Solving Partial Differential Equations using a Quantum Computer

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***Abstract*—The simulation of quantum systems currently constitutes one of the most promising applications of quantum computers. However, the integration of more general partial differential equations (PDEs) for models of classical systems that are not governed by the laws of quantum mechanics remains a fundamental challenge. Current approaches such as the Variational Quantum Linear Solver (VQLS) method can accumulate large errors and the associated quantum circuits are difficult to optimize. A recent method based on the Feynmann-Kitaev formalism of quantum dynamics has been put forth, where the full evolution of the system can be retrieved after a single optimization of an appropriate cost function. This spacetime formulation alleviates the accumulation of errors, but its application is restricted to quantum systems only. In this work, we introduce an extension of this formalism applicable to the non-unitary dynamics of classical systems including for example, the modeling of diffusive transport or heat transfer. In addition, we demonstrate how PDEs with non-linear elements can also be integrated to incorporate turbulent phenomena.**

***Index Terms*—quantum simulation, partial differential equations, Feynman–Kitaev Hamiltonian**

I. Introduction

Quantum computers are a promising tool with immediate applications in physics and chemistry [1]. Apart from electronic structure calculations of molecular systems, there is a growing interest across many industries in developing quantum algorithms for the integration of partial differential equations (PDEs) and other applications where a very large number of parameters is involved. Solving a PDE using a classical computer is typically carried out via numerical integration, where an initial state is propagated iteratively via infinitesimal time steps. When translating such a methodology into a variational quantum algorithm, an optimisation problem has to be solved for every timestep, and errors associated to the noisy nature of quantum processors quickly accumulate, restricting evolution to very short time intervals. Such a procedure can be readily implemented using the the well established Variational Quantum Linear Solver (VQLS) method that is able to solve the corresponding linear system of equations of the PDE in question.

Instead of propagating the initial state via a sequence of infinitesimal steps, a spacetime formulation of the original problem in a larger grid can directly provide the full time evolution of the system of interest and circumvent the accumulation errors associated with iterative approaches. We have applied VQLS to such a spacetime formulation of the PDE and found that the quantum circuits that minimise this global cost function are very hard to optimise, and we may well be facing a barren plateau problem where the cost function presents vanishing gradients when randomly sampled [3].

Following this spacetime approach, a recent method based on the Feynmann-Kitaev formalism of quantum dynamics has been put forth, where the full evolution of the system can be retrieved after a single optimization of a well-defined cost function [4]. This spacetime formulation alleviates the accumulation of errors, but its application is restricted to quantum systems only.

In this work, we introduce an extension of the Feynman–Kitaev formalism that is tailored to the integration of arbitrary PDE and provide proof-of-principle calculations that demonstrate that fundamental processes such as diffusion and turbulence can be well-reproduced within this framework.

These simulations constitute our first attempt to develop a quantum solver toolbox that is able to bring the power of quantum computing to a wider range of industries that rely on the integration of PDEs with non-linearities, such as the transport of ions in electrochemistry [2] or the aerodynamics of a wind turbine in mechanical engineering.

II. Method

A. Feynman–Kitaev Hamiltonian

The time evolution of a unitary, norm-conserving quantum system described by the Hamiltonian $\hat{H}_{\mathrm{S}}$ can be directly obtained as the ground-state of an expanded Hamiltonian that incorporates a clock quantum register [4]. The so-called Feynmann–Kitaev Hamiltonian is then given by

$$\hat{C} = \hat{C}_0 + \frac{1}{2}\left(\hat{C}_1 - \hat{C}_2\right), \tag{1}$$

with

$$\hat{C}_0 = \Big[\hat{I} - |\psi(0)\rangle\,\langle\psi(0)|\Big] \otimes |0\rangle\langle 0|, \tag{2a}$$

$$\hat{C}_1 = \sum_{i=0}^{n-1} \hat{I} \otimes |i\rangle\langle i| + \hat{I} \otimes |i+1\rangle\langle i+1|, \tag{2b}$$

$$\hat{C}_2 = \sum_{i=0}^{n-1} \hat{U}(dt) \otimes |i+1\rangle\langle i| + \hat{U}^{\dagger}(dt) \otimes |i\rangle\langle i+1|, \tag{2c}$$

where $\hat{C}_0$ enforces an specific initial state, and $\hat{C}_1$ and $\hat{C}_2$ guarantee that time evolution is governed by the propagator $\hat{U}(dt) = e^{-i\hat{H}_{\mathrm{S}}\,dt}$. The operator $\hat{C}$ can then be interpreted as a cost function whose minimum corresponds to the history state, a coherent superposition $\sum_t |\psi(t)\rangle \otimes |t\rangle$ in the joint System-Clock Hilbert space from which the time evolution of the system $|\psi(t)\rangle$ can be readily extracted. This minimization can be carried out using the standard *variational quantum eigensolver method* (VQE) where a parametrized quantum circuit is measured and optimized in an iterative manner.

B. Non-unitary time evolution with non-linearities

The validity of the formalism described above is sustained on the one hand in the conservation of quantum probabilities, and secondly, on the linearity of the quantum operations that are available in the quantum processor, i.e. the method is valid for systems that are governed by the Schrödinger equation $i\hbar\frac{\partial\psi}{\partial t} = \hat{H}_{\mathrm{S}}\psi$, on the condition that $\hat{H}_{\mathrm{S}}$ is Hermitian. Therefore, the method as it was published before is not suitable for the simulation of dissipative quantum systems and more importantly, it cannot be applied to classical systems whose evolution is governed by arbitrary PDEs that may contain non-linear elements.

We extend the Feynman–Kitaev method to deal with non-unitary time evolution, and demonstrate how important processes such as diffusive behaviour can be accommodated in this framework. We are preparing a follow-up publication to describe the details of our method.

III. Results

Firstly, we demonstrate the validity of such methodology to non-unitary systems to a simple model of diffusion, which constitutes an integral part of any mathematical model of charge transport in electrochemistry. Secondly, we turn our attention to the Burgers' equation equation [5], which constitutes a canonical model for the study of turbulent phenomena and PDEs with non-linear elements. These equations can be formally expressed as

$$\frac{\partial c}{\partial t} = \alpha\,\frac{\partial^2 c}{\partial x^2} + \beta\,c\,\frac{\partial c}{\partial x}. \tag{3}$$

When the coefficient $\beta = 0$, the solution of the corresponding diffusion equation is shown in Figure 1, where c is the concentration of some ionic species in a liquid, and $\alpha = 0.1\ \mathrm{cm}^2/\mathrm{s}$ is the diffusion constant. For this simulation, we have employed a *statevector* simulator from the IBM Qiskit toolkit with 2 time qubits (4 time steps) and 4 spatial qubits (16 spatial points). Notice how the resulting dynamics of the optimized quantum circuits overlap on the one hand with those obtained after an exact diagonalization of our adapted Feymann–Kitaev Hamiltonian, and secondly, with the dynamics resulting from a simple numerical integration of the associated PDE.

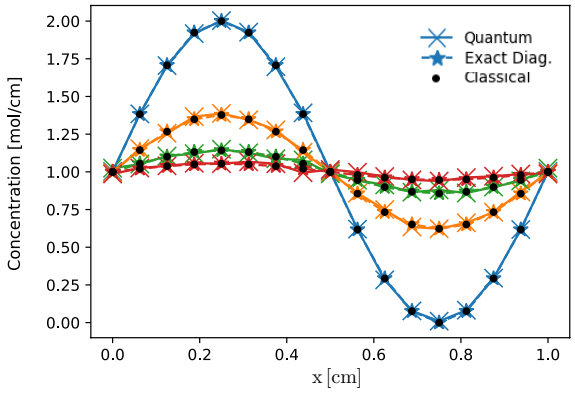

Fig. 1. Results from the diffusion equation with 2 time qubits (4 time steps) and 4 spatial qubits (16 spatial points), for $t = 0$ (blue), $t = dt$ (orange), $t = 2dt$ (green), and $t = 3dt$ (red), with $dt = 0.25$ s.

Finally, we incorporate the non-linear term in Eq. (3) with $\beta = -0.1\ \mathrm{cm}^2/(\mathrm{mol\ s})$. We performed this simulation with 3 spatial qubits (8 spatial points) as shown in Figure 2 on the same statevector simulator and compared it with a numerical integration of the equation.

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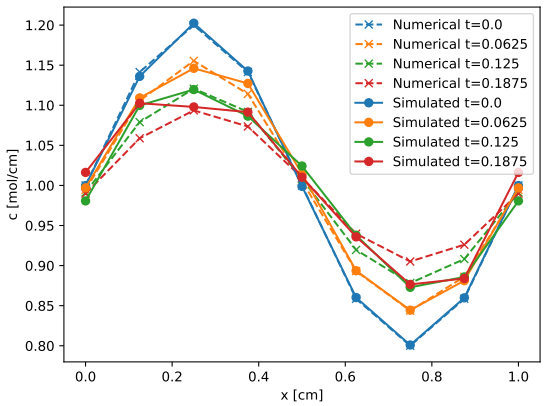

Fig. 2. Results from the Burgers' equation with 2 time qubits (4 time steps) and 3 spatial qubits (8 spatial points) comparing the quantum solution with numerical integration.

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