Research Plan

Accelerating the Solution of PDEs using Quantum Computers

Author: **Abdul Moiz Mehmood** , **abdulmoizmehmood@gmail.com**

Areas of interest & Domain of research*

1. Finite Element Method
2. Quantum Computing Algorithms
3. *Numerical Solutions to Partial Differential Equations
4. Graph Theory
5. Quantum Machine Learning

Objective

The aim here is to describe the landscape of possibilities while looking to accelerate PDEs solutions, in general, and via finite-element method for realtime (otherwise) physics based simulations in particular. This document, hence, seeks to merit an exploration of the aforementioned potential research areas.

Keywords: machine learning, deep learning, continuous quantum algorithms, quantum graphs, finite element analysis, machine experience persistence, tensorflow quantum, pennylane, qiskit, cirq, blockchain, crypto currency prediction, meta-learning, neural network, graph theory, recurrent neural network.

1. Current Landscape and Possibilities

With an emphasis on being concise, and to remain within the scope of this documents requirements, let us start by stating that most scientific phenomena can be described via PDEs and yet numerical solutions for these PDEs can generate a significant computational cost depending on the spatiotemporal complexity and required accuracy of the model.

Since quantum information processing algorithms show (polynomial and exponential in some cases) speedups over their classical counterparts [1, 2], numerical solutions for PDEs via quantum algorithms (QAs from here onwards) promise to be more efficient.

Efficiency contrast of QAs over other classical solutions is further exaggerated for complex physical systems. This efficiency is not only merely theoretical, nor limited to future quantum devices since several tech giants like Google, IBM, etc. (and some government backed startups) are already investing heavily in quantum tech and the practical results can be seen even in these small-scale (NISQ) quantum devices [3, 4].

That being said, [14] raises a question (do the claimed "*exponential*" speedups translate well from theory to practice?) on the implementation of suggested QAs on PDEs. This, however, doesn't takeaway anything from the proven potential of NISQ devices which will only improve in the coming decade [4].

At present most QAs for PDEs are mapped to (after discretization) either a PDE resembling Schrödinger's Equation or a system of Linear Equations, termed as Hamiltonian Solution and Harrow, Hassidim, Lloyd (HHL) algorithm, respectively. Both of these routes result in a quantum state from which a part (functional) of the solution can be obtained via "*Measurement*". Getting a full solution via state tomography is quite impractical at this measurement step as the quantum state contains the solution usually encoded in its amplitude, though, using phase encoding and variational quantum algorithms (VCAs) with this scheme can provide potential alternatives [5, 6] especially with NISQ and small-scale or cloud based quantum devices. Also VCAs approach [7] also links up PDE solutions via FEM with machine learning and meta-learning, but more on that in the coming sections.

Here, let us not delve much into the two well-known approaches mentioned above and also recognize that literature suggests other techniques to solve a PDE via QAs. For instance, [8], based on grover's algorithm or extending this further [9], both of which inturn can be linked to quantum graph structures (essentially quantum analogues for page rank and recommendation algorithms etc.) to take this approach further and [10] seems to back this idea as graph structures are closely linked to quantum random walks (for both Markovian and non-Markovian regimes).

For all the techniques mentioned above perhaps one of the most critical steps (and hence a general limiting factor for QAs for PDEs) is the initial quantum state preparation. While preparing a general quantum state isn't possible, an "*efficient*" and more specific initial quantum state, such as [11], hence requires state preparation algorithms like qGAN [12], uniformly controlled rotations [13], etc. Since the landscape and associated possibilities are quite extensive (complexity analysis of the PDE and Iteration of QAs to avoid errors, etc.), we therefore, in the upcoming sections, provide only a general overview of some of the possibilities associated with QAs in general and FEM in particular.

2. Quantum Algorithms targeting FEM

In section 1, we only mentioned discretization but when tasked with solving a PDE the error encountered within the discretization process needs to be considered for any acceleration a QA may suggest. This is because of [15]. A way to circumvent this problem is via introducing CVQAs (continuous variable quantum algorithms) which can store functions like, ***f(x,t)***, in a quantum state (***n*** dimensional) [16].

Since quantum information processing is essentially exploitation of the quantum phenomenon (continuous or discrete), CVQAs are rapidly developing. To make this much more digestible, let's say if discretization equals Dirac formulation then CVQAs would be good old wave mechanics (nothing that bra-ket notation can also be used for CVQAs). Also [17, 18] suggest that a viable hybrid approach can be further investigated. To apply CVQAs for discretization, it is important to note that there are two main types. 1, QAs designed for continuous domains and 2. QAs originally designed for discrete variable domains but later adapted as CVQAs [19, 20, 21, 22, 23].

Since we already mentioned graph structures and Grover's Algorithm association, expanding on that with [19] along with works such as [24], merit an investigation for developing quantum analogues for FEM. While another possible source of acceleration would be in development of QAs that solve the problem of model calibration (reducing uncertainty of the solution and/or increasing its accuracy), which in essence would be quantum analogues for the classical combinatorial FEM optimization via rank aggression [25], QAOA (Qiskit) [26], [27], etc.

Use of machine learning for FEM is an active field and quantum machine learning, QML, (can be implemented on present NISQ devices via pennylane, qiskit, tensorflow quantum, etc) can easily overcome the shortcomings, like modeling for a dataset with large degrees of freedom, of a classical system [28]. To that end, various basic (associative adversarial networks, qGANs) and complex (k-means, KNN, etc.) QAs can be employed.

To gauge the “acceleration” in such applications, the efficiency for the proposed complex QA may need other basic or complex QAs to be performed beforehand. For example, the quantum analogue for k-nearest neighbour algorithm (KNN), relies on a number of iterations of the SWAP-test [29] and quantum minimization [30]. Adding to that [31] shows the efficiency of using such QAs on a NISQ device (IBMQ).

As an example for ML and QML enhanced FEM, let's say we have a PDE that models for fluid dynamics domain given certain initial parameters. In a realistic case the size of the system can be huge (billions of degrees of freedom), and hence its numerical analysis would then demand significant computational power. Now after the process goes through the usual pipeline and we end up with only final numerical results, that is to say the entire machine experience gained by going through the iterations is lost. So even slight changes in initial conditions would demand the same time/computational costs each time.

QML preserves this machine experience in the form of datasets which can be used to train/predict future inputs/outputs. Since we may observe a high level of non-linearity (e.g a complex physical system in non-planar geometries [32]), utilization of the quantum version of deep neural networks may be quite beneficial [33, 34]. This can be done even with noisy devices like Reghetti and IBMQ, by including Qiskit, Matlab Simulink Quantum Module, Pennylane, TensorflowQ, Minesdb (generate training models via AI tables) etc. employing quantum analogues for classical algorithms suggested in [35].

3. Other Quantum Algorithms for PDEs

Building on the idea of ML and quantum neural networks, QNNs, let us now put forward QAs that are not directly linked to FEM. Something like “meta-learning” fits the bill as it improves any QNN and is not just limited to FEM based PDE solutions. Since QNNs are all highly practical in the context of present noisy quantum devices, meta-learning solves problems like parameter initialization etc. as described in [36].

Other viable approaches for solving PDEs on a quantum processor is by using a probabilistic approach like Monte Carlo Simulation (MCS) or the Density Matrix formalism. A QA from these can be established via borrowing concepts like quantum markovian (non-markovian) chains from open quantum systems dynamics. Although [37] and [38] do not use QAs but support the general idea behind the proposed approach nonetheless and at least merit further investigation. Also when we take into account that when talking about noisy quantum devices we can't really ignore the domain designed to cater for the “noise” especially when both classical and quantum noise can potentially be used as a quantum resource. [39, 40].

References

[1] Mosca, M., "Quantum algorithms", arXiv:0808.0369, 1-71 (2008).

[2] Coles, P.J.,Eidenbenz, S., Pakin, S. et al."Quantum Algorithm Implementations for Beginners", arXiv:1804.03719, 1-76 (2018).

[3] Filipe Fontanela & Antoine Jacquier & Mugad Oumgari, 2019. "A Quantum algorithm for linear PDEs arising in Finance," Papers 1912.02753, arXiv.org, revised Feb 2021.

[4] John Preskill , “Quantum Computing in the NISQ era and beyond”, arXiv:1801.00862v3, revised Jul 2018.

[5] Hiroshi Yano, et al.“Efficient Discrete Feature Encoding for Variational Quantum Classifier”, IEEE Transactions on Quantum Engineering, vol. 2, pp. 1-14, 2021, Art no. 3103214.

[6] Kiyoshi Tamaki, et al.”Phase encoding schemes for measurement device independent quantum key distribution and basis-dependent flaw” , Phys. Rev. A 85, 042307 (2012).

[7] Michael Lubasch, et al.“Variational quantum algorithms for nonlinear problems,” Physical Review A 101, 010301 (2020).

[8] Bolesław Kacewicz, “Randomized and quantum algorithms yield a speed-up for initial-value problems,” Journal of Complexity 20, 821–834 (2004).

[9] Frank Gaitan, “Finding flows of a navier–stokes fluid through quantum computing,” npj Quantum Information 6, 1–6 (2020).

[10] Noah Linden, et al.“Quantum vs. classical algorithms for solving the heat equation,” arXiv preprint arXiv:2004.06516 (2020).

[11] Lov Grover, et al.“Creating superpositions that correspond to efficiently integrable probability distributions,” arXiv preprint quant-ph/0208112 (2002).

[12] Mikko Mottonen,et al.“Transformation of quantum states using uniformly controlled rotations,” arXiv preprint quant-ph/0407010 (2004).

[13] Christa Zoufal, et al.“Quantum generative adversarial networks for learning and loading random distributions,” npj Quantum Information 5, 1–9 (2019).

[14] Ashley Montanaro, et al.”Quantum algorithms and the finite element method”. Phys. Rev. A 93, 032324, 17 March 2016.

[15] Arthur G Werschulz, “The computational complexity of differential and integral equations: An information-based approach”, (Oxford University Press, Inc., 1991).

[16] Juan Miguel Arrazola, et al.“Quantum algorithm for nonhomogeneous linear partial differential equations,” Physical Review A 100, 032306 (2019).

[17] Seth Lloyd. “Hybrid quantum computing” (2000). arXiv:quant-ph/0008057.

[18] Xiaoguang Wang. “Continuous-variable and hybrid quantum gates”. Journal of PhysicsA: Mathematical and General 34.44 (2001), pp. 9577–9584.

[19] Arun K. Pati, et al.“Quantum searching with continuous variables” (2000). arXiv:quant-ph/0002082.

[20] Arun K. Pati, et al.“Deutsch-Jozsa Algorithm for Continuous Vari-ables” (2002). arXiv:quant-ph/0207108.

[21] Rob C Wagner, et al.“The continuous-variable Deutsch–Jozsa algorithm using realistic quantum systems”. Journal of Physics A: Mathematical and Theoretical 45.24(2012), p.244015.

[22] Samuel J. Lomonaco Jr., et al.“Quantum Hidden Subgroup Problems:A Mathematical Perspective” (2002). arXiv:quant-ph/0201095.

[23] Samuel J. Lomonaco Jr., et al.“A Continuous Variable Shor Algorithm”(2002). arXiv:quant-ph/0210141.

[24] Kaveh, A., et al.”Formation of graph models for regular finite element meshes”, Computer Assisted Methods In Engineering And Science, 16(2), 101-115

[25] Gaetano Miraglia, et al.“Synergistic and combinatorial optimization of finite element models for monitored buildings”, Journal of Civil Structural Health Monitoring, 10.1007/s13349-020-00394-4, (2020).

[26] https://qiskit.org/textbook/ch-applications/qaoa.html

[27] Guillaume Verdon, et al.”Learning to learn with quantum neural networks via classical neural networks”, arXiv:1907.05415, Jul 2019.

[28] Sammut, C. et al.”Encyclopedia of machine learning and data mining”, Springer US, 1335 (2017).

[29] Aumeur, E., Brassard, et al.”Machine learning in a quantum world", Proc. Conference of the Canadian Society for Computational Studies of Intelligence, 431-442 (2006).

[30] Christoph, D. et al."A quantum algorithm for finding the minimum", arXiv:quant-ph/9607014, 1-2,(1996).

[31] Fastovets, D. V. et al. “Machine learning methods in quantum computing theory.” International Conference on Micro- and Nano-Electronics (2019).

[32] Mehmood, A., “Nonlinear Partial Differential Equations in NonPlanar Geometries”, BS thesis, Comsats University, Islamabad, Spring 2018.

[33] Liang L, et al. “A deep learning approach to estimate stress distribution: a fast and accurate surrogate of finite-element analysis”. J. R. Soc. Interface 15: 20170844.

[34] Mehdi Jokar, et al. “Finite element network analysis: A machine learning based computational framework for the simulation of physical systems, Computers & Structures”, Volume 247, 2021, 106484, ISSN 0045-7949.

[35] O. Kononenko, et al. “Machine Learning and Finite Element Method for Physical Systems Modeling”, arXiv:1801.07337.

[36] Guillaume Verdon, et al. “Learning to learn with quantum neural networks via classical neural networks”, arXiv:1907.05415v1, 11 Jul 2019.

[37] Marshall, G. (1989). “Monte Carlo methods for the solution of nonlinear partial differential equations”. Computer Physics Communications, 56(1), 51–61.

[38] Anker, F., et al.“SDE based regression for linear random PDEs”. SIAM J. Sci. Comput., 2017, 39(3), A1168–A1200.

[39] Mehmood, A., “The Swapping of Quantum Correlations through Teleportation under Quantum and Davies Environments”, MS thesis, Comsats University, Islamabad, Fall 2019.

[40] R. Lo. Franco, et al. “Revival of quantum correlations without system-environment back-action”, Phys. Rev. A 85, 032318 (2012).