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Machine learning and quantum computing for reactive turbulence modeling and simulation

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A B S T R A C T

A perspective is given on some prospects of machine learning and quantum computing for modeling and simulation of turbulent reactive flows. This perspective is a more comprehensive and extended form of the 13th Elsevier Distinguished Lecture in Mechanics delivered by the author.

1. Introduction

With the current *Big Data Revolution* [1], and the *Second Quantum Revolution* [2], the scientific community is witnessing remarkable scientific & technological progress and also challenges. Artificial intelligence (AI) and quantum information science (QIS) are influencing every fabrics of our society, and are rapidly making transformative changes in research and technology. With the rapid increase in the volume of data being generated, AI methods are playing a major role in utilizing data to construct new models of processes. In QIS, quantum computing (QC) is proving to be *real*, and to dramatically change the way computations will be conducted in the future. Both of these fields are now placed in top priorities in industrial societies, and will surely remain there within the upcoming decades.

Machine learning, originally emerged from computer science, has revolutionized fields such as vision, autonomous systems and natural language processing. Both the supervised and totally data driven form of ML have proven effective [3–6], and it is expected that the rate of progress would be even faster in the future. The rise of deep learning via neural networks has enabled researchers to perform complex classification and regression tasks that were not previously possible. As a result, data sciences have been recognized as the *fourth paradigm of scientific discovery* [7] offering an elegant path to construct predictive models of complex physical systems.

QIS represents the merger of the two most significant scientific and technological revolutions of the 20th century, notably quantum physics and information technology. As one of its constituents, QC can provide powerful resources for solving certain classes of problems, achieving cost scalings with the size of the problem that are not possible on existing "classical" computers [8,9]. Amongst the best known examples of quantum algorithms are Shor's algorithm of factorization [10,11], and Grover's search algorithm [12]. The gain in efficiency of the scaling of these algorithms is either exponential or polynomial [13,14]. These are known as *quantum speed-up* [8,15–23].

2. Applications in reactive turbulence

Turbulence transport and its interactions with chemistry remain as one of the most important unresolved problems with significant scientific and practical applications. The broad ranges of length and time scales in this transport makes its computational description very difficult [24,25]. Both ML and QC can become major forces in dealing with this complex phenomenon.

2.1. Perspectives in ML

Modeling of turbulent reactive flows is expected to be aided significantly via modern. ML optimization techniques in the contexts of both the Reynolds-averaged NavierStokes (RANS) and large eddy simulation (LES) [26–29]. For that, we need to consider the ways ML its into current modeling paradigms, and also develop new turbulence closure strategies that leverage ML strengths. We need to determine the best training procedures that accommodate specific features of turbulence descriptor. For example, coherent vs. stochastic structures, linear vs. non-linear physics, etc. [30]. Several specifics issues pertaining to ML applications in reactive turbulence modelings are listed here, along with some suggestions and guidelines for future work:

Amount, Quality and Complexity of Data: Currently, data in turbulent combustion is limited, and it is not totally clear how much data is required for training in ML/AI. More importantly if an accuracy target is

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set, it is difficult to understand if more data (and what data) is required to achieve the target. Extensive reactive flow data sets are currently available, such as Sandia TNF. Workshop (tnfworkshop.org). Such sets have been very useful in developments and evaluations of physical models. But they are not tailored for ML. For a dataset to be useful for ML, it should be well documented in terms of use, and be accessible by standard ML/data science packages (such as those in Python, and Matlab). A forum similar to *ImageNet* (image-net.org) in computer vision is needed. Such benchmark tests will also serve as excellent teaching materials for students and researchers.

Physics Discovery: One of the most useful application of ML/DL is for discovery of physical systems [31–35]. Work is needed to enhance current ML algorithms to reconstruct modelled transport equations of turbulent reacting flows. These algorithms must learn non-autonomous dynamical systems, and recover the symmetries including invariances. As DL/ML methods deal with data to capture physics, the process of optimization can be enhanced by including certain known physical characteristics. In this way, some additional unknowns can be determined in addition to the desired characteristics of the raw data. See Ref. [27] as an example. Also, "reinforcement learning" strategies involving the combination of proper ML tools with domains of expertise has the potential for optimizing the control strategies [34,36].

Solution of Inverse and Ill-Posed Problems: There are many situations where the physical quantities need to be inferred from data. There are also a relatively large number of physical ill-posed or inverse problems. See, for example Journal of Inverse and Ill-Posed Problems. For example, the inverse diffusion of scalar probability density function of scalars by their conditional expected dissipation [37]. In some of these cases, the optimization routine in a properly devised neural network can provide accurate solutions.

Algorithm Improvements: Data-driven algorithms expose the users to an extremely large number of options (number of layers & neurons, activation function, type of layers, etc.) Significant experience is required to sort through these options, This introduces a fundamental reprehensibility issue, since it would make it difficult to synthetically describe the various ML choices. Many of the options in these approaches are not clearly understood. Therefore, a theoretical framework for the description of these methods is of critical importance.

Using Physics to Improve ML: A successful ML routine must be interpretative and generalized for effective use beyond the training data. Also, as we develop and apply ML algorithms for turbulent combustion, the learning process can be also used to improve the ML algorithms in return. This is possible because of the extensive current knowledge in modeling and simulation of reactive turbulence (or any other domain field for that matter).

Similarities and Commonalities: It is useful to find similarities with other scientific areas to solve more general problems: How to couple domain-driven models with data-driven models from AI/ML. Modern methods have enabled non-linear dimensional reductions for large volume data, and offer opportunities for further model reduction and better generalizations compared to classical linear subspace methods, such as PCA or other dynamic mode decomposition methods [38]. Auto-differentiation could enable efficient analysis of simulation results, which will make the uncertainty quantification of expensive systems to be computationally tractable. See Ref. [39] as an example.

Along similar lines, the universality of the data driven models must be assessed and documented. Will the ML-assisted turbulent combustion model only act as an interpolator within the domain of the training data, or will it provide useful predictions outside that domain? If yes, what is the domain of applicability? For example: premixed and/or non-premixed and/or partially premixed flames? distributed or flamelet-like reaction zones? etc.

Despite all of its popularity, it is to be emphasized that ML is not a *magic*! It essentially consists of four basic elements: linear algebra, optimization, probability & statistics and algorithms. The subject's broad popularity has been, in part, motivated by developments of excellent software such as Tensorflow [40]. While ML will surely remain as a powerful research tool, it must be utilized in the context of a very strong domain modeling.

2.2. Perspectives for QC

The unit of quantum information is a "qubit" (or quantum bit) [41]. In QC the qubits have the quantum mechanical property of being in *both* states 0 and 1 simultaneously. It is currently possible to conduct digital quantum computation with about 30 qubits with gate error rates of order 1-2 percent. To achieve an advantage for quantum over classical computing, it is required to increase the number of qubits to about 50-100, and to decrease the error rates to less than 0.1%. This is expected to happen within the next decade or so. Solution of multi-dimensional non-linear partial differential equations as required for turbulent combustion computations on a digital universal quantum computer would require a fault-tolerant computer along with millions of gates and qubits [23,42]. This would not be possible for another decade or somewhat longer. In the meantime, other near-term alternatives are available. Some of these are listed here:

Noisy Intermediate-Scale Quantum (NISQ): These devices typically consist of order several hundreds of imperfect qubits, which can only operate for some fixed maximum number of cycles.. The algorithms in these machines are based on those in gate operations, but without any error corrections [20]. Some prospects for such computing are currently being examined in many fields including machine learning, optimization, chemistry and materials science amongst others. All of these are useful for turbulent combustion.

Analogue Computers, Quantum Simulators and Annealers: These machines are designed to deal with specific problems and potentially provide quantum speedups [43]. In these devices, operations are implemented as controlled interactions between qubits that operate continuously in time. In the actual operation, the physical problem is mapped onto the an evolution of a quantum system. D-Wave computers are considered to belong to this category of quantum computers [44]. It is useful to identify research areas in which the governing equations can be mapped into a format suitable for quantum annealers & simulators.

Hybrid Quantum-Classical Computing (HQQC): All of the alternatives listed here can be used as a potential co-processor to a calculation on a classical computer. These type of computing has proven functional [45–47], and is expected to gain more popularity as quantum computers become widely accessible.

Quantum-Inspired Algorithms: Work is in progress in identifying classical algorithms that are"*quantum-inspired*" [23]. For example, *matrix product state* (MPS) algorithms are deemed suitable for large scale turbulence simulations. The MPS is an important sub-type of tensor networks [48,49]. Essentially, the algorithm works by mapping the differential equations (Navier-Stokes, reactiondiffusion, energy, etc.) onto a tensor network, and evolving the network towards the solution. These networks provide one of the most effective means of dealing with strongly correlated quantum systems [50]. Work along this path is in progress by Jacksch and co-workers [51].

The success rate of QC for simulating turbulence, or any other classical phenomena, is directly related to the progress in establishing and sustaining a "virtuous cycle" in QC [21]. Similar to that in semi-conductor technology, it is crucial to consider QC and its prospects for as many problems and applications as possible.

Future programs in both ML and/or QC should encourage partnerships and collaboration of both domain scientists and ML/QC experts. The turbulent combustion community is not very far into coupling with these modern disciplines. Therefore, shall be ready for dealing with issues that are inevitable in multidisciplinary programs including social, behavioral, and economic challenges [21,52].

Declaration of Competing Interest

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