Quantum Science and Technology

PAPER

Generalized quantum assisted simulator

Tobias Haug* and Kishor Bharti*
Centre for Quantum Technologies, National University of Singapore, 117543, Singapore
* Authors to whom any correspondence should be addressed.
E-mail: tobias.haug@u.nus.edu and kishor.bharti1@gmail.com

Keywords: noisy intermediate scale quantum algorithms, quantum simulation, open quantum system, quantum computing, differential equations

Abstract
We provide a noisy intermediate-scale quantum framework for simulating the dynamics of open quantum systems, generalized time evolution, non-linear differential equations and Gibbs state preparation. Our algorithm does not require any classical—quantum feedback loop, bypass the barren plateau problem and does not necessitate any complicated measurements such as the Hadamard test. We introduce the notion of the hybrid density matrix, which allows us to disentangle the different steps of our algorithm and delegate classically demanding tasks to the quantum computer. Our algorithm proceeds in three disjoint steps. First, we select the ansatz, followed by measuring overlap matrices on a quantum computer. The final step involves classical post-processing data from the second step. Our algorithm has potential applications in solving the Navier–Stokes equation, plasma hydrodynamics, quantum Boltzmann training, quantum signal processing and linear systems. Our entire framework is compatible with current experiments and can be implemented immediately.

1. Introduction

The quest for quantum advantage for practical use-cases in the noisy intermediate-scale quantum (NISQ) era [1, 2] has spurred the development of algorithms, which can be executed on shallow quantum circuits and do not necessitate error correction. Despite the hope rendered by the recent Google quantum supremacy experiment [3] at the hardware frontier, it remains to devise algorithms which can harness the power of the NISQ devices for problems of practical relevance.

The task of estimating the ground state and ground state energy of a Hamiltonian is one such model problem, for which one could expect to conceive algorithms for quantum advantage. Another canonical problem is the broader challenge of simulating the quantum dynamics. In fact, the birth of the field of quantum computation can be attributed to Feynman’s dream of simulating the quantum dynamics [4]. While the Hamiltonian ground state problem has applications in combinatorial optimization, solid-state physics and quantum chemistry, quantum simulation offers the possibility to explore topics such as high-temperature superconductivity and drug design. Interestingly, both Hamiltonian ground state problem and quantum simulation can be tackled via variational principles, based on static and dynamical methods respectively.

The leading canonical NISQ era algorithm for approximating the ground state and ground state energy of a Hamiltonian is variational quantum eigensolver (VQE) [5–12]. The aforementioned algorithm is based on the Rayleigh–Ritz variational principle and employs a classical–quantum feedback loop to update the parameters of the corresponding parametric quantum circuit (PQC). The classical optimization program corresponding to VQE is highly non-convex and in general uncharacterized [13]. The classical–quantum feedback loop further impeded the possibility to utilize the quantum computer, until the classical computer has calculated its output. In general the ansatz is either not compatible with the existing hardware capabilities or chosen in a heuristic fashion. The absence of a mathematically rigorous structure renders any systematic investigation challenging. Moreover, the recent results revealing the existence of the barren plateau as the hardware noise, number of qubits or amount of entanglement increase, has led to genuine
concerns about the fate of VQE [14–19]. Even gradient-free optimization techniques fail to evade the fatality of the barren plateaus [20].

For simulating the dynamics of closed quantum systems, the leading canonical NISQ era algorithm is the variational quantum simulation (VQS) algorithm [21–23]. The VQS algorithm utilizes a hybrid classical–quantum feedback loop to update the parameters of a PQC using dynamical variational principles. The aforementioned algorithm as well as its VQE based variant, i.e. the subspace variational quantum simulator [24], share resemblances and hence many of the problems of VQE such as the barren plateau problem. The VQS algorithm furthermore requires complicated measurements, does not provide a systematic strategy to choose the ansatz and mandates the adjustable parameters to be real-valued [23].

Recently algorithms as alternative beyond VQE and VQS were proposed in the literature [25–27]. The quantum assisted eigensolver and iterative quantum assisted eigensolver (IQAE) demonstrate a systematic structure in their algorithm [25, 26]. Their classical optimization program is well-characterized quadratically constrained quadratic program with a single equality constraint. In particular, the IQAE algorithm offers an organized path to construct the ansatz, circumvents the barren plateau problem, does not mandate any quantum–classical feedback loop and can be efficiently executed on the current quantum hardware without the need of complicated measurements. To tackle the challenges encountered by VQS, the quantum assisted simulator (QAS) can simulate dynamics of quantum systems while boasting the same advantages as IQAE [27].

The task of simulating the dynamics for open quantum systems is relatively more demanding than for closed quantum systems. Here, challenging tasks related to dynamics are generalized time evolution with a non-Hermitian or nonlinear Hamiltonian as well as Gibbs state preparation. In the literature, various algorithms have been proposed to solve the aforementioned tasks [28–36]. However, the existing algorithms are either not compatible with current hardware capabilities or share the troubles faced by VQS.

In this work, we provide the generalized quantum assisted simulator (GQAS) to simulate open system dynamics, generalized time evolution, nonlinear differential equations and Gibbs state preparation. The GQAS algorithm furnish an antidote to the hardships faced by the current NISQ alternatives. In particular, the GQAS does not mandate any classical–quantum feedback loop, circumvents the barren plateau problem and does not require any complicated measurements. The whole framework is compatible with existing hardware capabilities.

We introduce our algorithm in section 2. Then, we show four different applications of our algorithm. First, we solve open system dynamics in section 3, then generalized time evolution in section 4, followed by nonlinear differential equations in section 5 and Gibbs state preparation in section 6. Finally, we discuss the results in section 7.

2. Algorithm

The execution of GQAS algorithm involves in general three steps (see figure 1 for pictorial synopsis), which we show in the following. The specific details of GQAS vary depending on the application, which we defer to the application part in sections 3–6. Our algorithm proceeds as follows

(a) The ansatz is selected as a linear combination of quantum states
(b) Calculation of the overlap matrices on a quantum computer
(c) Solving the dynamical evolution equation on a classical computer

First, we choose a set of quantum states \( \mathcal{S} = \{ | \psi_j \rangle \} \). The states should be chosen such that they span the space of the problem, and can be selected adapted to the application as shown in section 3. The ansatz is either a linear combination of states \( | \phi \rangle = \sum_{i=1}^{M} \alpha_i | \psi_i \rangle \) with classical combination coefficients \( \alpha_i \in \mathbb{C} \) (sections 4 and 5) or a hybrid density matrix with a coefficient matrix \( \beta_{ij} \in \mathbb{C} \) as introduced in equation (1) (sections 3 and 6). Note that the ansatz states are fixed and only classical combination coefficients are updated later on.

For step 2, the quantum computer measures overlap matrices of the form \( \langle \psi_j | O | \psi_i \rangle \) with some observable \( O \). As we will show in section 3, step 2 can be performed efficiently on a quantum computer, without the requirement of any complicated measurements such as the Hadamard test. When the ansatz states \( | \psi_j \rangle = P_i | \psi \rangle \) are generated by applying a set of Pauli strings \( \{ P_i \}_{i=1}^{M} \) to a reference state \( | \psi \rangle \), the overlaps can be calculated as simple measurements of Pauli strings of the form \( \langle \psi | P_i | \psi \rangle \) with some Pauli string \( P \). This is because products of Pauli strings are again Pauli strings up to a pre-factor \( \pm 1, \pm i \), which can be calculated trivially.

As last step, we perform evolve the combination coefficients using the measured overlaps. Note that the equations depend on the particular application and will be discussed in detail in the following sections.
Figure 1. Concept of the general quantum assisted algorithm (GQAS). It consists of three steps. The first step selects the ansatz as a linear combination of states $|\psi_i\rangle \in S$ from a set $S$. The ansatz can be either a pure state or a mixed state $\rho$. We introduce the concept of hybrid mixed state $\rho = \sum_{i,j} \beta_{ij}(t) |\psi_i\rangle \langle \psi_j|$. Only the coefficients $\beta_{ij}(t)$ which are stored on a classical computer are varied in time, thus avoiding any classical–quantum feedback loop. The second step computes the overlap matrices on a quantum computer, which can be measured efficiently using Pauli strings [27]. Finally, the differential equation to be computed is solved on a classical computer.

2.1. Hybrid density matrix

Here, we introduce the concept of the hybrid density matrix which will be used for applications in sections 3 and 6. The ansatz is constructed from a set of fixed quantum states, which we define as follows

**Definition 1.** Hybrid density matrix. Given a Hilbert space $\mathcal{H}$ and a set of $M$ quantum states $S = \{|\psi_j\rangle \in \mathcal{H}\}_j$, a hybrid density matrix $\rho$ is given by

$$\rho = \sum_{(i,j) \in S \times S} \beta_{ij} |\psi_i\rangle \langle \psi_j|$$

for $\beta_{ij} \in \mathbb{C}$. The coefficients $(\beta_{ij})_{ij}$ are stored on a classical device and the quantum states correspond to some quantum system. A hybrid density matrix represents a valid density matrix if $\text{Tr}(\rho) = 1$ and $\rho \succeq 0$.

The normalization condition is fulfilled when

$$\text{Tr}(\rho) = \text{Tr}(\beta E) = 1,$$

where the coefficient matrix $\beta$ is a positive semidefinite matrix and we define the overlap matrix via

$$E_{ij} = \langle \psi_i | \psi_j \rangle.$$

The positive semidefinite condition of $\rho$ is automatically fulfilled when $\beta$ is a positive semidefinite matrix as we have

$$\langle x | \rho | x \rangle = \sum_{ij} \langle x | \psi_i \rangle \beta_{ij} \langle \psi_j | x \rangle = c_x^\dagger \beta c_x \geq 0 \quad \forall |x\rangle,$$

where $c_x$ is a vector with $c_{i\psi} = \langle \psi | x \rangle$. We note that the purity of the hybrid density matrix is given by $\text{Tr}(\rho^2) = \text{Tr}(\beta^2 E^2)$. The notion of hybrid density matrix helps us remove the quantum–classical feedback loop and thus renders the different steps of our GQAS algorithm disjoint. Here, the hybrid density matrix can be classically updated by tuning the classical coefficients $\beta_{ij}$ without requiring a change to the quantum states $|\psi_i\rangle \in \mathcal{H}$ on the quantum computer. We note that expressing the ansatz state via a classical combination of quantum states is a powerful concept that has been used in a number of papers [26, 37–44] for calculating ground and excited states. A representation of density matrices with variational quantum circuits has been proposed in references [35, 44].

In the following sections, we proceed to discuss GQAS algorithm for simulating the dynamics of open systems, generalized time evolution, solving nonlinear differential equations and Gibbs state preparation.
3. Open system dynamics

A system interacting with a bath within the Born–Markov approximation can be described with the Lindblad master equation [45]

$$\frac{d}{dt}\rho = -i[H, \rho] + \sum_{n=1}^{f} \gamma_n \left( L_n \rho L_n^\dagger - \frac{1}{2} L_n^\dagger L_n \rho - \frac{1}{2} \rho L_n^\dagger L_n \right),$$

(5)

where $\rho$ is the density matrix of the system, $H$ describes the Hamiltonian of the system and $f$ operators $L_k$ encode the action of the bath on the system and $\gamma_n \geq 0$. This type of equation has been employed to describe a wide range of systems interacting with the environment. This equation is valid as long as the interaction between system-bath is weak, and the correlation between system and bath decay fast.

To evolve the open system problem, we now introduce the following notations

$$D_{\psi} = \langle \psi | H | \psi \rangle,$$

(6a)

$$R_{\psi}^n = \langle \psi | L_n | \psi \rangle,$$

(6b)

$$F_{\psi} = \langle \psi | L_n^\dagger L_n | \psi \rangle.$$  

(6c)

Using above overlap matrices and equation (1), we can now use the Dirac and Frenkel variational principle [23]

$$\text{Tr} \left( \delta \rho \left( \frac{d}{dt} \rho - \mathcal{L}(\rho) \right) \right) = 0,$$

(7)

where $\mathcal{L}(\rho)$ is the right-hand side of equation (5). We then find the following differential equation for the time dependent parameters $\beta(t)$,

$$\mathcal{E} \frac{d}{dt} \beta(t) \mathcal{E} = -i(D \beta(t) \mathcal{E} - \mathcal{E} \beta(t) D) + \sum_{n=1}^{f} \gamma_n \left( R_n \beta(t) R_n^\dagger - \frac{1}{2} F_n \beta(t) F_n - \frac{1}{2} \mathcal{E} \beta(t) \mathcal{E} \right).$$

(8)

Assuming that $H = \sum_i a_i U_i$ and $L_k = \sum_j b_j V_j$ is a linear combination of $N$-qubit unitaries $U_i$ and $V_i$, where each unitary acts non-trivially on at most $O(\log N)$ qubits, then the overlap matrices can be measured efficiently using methods of [46]. For $U_i$, $V_i$ being Pauli strings, the overlaps can be easily calculated as measurements of Pauli strings and one can relax the aforementioned $O(\log N)$ constraint.

Note that for an ansatz that does not cover the full Hilbert space the evolution with the Lindblad terms may not preserve the trace of the ansatz $\text{Tr}(\mathcal{E} \beta)$. To accommodate for this, we numerically normalize $\beta(t)$ during the classical integration after every time step.

We show an example dissipative problem in figure 3 which first has been discussed in [28]. The Hamiltonian is an Ising model in a ladder configuration

$$H_L = \sum_{\langle ij \rangle} J \sigma_i^z \sigma_j^z + \sum_i h \sigma_i^x,$$

(9)

where $\langle ij \rangle$ denotes the set of nearest-neighbor couplings, $\sigma^z_i$ is the $z$ Pauli operator acting on the $i$th qubit. The qubits are arranged in a ladder configuration. Dissipation acts on the system in form of a spontaneous creation of excitations realized by $L_i = \sqrt{\gamma} \sigma^+$, where $\gamma$ is the creation rate and $\sigma^+ = |1\rangle \langle 0|_i$ is the raising operator acting on qubit $i$.

As first step, we choose a problem-aware ansatz that captures the evolving subspace by using the Hamiltonian. We generate a set of $M$ basis states $|\psi\rangle$ with the $K$-moment expansion [27]. This method of construction is inspired by the Krylov subspace expansion, which uses an expansion in terms of higher orders of the Hamiltonian $H$ to represent the solution space $\text{span}\{\psi, H\psi, H^2\psi, \ldots, H^K\psi\}$ [47]. The $K$-moment expansion is an adaption of this method which is suitable for NISQ devices here. The basis states are taken from the cumulative $K$-moment states [27]

$$\mathcal{CS}_K = \{|\psi\rangle \cup \{U_i |\psi\rangle\}_i \cup \cdots \cup \{U_k \cdots U_i |\psi\rangle\}_i \cdots \cup \{U_1 |\psi\rangle\} \},$$

(10)

where $|\psi\rangle$ is some efficiently preparable reference state and $U_i$ are taken from the set of $r$ Pauli strings that make up equation (9) with $H = \sum_{i=1}^{r} a_i U_i$.

As second step, we calculate the overlap matrices given in equation (6). This step is performed on a quantum computer, which we simulate here numerically. Our choice of $U_i$ as Pauli strings allows us to
determine all the overlaps as simple measurements of Pauli strings, which can be efficiently done on the current quantum hardware. We choose the initial state for the evolution to be $|0\rangle$ and a choice adapted to the problem instead of a randomized circuit could improve the fidelity \[48\].

The type of reference state is crucial for the representation power of the ansatz $M$. Increasing the full dynamical space, such that the fidelity decreases with time. We find the fidelity improves with gates arranged in a hardware-efficient manner in a chain topology (see figure 2).

In figure 3(a), we plot the evolution of the correlation of nearest-neighbor spins $\sum |i,j\rangle \sigma^z_i \sigma^z_j / 7$. The exact dynamics in both closed and dissipative regime can be reproduced exactly for the second $K$-moment expansion. In figures 3(b) and (c) we plot the fidelity between the simulation and the exact state as function of time and number of basis states $M$ of the ansatz without and with dissipation. We find similar performance when the states are picked randomly from the $K$-moment expansion. We find that for $M \geq 64 = 2^6$, we achieve unit fidelity. For smaller $M$, the ansatz does not cover the full dynamical space, such that the fidelity decreases with time. We find the fidelity improves with increasing $M$. We find higher fidelity for open dynamics due to the simulated state being highly mixed, which is easier to represent. The type of reference state is crucial for the representation power of the ansatz and a choice adapted to the problem instead of a randomized circuit could improve the fidelity \[48\].

---

**Figure 2.** Circuit of $N$ qubits to generate reference state $|\psi\rangle$. This state is used to generate ansatz states $|\psi_i\rangle = |\psi\rangle P_i$ by applying different Pauli strings $P_i$, $|\psi\rangle$ consists of $p$ layers of $N$ single qubit rotations around the $y$ axis with parameters $\theta_i$, followed by CNOT gates arranged in a nearest-neighbor chain topology. The parameters $\theta_i$ are chosen at random and then kept fixed for the entirety of the GQAS algorithm.

**Figure 3.** Simulation of the dynamics of an Ising ladder without and with dissipation. Circuit used to generate moment expansion is shown in figure 2. Initial coefficients $\beta(0)$ are calculated via IQAE such that the initial state $\rho(0)$ is a product state with all qubits in state zero. Parameters are $N = 6$, $J = 1$, number of layers $p = 6$, $h = 1$ and optional dissipative Lindblad term $L_i = -\gamma \sigma^z_i$ with $\gamma = 1$. (a) Dynamics of the nearest-neighbor spin correlation $\sum |i,j\rangle \sigma^z_i \sigma^z_j / 7$ without dissipation (closed) and with dissipation (open). Number of basis states is $M = 64$. (b) Fidelity $F$ of GQAS with exact time evolution for varying number of basis states $M$ without dissipation. (c) Fidelity $F$ with dissipation $\gamma = 1$. 

For the numerical demonstrations in this paper, we generate the reference state $|\psi\rangle$ by a hardware efficient circuit that is hard to simulate classically, given by random $y$-rotations followed by control not gates arranged in a hardware-efficient manner in a chain topology (see figure 2).

In figure 3(a), we plot the evolution of the correlation of nearest-neighbor spins $\sum |i,j\rangle \sigma^z_i \sigma^z_j / 7$. The exact dynamics in both closed and dissipative regimes can be reproduced exactly for the second $K$-moment expansion. In figures 3(b) and (c) we plot the fidelity between the simulation and the exact state as function of time and number of basis states $M$ of the ansatz for closed and open dynamics. We select the $M$ basis states by generating the two-moment expansion, and then select the first $M$ states in the order they were generated. We find similar performance when the states are picked randomly from the $K$-moment expansion. We find that for $M \geq 64 = 2^6$, we achieve unit fidelity. For smaller $M$, the ansatz does not cover the full dynamical space, such that the fidelity decreases with time. We find the fidelity improves with increasing $M$. We find higher fidelity for open dynamics due to the simulated state being highly mixed, which is easier to represent. The type of reference state is crucial for the representation power of the ansatz and a choice adapted to the problem instead of a randomized circuit could improve the fidelity \[48\].
4. Generalized time evolution

Next, we want to solve general linear equations with our algorithm. The generalized time evolution is given by

\[ B(t) \frac{d}{dt} |v(t)\rangle = |dv(t)\rangle, \]

such that \(|dv(t)\rangle = \sum_j A_j(t)|v'_j(t)\rangle\), where \(A_j(t)\) and \(B(t)\) are time-dependent operators and \(|v(t)\rangle\) is the system state. We use the following ansatz for the system states

\[ |v(t)\rangle = \sum_{i=0}^{m-1} \alpha_i(t)|\psi_i\rangle \]

\[ |v'_j(t)\rangle = \sum_{i=0}^{n-1} \gamma_{j\alpha}(\alpha, t)|\phi_{i\alpha}\rangle, \]

where we define the state \(|v'_j(t)\rangle\) as a linear combination of arbitrary quantum states \(|\phi_{i\alpha}\rangle\) with \(s_j\) coefficients \(\gamma_{j\alpha}(\alpha, t)\). We now use McLachlan’s principle for the square of the absolute value and find [23, 49]

\[
0 \leq \delta \left\| B(t) \frac{d}{dt} |v(t)\rangle - |dv(t)\rangle \right\|^2 \\
= \sum_k \left( \frac{\partial|v(t)\rangle}{\partial\alpha_k^*} B(t) \left( B(t) \sum_j \frac{\partial|v(t)\rangle}{\partial\alpha_j} \hat{\alpha}_j - |dv(t)\rangle \right) \right) \delta \hat{\alpha}_k^* \\
+ \sum_k \left( \sum_j \frac{\partial|v(t)\rangle}{\partial\alpha_j^*} B(t) \hat{\alpha}_j - \langle dv(t) \rangle B(t) \frac{\partial|v(t)\rangle}{\partial\alpha_k} \right) \delta \hat{\alpha}_k 
\]

By demanding that McLachlan’s principle is fulfilled for arbitrary variations \(\delta \hat{\alpha}_k, \delta \hat{\alpha}_k^*\) and by using \(\frac{\partial|v(t)\rangle}{\partial\alpha_j} = |\psi_j\rangle\), we get

\[
\sum_j \langle \psi_k | B(t) B(t)|\psi_j\rangle \delta \hat{\alpha}_j = \langle \psi_k | B(t) |v'_j(t)\rangle. 
\]

We assume that \(A_j(t)\) and \(B(t)\) can be written as linear combination of unitaries \(U_{jk}\) and \(V_k\) with coefficients \(\nu_{j\alpha}(t)\) and \(\lambda_k(t)\) respectively

\[ A_j(t) = \sum_k \nu_{j\alpha}(t) U_{jk}, \]

\[ B(t) = \sum_k \lambda_k(t) V_k. \]

For the sake of convenience, we define following overlap matrices

\[ V_{kj} \equiv \langle \psi_k | B^\dagger(t) B(t)|\psi_j\rangle \]

\[ D_{kj} \equiv \langle \psi_k | B^\dagger(t) A_j(t)|v'_j(t)\rangle. \]

We observe that

\[ V_{kj} = \sum_{m,n} \lambda^*_m(t) \lambda_n(t) \langle \psi_k | V_m^\dagger V_n|\psi_j\rangle, \]

\[ D_{kj} = \sum_{j,m,n,p} \lambda^*_m(t) \nu_{j\alpha}(t) \gamma_{j\beta}(\alpha, t) \langle \psi_k | V_m^\dagger U_{jk}|\phi_{i\beta}\rangle. \]

In terms of the overlap matrices \(D\) and \(V\), we get the following evolution equation,

\[ V(t)|\alpha\rangle = D(\alpha, t), \]

where the parameters of \(D(\alpha, t)\) can also be function of \(\alpha\). Real and imaginary time evolution of the Schrödinger equation with a Hamiltonian \(H\) is a special case of the GQAS with \(B(t) = 1\) and \(|dv(t)\rangle = |v(t)\rangle\), which has been investigated in [27]. For real time evolution, we set \(A_1 = -iH\) and for imaginary time evolution \(A_1 = -H\).
The generalized time evolution can be applied for various other problems, such as linear algebra [28]. Here we show as example how to find the inverse of an invertible matrix $M$

$$M|v_{M^{-1}}⟩ = |v_b⟩ \tag{23}$$

with given vector $|v_b⟩$ and solution to be found $|v_{M^{-1}}⟩$. This problem can be converted into a time evolution problem [28] with

$$E(t)|v(t)⟩ = |v_b⟩ \tag{24}$$

$$E(t) = \frac{t}{T}M + \left(1 - \frac{t}{T}\right)I \tag{25}$$

where $I$ is the identity matrix, $T$ the final evolution time and $|v(0)⟩ = |v_b⟩$, $|v(T)⟩ = |v_{M^{-1}}⟩$. The derivative of $|v(t)⟩$ gives the differential equation

$$E(t) \frac{d}{dt} |v(t)⟩ = -G(t)|v(t)⟩ \tag{26}$$

with $G(t) = (M - 1)/T$. We can identify this equation with equation (11), where $B(t) = E(t)$, $|\psi(t)⟩ = |v(t)⟩$ and $A(t) = -G(t)$. We assume that $M = \sum_k \mu_k V_k$ can be represented as a linear combination of unitaries $V_k$.

We now apply the GQAS algorithm to this problem. First, we represent the evolving state as a linear combination of states $|\psi(t)⟩ = \sum_i \alpha_i(t)|\psi_i⟩$. An efficient way to generate $|\psi⟩$ for a given problem matrix $M$ could be found using similar methods as the cumulative K-moment expansion [26]. As second step, the overlap matrices equations (20) and (21) are to be measured on the quantum computer. For the last step, one integrates equation (22) on a classical computer using the measured overlaps for a time $T$ to get $\alpha(T)$ that parameterize the solution vector $|v(t)⟩ = \sum_i \alpha_i(T)|\psi_i⟩$.

5. Nonlinear differential equation

Nonlinear differential equations are ubiquitous in many areas of science, from hydrodynamic problems such as the Navier–Stokes equations to weather forecasts. It has been recently shown that quantum computers promise exponential speed-up for solving non-linear equations [32]. Further, several other quantum algorithms for non-linear equations have been proposed [29–31]. GQAS for generalized time as shown in equation (11) can be extended to solve non-linear dynamics. Here, we demonstrate the case where $B(t) = 1$ with a single non-linear operator $A(t, |v(t)⟩)$. However our algorithm can be easily extended to include linear and non-linear $B(t)$. We define

$$\frac{d}{dt} |v(t)⟩ = A(t, |v(t)⟩)|v(t)⟩, \tag{27}$$

We decompose the operator as linear combination of $r$ unitaries $U_k$ and nonlinear functions $f_k(t, |v(t)⟩)$

$$A(t, |v(t)⟩) = \sum_{k=1}^r f_k(t, |v(t)⟩)U_k \tag{28}$$

We now assume that $f_k$ is a nonlinear function of the expectation values of the unitaries $U_k$ with the state $|v(t)⟩$

$$f_k(t, |v(t)⟩) \equiv f_k(t, \langle v(t)|U_1|v(t)⟩, \ldots, \langle v(t)|U_r|v(t)⟩) \tag{29}$$

As first step, we define the state $|v(t)⟩$ as a linear combination of basis states $|\psi⟩$

$$|v(t)⟩ = \sum_{i=0}^{m-1} \alpha_i(t)|\psi_i⟩. \tag{30}$$

As second step, one uses a quantum computer to measure the overlaps $E$ as defined in equation (3) and

$$S_k^\alpha = \langle \psi_i|U_k|\psi⟩, \tag{31}$$

As third and final step, we rewrite equation (27) in terms of above definitions to find

$$E\frac{d}{dt} \alpha = -i \left( \sum_k f_k(t, \alpha_1^∗ S^1 \alpha, \ldots, \alpha_r^∗ S^r \alpha) S^k \right) \alpha. \tag{32}$$
This nonlinear differential equation is then solved on a classical computer. We now demonstrate how to solve the non-linear Schrödinger equation [50] with our method. This type of equation is for example used in nonlinear optics and describes Bose–Einstein condensates with weakly interacting particles. A simple discrete version of this equation in one dimension is given by

\[
\frac{d}{dt} \eta_i = -J(\eta_{i+1} + \eta_{i-1}) + V_i \eta_i + g|\eta_i|^2 \eta_i,
\]

where \(\eta_i\) are \(N\) complex numbers that are normalized with \(\sum_{i} |\eta_i|^2 = 1\), \(J\) is the coupling strength of neighboring discrete states \(i\) and \(i+1\), \(V_i\) the local energy and \(g\) the non-linear interaction strength. We encode the \(\eta_i\) into a quantum state via \(|\phi(t)\rangle = \sum_i \eta_i \sigma^z_i |0\rangle\). Now, the discrete nonlinear Schrödinger equation can be mapped to a spin Hamiltonian of \(N\) qubits with nonlinear coefficients, under the condition that the state \(|\phi(t)\rangle\) is an eigenstate of \(M = \sum_i n_i\) with \(M|\phi\rangle = |\phi\rangle\) with eigenvalue \(\lambda_M = 1\), where we define the density \(n_i = \frac{1}{2}(1 - \sigma_i^z)\). We now define the nonlinear spin Hamiltonian

\[
H = -\frac{1}{2} \sum_i (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + \sum_i V_i n_i + g \sum_i \langle \phi | n_i | \phi \rangle n_i.
\]

We can now solve the discrete non-linear Schrödinger equation (equation (33)) by mapping it to equation (34). In figure 4, we simulate both the linear regime \((g = 0)\) as well as the nonlinear dynamics \((g > 0)\). We use an ansatz a linear combination of the states \(|\psi_i\rangle = \sigma_i^z |0\rangle\). The initial state of the simulated evolution at \(t = 0\) is a superposition state with non-zero density at odd number of sites, e.g. \(\sum_{i\text{ odd}} |n_i\rangle = 1\) and zero density at even sites \(\langle n_{\text{even}} \rangle = \sum_{i\text{ even}} \langle n_i \rangle = 0\), with density at site \(i\) \(n_i = \frac{1}{2}(-\sigma_i^z + 1)\). We observe with increasing \(g\) that the density oscillation is suppressed, demonstrating the onset of non-linear behavior and self-trapping [51].

### 6. Quantum assisted Gibbs state preparation

Preparation of quantum states at a given temperature is an important task relevant for many quantum algorithms. However, generating these Gibbs state can be quite challenging. A common approach is to evolve the totally mixed state in imaginary time [52]. However, in general preparing the totally mixed state is very resource demanding. Further, imaginary time evolution requires non-unitary dynamics, which can be hard to implement on quantum computers. Here, we propose to approximate the totally mixed state using the hybrid density matrix and apply QAS as primitive to implement the imaginary time evolution to generate Gibbs states.

The Gibbs state is given by

\[
\rho(T) = \frac{e^{-H/T}}{\text{Tr}(e^{-H/T})},
\]

where \(H\) is some Hamiltonian and \(T\) the temperature. To get this state, the totally mixed state \(\rho_I = 1_{N}/N\) can be evolved in imaginary time \(\tau\) to get the state with temperature \(T = 1/(2\tau)\). The evolution of a density matrix in imaginary time is given by

\[
\frac{d}{d\tau} \rho = -(H\rho + \rho H).
\]

We now solve this equation using QAS. First, we expand \(\rho = \sum_i \beta_i |\psi_i\rangle \langle \psi_i|\) as hybrid density matrix corresponding to equation (1) with combination parameters \(\beta\). The basis states \(|\psi_i\rangle\) can be for example generated via K-moment expansion (see equation (10)). Then, we measure the overlap matrices \(E\) and \(D\) as...
In this work, we presented a NISQ era algorithm to simulate open system dynamics, generalized time evolution, nonlinear differential equations and Gibbs state preparation. The GQAS proceeds in three steps. The first step selects the ansatz as a linear combination of basis states defined in equations (3) and (6a) on a quantum computer. Finally, we solve the corresponding equations for imaginary time evolution, nonlinear differential equations and Gibbs state preparation. The GQAS proceeds in three steps. The first step selects the ansatz as a linear combination of basis states evolving the totally mixed state $\rho = 1/N$ in imaginary time $\tau = T/2$. We show the expectation value of energy $\langle H(\tau) \rangle$ for varying number of basis states $M$. The Hamiltonian is the transverse Ising model given by equation (39) with parameters $N = 6$, $p = 6$, $J = 1$ and $h = 1$.

As example, we show in figure 5 the preparation of the Gibbs state with QAS for different moment expansion $K$ of the transverse field Ising model, allowing us to prepare Gibbs state with arbitrary temperature approaching the exact Gibbs state with increasing $M$, reaching the exact state for $M = 64$ and allowing us to prepare Gibbs state with arbitrary temperature $T$ by varying the evolution time $\tau$. Alternatively, one can start with maximally entangled state $|\zeta\rangle_{AB}$ of system $AB$, evolve the whole system under the Hamiltonian $H_A \otimes H_B$ via imaginary time evolution using QAS for time $\tau$ [23]. The state of system $A$ at time $\tau$ is then given by the Gibbs state with temperature $T = \frac{1}{2\tau}$.

7. Discussion and conclusion

In this work, we presented a NISQ era algorithm to simulate open system dynamics, generalized time evolution, nonlinear differential equations and Gibbs state preparation. The GQAS proceeds in three steps. The first step selects the ansatz as a linear combination of basis states $|\psi_i\rangle \in \mathcal{S}$ from a set $\mathcal{S}$. The ansatz can be either a pure state or mixed state $\rho_i$ depending on the problem. Here, we introduce the concept of hybrid density matrix (equation (1)) to represent a mixed state as a linear combination of parameters, where the combination parameters can be updated on a classical computer without the need of tuning the quantum states. The second step involves the computation of overlap matrices on a quantum computer, which can be performed efficiently using techniques of [46] or by assuming construction from Pauli strings [27]. After the overlap matrices have been computed, the differential equation to be computed is solved on a classical computer. Note that once the ansatz has been decided, our algorithm does not mandate any quantum–classical feedback loop as the quantum states defining the ansatz are fixed, and only the variational parameters are (classically) updated. The algorithm does not require the computation of gradients using the quantum computer and thus circumvents the barren plateau problem by construction.
Our algorithm simulates the dynamics within an ansatz space spanned by $M$ states. The ansatz states are prepared on a quantum computer and we measure corresponding overlaps. By choosing ansatz states that are intractable for classical simulation, our algorithm has the potential to exceed classical simulation methods. Our algorithm achieves high fidelity when the ansatz spans the subspace of the dynamics (see figures 3(b) and (c)), else we observe a decay in fidelity with increasing time. To run our algorithm with high fidelity, a main challenge is to keep the number of ansatz states small by choosing the most important states. In the worst case, an exponential number of states is needed when the dynamics is highly ergodic and spans the whole Hilbert space. For short times or constrained problems with many-body scars [53], symmetries or many-body localization, dynamics is restricted to a small part of the Hilbert space, which can be spanned by a polynomial number of states. For simulating dynamics, we use the cumulative $K$-moment expansion with equation (10) to construct the ansatz. This method is inspired by the Krylov subspace expansion, a powerful classical method for simulation that uses the Hamiltonian to find a suitable subspace [47]. We highlight that the cumulative $K$-moment expansion has been recently shown to find a good subspace with polynomial scaling for a spin model by choosing a reference state inspired by quantum annealing [48]. As another example, for fermionic problems one can use fermionic excitation subspace [47]. We believe that the cumulative $K$-moment expansion could be found for many problems.

For the classical post-processing step, our algorithm requires inversion of the $E$ matrix. If $E$ has small eigenvalues, the inversion can be sensitive to experimental noise, which can negatively impact the accuracy. Recent work has found improved methods to reduce the error of the inversion step [54].

Note that the overlaps corresponding to equations (6a)–(6c) can be exponentially small when using random circuits to generate $|\psi_i\rangle$. However, we would like to emphasise that this problem corresponds to the calculation of expectation values for random quantum states and is fundamentally different from that of gradients. For random circuits, one can have both exponentially small expectation values as well as vanishing gradients. The former problem exists in our approach as well as variational quantum algorithms. However, our approach bypasses the vanishing gradient problem by construction as no gradients are measured with the quantum computer. The measurements involved in the estimation of the overlap matrices can be performed efficiently without the requirement of any complicated measurements, such as the Hadamard test. Refer to the appendix of reference [26] for details. The GQAS algorithm can trivially subsume the algorithms based on VQE (or VQS) by allowing the quantum states defining the ansatz to be variationally adjusted. See the appendix A for an illustration. Apart from straightforward applications, our algorithm could be used as primitive for more involved algorithms such as quantum Boltzmann training, quantum signal processing and algorithms for quantum machine learning. Our algorithm also harbour potential applications in solving the Navier–Stokes equation and plasma hydrodynamics.

The algorithms designed for fault-tolerant quantum computers, such as Shor’s factoring and Grover search, allow a rigorous mathematical analysis. On the contrary, algorithms such as VQE and VQS, which do not require fault-tolerant architecture, are heuristic in nature and often render any systematic analysis challenging. A borderline exception is the quantum approximate optimization algorithm [8], which can be analyzed though its implementation can be challenging on the existing quantum hardware. In contrast, our algorithm are compatible with the existing NISQ capabilities and provide proper mathematical analysis of its optimization program.

Most of the quantum computers nowadays are being accessed via cloud platforms by submitting jobs into a queue, which is then executed at some later time. The classical–quantum feedback loops of VQE require a lot of time, as each step of the loop has to wait for the previous job to finish in the queue. Only then, one can perform the classical part of the algorithm and submit the next job for the quantum computer. The sequential nature of classical–quantum feedback loop severely slows down the execution of these algorithms. In contrast, our algorithm do not require any classical–quantum feedback loop and are embarrassingly parallel as all quantum computations are independent of each other, allowing for much faster termination.

In future, it would be interesting to study GQAS algorithms in the presence of noise. A proper error analysis is in order. Providing complexity-theoretic guarantees would be another exciting direction.

Acknowledgments

We are grateful to the National Research Foundation and the Ministry of Education, Singapore for financial support.
Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Appendix A. Quantum assisted variational simulator

One can select a linear combination of variational quantum states and thus allow to update the quantum states defining the ansatz. The aforementioned strategy furnishes a method to allow QAS based algorithms to subsume VQS based algorithms. For the sake of illustration, let us consider the ansatz state as

\[ |\psi(\theta, \alpha)\rangle = \sum_{i=1}^{M} \alpha_i |\psi_i(\theta)\rangle, \]

where \(|\psi_i(\theta)\rangle = U_i |\psi(\theta)\rangle\) for some unitary \(U_i\) (constructed using the unitaries defining the underlying Hamiltonian) and \(\theta = \theta_1 \ldots \theta_K\). We assume the variational parameters to be real valued and leave the more detailed analysis for involved cases such as \(\alpha_i \in \mathbb{C}\) and \(\theta_j \in \mathbb{R}\) for future works. Simple algebraic calculations based on McLachlan principle yields the following update equation,

\[
\begin{pmatrix}
P \\ Q \\ S \\ T 
\end{pmatrix}
\begin{pmatrix}
\dot{\theta} \\ \dot{\alpha}
\end{pmatrix}
= \begin{pmatrix}
R \\ W
\end{pmatrix},
\]

(A1)

Here, \(P, Q, S, T, R\) and \(W\) are \(K \times K, K \times M, M \times K, M \times M, K \times 1\) and \(M \times 1\) matrices with the following description,

\[
P_{ij} = \frac{\partial \langle \phi | \partial \theta_i \rangle}{\partial \theta_j} + \frac{\partial \langle \phi | \partial \theta_j \rangle}{\partial \theta_i},
\]

\[
Q_{ij} = \frac{\partial \langle \phi | \partial \theta_i \rangle}{\partial \theta_j} + \langle \psi_j | \partial \theta_i \rangle |\psi_i\rangle,
\]

\[
S_{ij} = \langle \psi_i | \partial \theta_j \rangle |\psi_j\rangle + \langle \psi_i | \partial \theta_j \rangle |\psi_j\rangle,
\]

\[
T_{ij} = \langle \psi_i | \psi_j \rangle + \langle \psi_i | \psi_j \rangle,
\]

\[
R_i = -t \left( \frac{\partial \langle \phi | H | \phi \rangle}{\partial \theta_i} - \langle \phi | H | \partial \theta_i \rangle \right),
\]

and

\[
W_i = -t \left( \langle \psi_i | H | \phi \rangle - \langle \phi | H | \psi_i \rangle \right).
\]

Here, for the sake of brevity, we have denoted \(|\phi(\theta, \alpha)\rangle\) by \(|\phi\rangle\), and \(|\psi_i(\theta)\rangle\) by \(|\psi_i\rangle\).

ORCID iDs

Tobias Haug https://orcid.org/0000-0003-2707-9962

References

[1] Preskill J 2018 Quantum computing in the NISQ era and beyond Quantum 279
[2] Deutsch I H 2020 Harnessing the power of the second quantum revolution (arXiv:2010.10283)
[3] Arute F et al 2019 Quantum supremacy using a programmable superconducting processor Nature 574 505
[4] Feynman R P 1982 Simulating physics with computers Int. J. Theor. Phys. 21 467
[5] Peruzzo A, McClean J, Shadbolt P, Yung M-H, Zhou X-Q, Love P J, Aspuru-Guzik A and O’Brien J L 2014 A variational eigenvalue solver on a photonic quantum processor Nat. Commun. 5 4213
[6] McClean J R, Romero J, Babbush R and Aspuru-Guzik A 2016 The theory of variational hybrid quantum–classical algorithms New J. Phys. 18 023023
[7] Kandala A, Mezzacapo A, Temme K, Takita M, Brink M, Chow J M and Gambetta J M 2017 Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets Nature 549 242
[8] Farhi E, Goldstone J and Gutmann S 2014 A quantum approximate optimization algorithm (arXiv:1411.4028)
[9] Farhi E and Harrow A W 2016 Quantum supremacy through the quantum approximate optimization algorithm (arXiv:1602.07674)
[10] Harrow A W and Montanaro A 2017 Quantum computational supremacy Nature 549 203
[11] MccArdle S, Endo S, Aspuru-Guzik A, Benjamin S C and Yuan X 2020 Quantum computational chemistry Rev. Mod. Phys. 92 015003
[12] Endo S, Cai Z, Benjamin S C and Yuan X 2020 Hybrid quantum–classical algorithms and quantum error mitigation (arXiv:2011.01382)
