sandia/Sydney swirl burner [35]. This configuration is selected as it is one of the most challenging turbulent flames for prediction. Figure 3 shows the contours of the azimuthal velocity field as predicted by our FDF. The simulated results agree with experimental data better than any other classical methods currently available [36]. But the computational time requirements are excessive. As another example, Fig. 4 shows the contour of filtered temperature field for the symbolic Taylor-Green vortex flow as obtained via FDF coupled with a discontinuous Galerkin flow solver [37]. Quantum computation may potentially provide a much more efficient means for such simulations.

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