IRSTI 27.35.17 https://doi.org/10.26577/ijmph.2021.v12.i1.01

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Computational turbulent combustion in the age of artificial intelligence and quantum information

Abstract. The impact of high-performance computing on the society has been enormous, but it is easy to be taken for granted. In today's world, it is virtually impossible to imagine system design or major decision making not aided via predictive modeling and simulation. Now that we are experiencing the *Data Revolution* and the emergence of the *Second Quantum Revolution*, it is wise to consider both of these elements in computational science and engineering. Data-driven modeling approaches and demonstrated speed-ups of quantum algorithms have the potential to transform scientific discovery. This will affect the fabrics of industrialized societies in diverse disciplines. A research arena which can substantially benefit from these technologies is combustion. This field has been the subject of heavy computational research for many decades now. In this review, some examples taken from the previous works of the author are presented to demonstrate how the field of computational turbulent combustion is benefiting from modern developments in machine learning (ML) and quantum computing (QC).

Key words: computational turbulent combustion, computational science and engineering, speed-ups of quantum algorithms, machine learning, quantum computing.

Introduction

Computer modeling and numerical simulation have been rapidly growing in importance throughout the sciences, engineering, medicine as well as in most other disciplines. We are now in an era where, increasingly, experimental and computational researchers are teaming up to tackle grand challenge problems. For over two decades the case has been made for recognizing computational science and engineering (CSE) as a priority interdisciplinary area for funding agencies, and to expand and strengthen the education in its related disciplines [1–3]. We are also in the midst of experiencing both the *Big Data Revolution* [4], and the emergence of the *Second Quantum Revolution* [5]. The amount of data available is doubling yearly, and artificial intelligence (AI), in particular machine learning (ML) methods are playing an increasingly important role in analyzing this data and using it to deduce new models of processes. Moreover, quantum mechanical phenomena have evolved into many core technologies and are expected to be responsible for many of the key advances of the future. Quantum computing (QC), in particular, has the potential to revolutionize computer modeling and simulation. The importance of these fields to the global economy and security are well recognized, promoting an even more rapid growth of the related technologies in the upcoming decades. This growth is fueled by large investments by many governments and leading industries. An arena in which both QC and AI are promoted to play a more significant role is CSE [2, 3, 6, 7]. Since the early 1980s, computational simulations have been known as the *3rd pillar of science* [8, 9], and are now being augmented by this *4th paradigm* because of the big data revolution [10].

In the arena of computation, now there are some doubts about the longevity of Moore's law [11] which has largely held true for over five decades [12]. As silicon-based processors shrink to smaller and smaller sizes, physical limitations start to play an important role. As a result, the expense and effort required to continue the increase in performance of supercomputers are now much greater than ever before. In order to provide new disruptive means to perform computations with increased complexity, the CSE community will need a radical departure from the conventional classical computing platforms. Quantum computing is a particularly promising candidate to be this disruptive technology for many computational problems [13–23].

The rate of progress in QC technology is very promising. In fact, the rapid development of this

technology has led to what is now known as the "*Neven's law*," stating that: "quantum computers are gaining computational power relative to classical ones at a doubly exponential rate." The QC community as a whole has an overarching goal to build a general purpose, universal quantum computers [24]. Google, IBM, Intel, Microsoft, and a large and growing number of start-ups in the US and abroad are developing such machines [23]. Quantum computers are increasingly available on the cloud, with commercial offerings from IBM, Microsoft, and Amazon recently being announced. There is also increasing momentum and excitement in the field, with rapid progress in building non-corrected, so called *noisy intermediate scale quantum* (NISQ) computers [19], and the promise of error-corrected machines in the not-too-distant future.

Applications in Turbulent Combustion

Despite all of the dedicated efforts towards the development of alternative and/or sustainable energy resources, combustion still provides a large portion of the energy needs worldwide, a situation that will likely remain the same within the foreseeable future. Associated with combustion is air pollution and the greenhouse effect; thus the need for the reduction of CO_2 emissions while maintaining high combustion efficiency. These concerns, along with stringent demands to reduce petroleum consumption, are putting a high priority on combustion research. In most cases, combustion is accompanied by turbulence where the latter provides the means of enhanced fuel-air mixing. The physics of turbulent reactive flows is notoriously difficult due to the intricacies of the interactions between chemistry and turbulence. The phenomenon of mixing at both micro and macro scales and its role and capability (or lack thereof) to provide a suitable environment for combustion, and the subsequent effects of combustion on hydrodynamics, have been at the heart of turbulent combustion research for over half a century now [25–27].

Researchers in computational turbulence and combustion are well versed in advanced numerical algorithms, and how to use them effectively in parallel numerical simulations. For over 40 years, the fields of computational turbulent combustion have been one of the most intense fields of CSE [28]. Statistical methods continue to constitute the most practical means of turbulent combustion predictions. These methods involve stochastic representation of the transport equations, augmented with closures to account for the effects of unresolved scales. Among the variety of stochastic tools developed within the past century, the probability density function (PDF) methods have proven to be particularly effective [29]. This is due to the fundamental property of PDF as it accounts for all of the statistical variations of the transport variable [30–32]. This feature is particularly appealing for modeling of chemically reactive flows, as it accounts for the effects of chemical reactions in an *exact* manner [33–35].

A major challenge in utilizing PDF is associated with its modeling and computational simulations. Combustion engineers have been trying to deal with this issue [36], and there is a continuing need to make use of advanced computational methodologies for turbulent combustion research. In this article, two examples are presented to demonstrate how ML/DL and QC can be useful in this regard. These examples are taken from this previous publications in which this reviewer is a co-author.

a. Deep-Learning of Turbulent Scalar Mixing

In this example, detailed in Ref. [37], we consider the problem of mixing of a Fickian passive scalar $\psi = (t, \boldsymbol{x})$ (t denotes time and $\boldsymbol{x}$ is the position vector), with diffusion coefficient Γ from an initially symmetric binary state within the bounds $-1 \leq \psi \leq +1$. Therefore, the single-point PDF of ψ at the initial time is $P_L(0,\psi) = \frac{1}{2}[\delta(\psi-1) + \delta(\psi+1)]$. In homogeneous turbulence, the PDF is governed by [33] $\frac{\partial P_L}{\partial t} + \frac{\partial (D P_L)}{\partial \psi} = 0$, where D denotes the conditional expected diffusion of the scalar field. The closure problem in the PDF transport is associated with this diffusion, and modeling of this term has been a stumbling block since the early days of PDF modeling [33, 34, 38].

Modern ML techniques have the potential to be utilized for PDF model developments [39, 40]. Given data $\{t^n, \psi^n, P_L^n\}_{n=1}^N$ on time and the PDF, we approximate the functions P_L and D by two deep neural networks to obtain the physics-informed neural network $R := \frac{\partial P_L}{\partial t} + \frac{\partial (D P_L)}{\partial \psi}$ as illustrated in Fig. 1. We obtain the required derivatives to compute the residual network $R(t,\psi)$ via automatic differentiation [41]. This allows accurate evaluation of derivatives at machine precision with ideal asymptotic efficiency. To assess the performance of this deep learning algorithm, we considered the PDF model obtained by the amplitude mapping closure (AMC) [42–44]. The AMC captures many of the

basic features of the binary mixing problem. Namely, the inverse diffusion of the PDF in the composition domain from a double delta distribution to an asymptotic approximate Gaussian distribution, as the variance goes to zero. Figure 2 depicts the exact [44] and the learned conditional expected diffusion $D(t,\psi)$. As demonstrated the agreement is excellent even though the algorithm has seen no data whatsoever on the conditional expected diffusion.

b. Quantum Computing for Combustion

In this example, detailed in Ref. [45], we demonstrate some potentials of QC for turbulent combustion simulations. We consider the transport of two initially segregated reactants $F(\boldsymbol{x},t)$ and $O(\boldsymbol{x},t)$, where $\boldsymbol{x}$–t denote the (homogeneous) space-time. An idealized irreversible binary reaction of the type $F + rO \rightarrow (1+r)Product$ is considered, and turbulent mixing is modelled by the coalescence/dispersion (C/D) closure of Curl [38, 46, 47]. Subsequently, all of the pertinent single-point statistics of the reacting field are determined. The most important of these statistics are the mean rates of reactant conversion, denoted by $\mathcal{Z}(t)$.

A Monte Carlo (MC) methodology is used for the stochastic simulation of the C/D model. The quantum algorithm is based on quantum phase estimation [48]. Figure 3 shows classical simulations of the quantum algorithm for estimating the rate of mean fuel conversion $\mathcal{Z}_{MC}(t)$. The increasing behavior of $\mathcal{Z}_{MC}(t)$ as a function of t is demonstrated in Fig. 3 (a). The results of the quantum algorithm are in agreement with the highly accurate results via classical MC calculations obtained with $N_r = 2^{20} \times 60$ runs, allowing to obtain estimates $\tilde{\mathcal{Z}}_{MC}(t)$ that are very close to the actual value of $\mathcal{Z}_{MC}(t)$. The estimated rates of reactant conversion from the quantum algorithm relative to $\tilde{\mathcal{Z}}_{MC}(t)$, for two values of MC samples (N_r), are shown in Fig. 3 (b). The relative errors decrease as a function of time because the $\mathcal{Z}(t)$ approaches 1 as t increases. Figure 4 shows comparisons of estimation errors from classical MC methods (ϵ_C) and the quantum algorithm (ϵ_Q) as functions of the total number of computational elements (N_r). It is observed that ϵ_C decreases as $1/\sqrt{N_r}$ while ϵ_Q decreases as $1/N_r$, demonstrating a quadratic quantum speedup of the quantum algorithm with respect to the classical methodology. The advantages of the quantum algorithm are more obvious for values of N_r for which $\epsilon_Q \leq \epsilon_C$. However, the genuine advantage is in the different scaling of the algorithm. This example has substantial applications in practical engineering combustion systems. In the near future, it is expected that the current classical turbulent combustion simulations [49, 50], exemplified by Fig. 5 can benefit from quantum speed-up.

Concluding Remarks

The emergence and increased importance of massive data sets in many disciplines, coupled with the emergence of ML/DL to analyze these data sets is already transforming the world, and QC has the potential to revolutionize CSE. Data-driven modeling approaches, and demonstrated speed-ups of quantum algorithms have the potential to transform scientific discovery. This will affect the fabrics of industrialized societies in diverse disciplines far beyond science and engineering. The paradigm of scientific discovery offers an elegant path to generalization and enables computing with probability distributions rather than solely relying on deterministic thinking. We have also been witnessing demonstration of quantum speed-up. With emergence of quantum simulators, quantum annealers and analog quantum machines [51–53], and the arrival of universal quantum computers with 50+ qubits, we are now in the era where *quantum supremacy* exists both as a theoretical proposal [54, 55] and experimental realization [56].

Machine learning is currently one of the most popular areas in almost all disciplines. Significant efforts are being devoted to this field, not just in its basic developments, but also in numerous diverse applications. However, it is to be emphasized that ML is not *magic*! It consists of four basic elements: linear algebra, optimization, probability & statistics and algorithms. Machine learning's broad popularity has been, in part, motivated by production of excellent software such as Tensorflow [57]. While ML will surely remain as a powerful research tool, it must be utilized in the context of a very strong physical & mathematical modeling. It is also clear that the era of QC is here and the community is moving towards developments that could potentially have a profound impact on CSE. The challenge lies in understanding the new technology, and identifying the highest-impact applications. As the Nobel Laureate Bill Phillips said: "...Quantum information is a radical departure in information technology, more fundamentally different from current technology than the digital computer is from the abacus..." The computational combustion

community needs to recognize that this is not a short-term endeavor. There is a need to build infrastructure and expertise in this technological frontier of the 21st century.

Acknowledgements

I am honored to participate at this meeting in honor of Professor Aidarkhan Kaltayev of Satbayev University, and I am grateful to him for many technical discussions on the subject matters covered in this review. I am also grateful to my co-authors of previous publications which have been cited here. Our current related work is sponsored by NSF under Grant CBET2042918, and the NASA Transformational Tools and Technologies (TTT) Project under Grant 80NSSC18M0150.

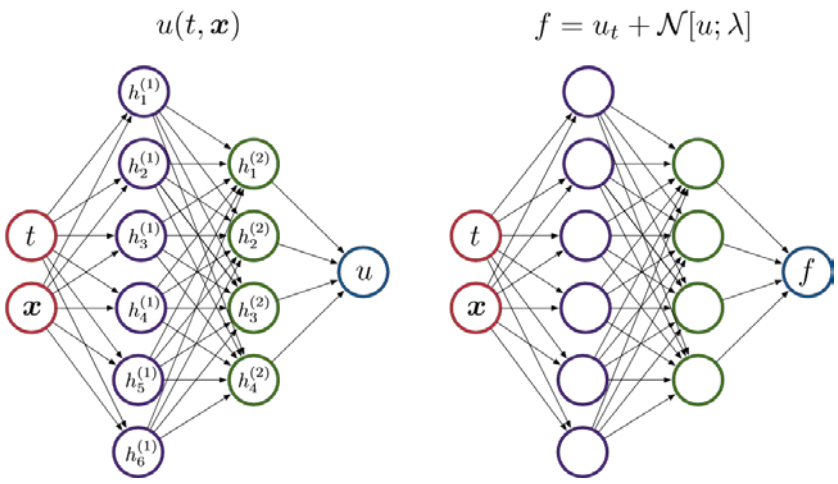

Figure 1– *Physics-Informed Neural Network:* The residual neural network f is obtained by approximating the unknown solution u by a deep neural network and by taking the required spatial and temporal derivatives using automatic differentiation. Taken from Ref. [37]

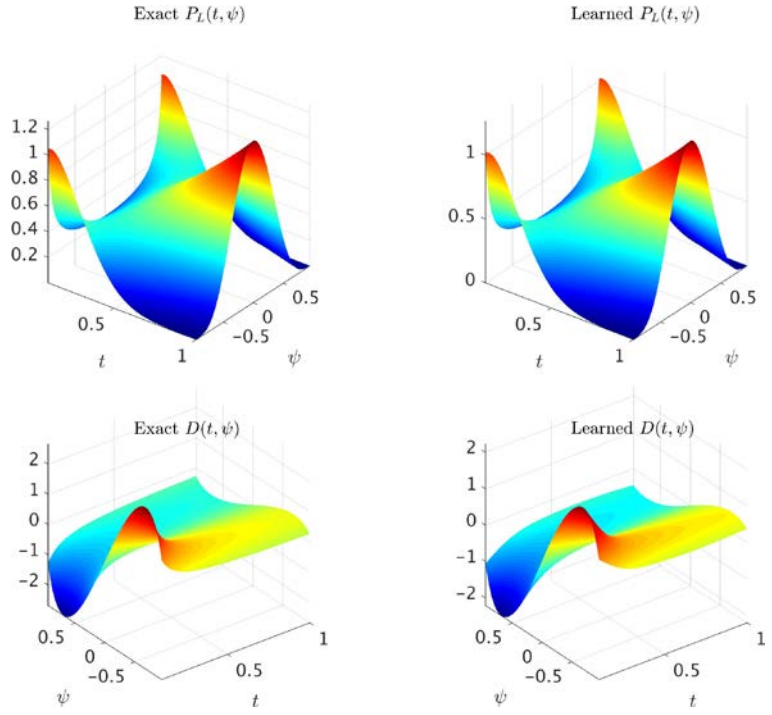

Figure 2 – The exact P_L via the exact model and the learned one are on the top, while the exact and learned Ds are in the bottom panels. Taken from Ref. [37].

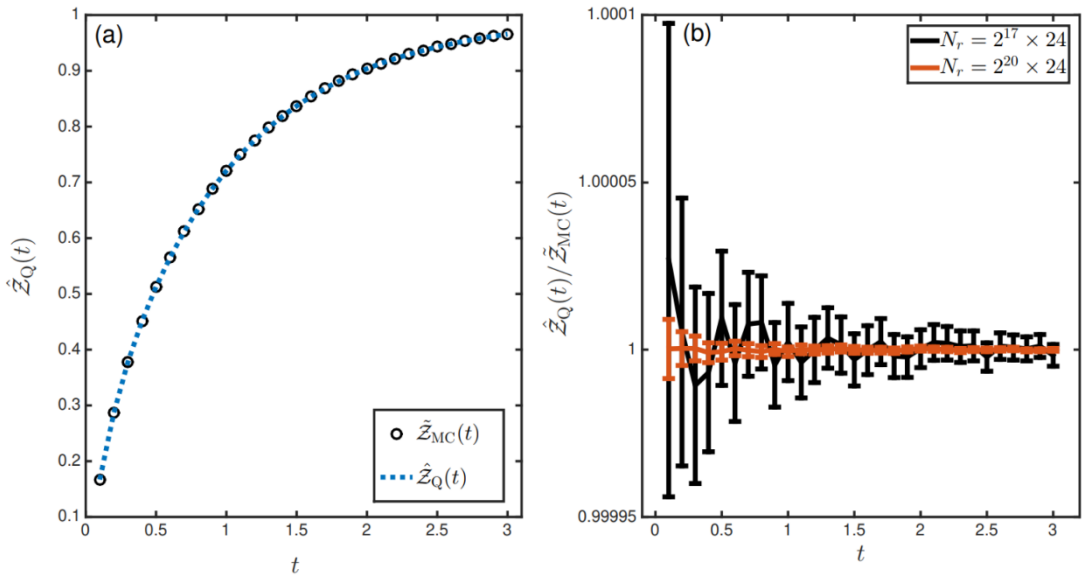

Figure 3 – Estimates of the rate of reactant conversion obtained from classical simulations of the quantum-algorithm that would solve a reacting flow process using Curl's model [46]. (a) Growth of the estimated rate of reactant conversion as a function of time. (b) Comparison of two estimated rates of reactant conversion for $N_r = 2^{17} \times 24$ (black line) and $N_r = 2^{20} \times 24$ (red line), given by the quantum algorithm, with $\tilde{Z}_{MC}(t)$. Taken from Ref. [45].

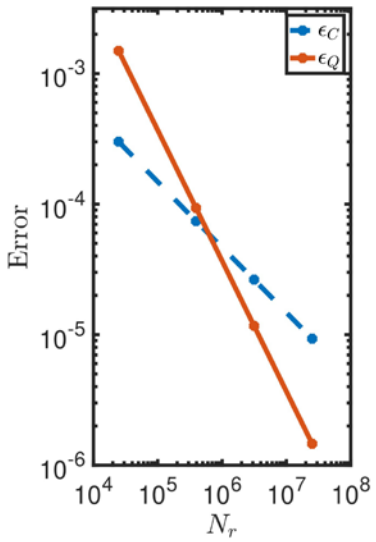

Figure 4 – Comparisons of errors output by the Classical MC method (ϵ_C) and the Quantum MC algorithm (ϵ_Q). Taken from Ref. [45].

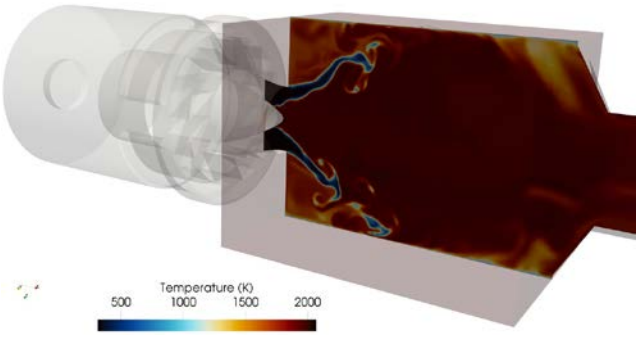

Figure 5 – Simulation results of the reactor in experiments of Ref. [58].

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