Methodology for the digital simulation of open quantum systems

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Abstract. Quantum simulation of quantum systems is an extremely active field of contemporary research. In this paper a brief introduction is given to this field, with an emphasis on the distinction between analog and digital quantum simulations. Furthermore, conventional methods for the digital quantum simulation of Hamiltonian simulation are discussed and generalisations of these methods for the digital simulation of open quantum systems are presented.

1. Introduction

It has been known for some time that the simulation of quantum systems is a challenging problem [1]. In particular, one immediately apparent difficulty inherent in simulating quantum systems on conventional classical computers arises from the so called *exponential explosion* [2] - a description of the fact that a classical encoding of an N qubit quantum state (one may think of a qubit as a spin 1/2 particle [3]) typically requires the storage of 2^N probability amplitudes. As such, even writing the initial state of some desired simulation (before a discussion of the simulation itself can even take place) may require totally unrealistic memory resources. As an illustration, encoding the state of 40 spin 1/2 particles may require the storage of $2^{40} \approx 10^{12}$ complex numbers, which at standard precision requires approximately 4 terabytes of memory [2].

Due to such difficulties and the large number of potential applications for simulation of quantum systems in fields such as physics, biology and chemistry, the development of methods for the efficient simulation of quantum systems has become an extremely active area of contemporary research [2]-[4]. As we are concerned in this paper with a presentation of potential methodologies for the efficient quantum simulation of open quantum systems, it is useful to begin by defining what is meant by ""efficient simulation of quantum systems". Firstly, a simulation of a quantum system is understood as some process via which certain *pre-specified* properties of the the quantum system are accurately predicted [4]. It is important to note that we do not require our simulation to predict *all* properties of the quantum system of interest. For example, one may be interested in the expectation value of specific observables, scattering amplitudes within a quantum field theory or the state of the system at some particular time. The predictions of the simulation are considered accurate if the error is less than some pre-specified error tolerance

ϵ, and the simulation is considered successful if the specific properties of interest are accurately predicted, regardless of whether or not other properties of the quantum system are accurately predicted, or even accessible. Secondly, a simulation is considered efficient if the time and space resources required to obtain the required predictions can be determined as a polynomial function of the length of the bit string specifying the problem inputs and of $1/\epsilon$ [4, 5].

In the early 1980's Richard Feynman suggested that it may be possible to use quantum systems themselves as a means to efficiently simulate other quantum systems and simultaneously avoid difficulties such as the exponential explosion [1]. This suggestion has turned out to be remarkably prescient and while many approximation methods, such as Monte-Carlo techniques [6], have been developed for the efficient simulation of quantum systems on classical computers, we are concerned here with simulations in line with Feynman's original vision - so called "efficient *quantum* simulation of quantum systems".

2. Analog and digital quantum simulation

Quantum simulation, as envisaged by Feynman, requires a *quantum simulator*, which is understood as a *controllable quantum system used for the simulation of other quantum systems* [2]. For the purposes of illustration we will discuss in this section the simulation of closed quantum systems, undergoing Hamiltonian generated unitary evolution, but it is important to bear in mind that these principles may be applied to a broad class of quantum systems, such as quantum field theories and open quantum systems, as discussed in the review of Georgescu et. al. [2].

Consider a closed quantum system, initially in the state $|\phi(0)\rangle$ evolving via the Hamiltonian H_{sys} into the final state $|\phi(t)\rangle = U|\phi(0)\rangle$ where $U = \exp(-i\hbar H_{sys}t)$. As illustrated in Figure 1, any quantum simulation of such a system requires three distinct steps: The first step, or preparation phase, is an efficient preparation of the initial quantum state of the quantum simulator $|\psi(0)\rangle$, where there exists some well defined mapping between the states $|\psi(0)\rangle$ and $|\phi(0)\rangle$. The second step is a simulation of the system dynamics, i.e. an implementation of the unitary dynamics $\hat{U}$ where $\hat{U}$ approximates U, and the final step is an extraction of the desired system properties via measurements of the final state of the simulator $|\psi(t)\rangle = \hat{U}|\psi(0)\rangle$. It is important to note that *all steps* in the above process need to be efficient according to the criterion discussed in the introduction.

2.1. Digital quantum simulation

Digital quantum simulation refers to quantum simulation utilising the conventional quantum circuit model implemented on some universal quantum computer [3]. In order to perform a digital quantum simulation it is therefore necessary that the initial state of the simulator $|\psi(0)\rangle$ is some multi-qubit state. Furthermore, the unitary transformation $\hat{U}$ is then implemented via a sequence of one and two qubit gates from some appropriate universal gate set [3]. It is interesting to note that in principle *any* unitary operation can be decomposed into a sequence of gates from any universal gate set (hence the name *universal* gate set) however not all such decompositions are efficient - i.e. not all unitary operators can be decomposed into a polynomial number of gates from some universal set. The question of which Hamiltonians can be efficiently simulated via digital quantum simulation has been exhaustively addressed [2, 4] and in Section 3 we provide an illustration of the prevailing methodology by using local Hamiltonians as an example. Digital quantum simulation is advantageous in that any universal quantum computer can be used as a digital quantum simulator. However, this advantage comes at the price of requiring a sufficiently sized universal quantum computer, which in itself is a significant theoretical and technological challenge, whose realisation has not yet been achieved.

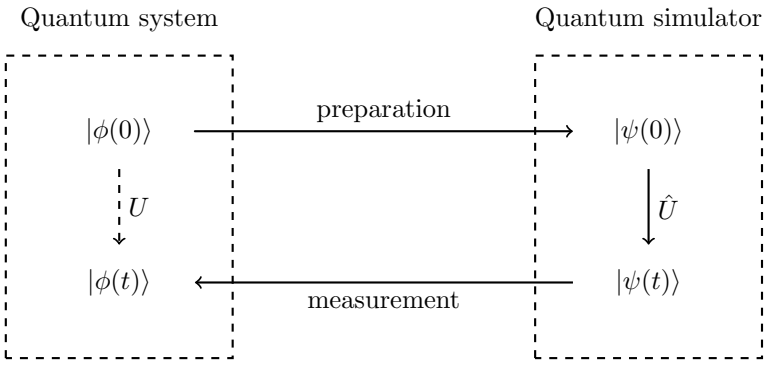

Figure 1. Schematic representation of a typical quantum simulation of a closed quantum system undergoing Hamiltonian generated unitary evolution $U = \exp(-i\hbar H_{sys}t)$. The first stage of the simulation is preparation of the initial state of the simulator $|\psi(0)\rangle$, which is in direct correspondence with $|\phi(0)\rangle$, the initial state of the system. The simulator then evolves via $\hat{U}$, an approximation to U, after which the desired system properties are obtained from measurements of the final simulator state $|\psi(t)\rangle$.

2.2. Analog quantum simulation

Analog quantum simulation, also known as quantum emulation, refers to quantum simulations in which one designs a quantum system (the quantum simulator) whose Hamiltonian H_{sim} is in direct correspondence with the Hamiltonian of the system which is to be simulated H_{sys}. The simulation then proceeds by letting the simulator evolve naturally via $\hat{U} = \exp(-i\hbar H_{sim}t)$. As an example [2] consider the Hamiltonian describing a gas of interacting bosonic atoms in a periodic potential

$$H_{sim} = -J\sum_{i,j}\hat{a}_i^\dagger\hat{a}_j + \sum_i \epsilon_i\hat{n}_i + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1) \tag{1}$$

where $\hat{a}_i^\dagger$ and $\hat{a}_i$ are the bosonic creation and annihilation operators on the i'th lattice site, $\hat{n}_i = \hat{a}_i^\dagger\hat{a}_i$ is the atomic number operator and ϵ_i denotes the energy offset of the i'th lattice site. The coefficient J provides a measure of the hopping strength between lattice sites and U quantifies the interaction strength between atoms at the same lattice site. The Hamiltonian H_{sim} is extremely similar to the Bose-Hubbard Hamiltonian

$$H_{BH} = -J\sum_{i,j}\hat{b}_i^\dagger\hat{b}_j - \mu\sum_i \hat{n}_i + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1) \tag{2}$$

where J and U are the same as above and μ is the chemical potential. The correspondence between H_{sim} and H_{BH} is clear and as such it is evident that one may straightforwardly simulate the Bose-Hubbard model, via identification of appropriate parameters, using an analog quantum simulator consisting of atoms in an optical lattice. Analog quantum simulation is advantageous in that one does not require an entire universal quantum computer for such simulations, and as a result analog quantum simulations have already been successfully demonstrated [2].

3. Hamiltonian simulation

In 1996 Lloyd [7] demonstrated a method for the digital simulation of Hamiltonian systems, and since then this method has provided the fundamental methodology for more sophisticated digital Hamiltonian simulation algorithms [4]. In this section we briefly review these methods as they

provide the inspiration for the open quantum system digital simulation methods presented in Section 4. Lloyd considers a Hamiltonian which may be written as the sum of local Hamiltonians

$$H = \sum_{l=1}^{M} H_l \tag{3}$$

where each H_l may be efficiently simulated - i.e. there exists a known efficient gate decomposition for $U_l = \exp(-i\hbar H_l t)$. In the case that $[H_l, H_{l'}] = 0$ for all l and l' we then have that

$$U = \exp(-i\hbar H t) = \prod_l \exp(-i\hbar H_l t) = \prod_l U_l \tag{4}$$

and the efficient gate decomposition for U is easily achieved via the known gate decompositions for U_l. However in general it is not true that all constituent local Hamiltonians commute and for this case Lloyd recognized that the Hamiltonian H could be efficiently simulated via a discretization of time, where the errors resulting from such a discretization are bounded via the Lie-Trotter product formula [3]. In particular, if H_1 and H_2 can be efficiently simulated, then as a result of the Lie-Trotter formula

$$e^{-i\hbar(H_1+H_2)t} = \lim_{n\to\infty} \left(e^{-i\hbar H_1 t/n} e^{-i\hbar H_2 t/n}\right)^n, \tag{5}$$

one has that

$$\left|\left|\left(e^{-i\hbar H_1 t/n} e^{-i\hbar H_2 t/n}\right)^n - e^{-i\hbar(H_1+H_2)t}\right|\right| \leq \epsilon \tag{6}$$

provided $n = \mathcal{O}((\nu t)^2/\epsilon)$ where $\nu := \max\{||H_1||, ||H_2||\}$. This result is easily extended to the sum in Eq. 3 and provides an effective method, via time discretization, for the simulation of any Hamiltonian which can be written as a sum of efficiently implementable Hamiltonians. Since this initial result new digital simulation algorithms have been developed which have broadened the class of Hamiltonians which may be simulated while simultaneously decreasing the algorithmic costs [4]. However all such methods rely on the following fundamental strategy:

(i) Decompose the Hamiltonian H into a sum of Hamiltonians which can be efficiently simulated, as in Eq. 3.

(ii) Simulate the Hamiltonian H through recombination of the constituent Hamiltonians, via a Lie-Trotter product formula or suitable generalisation.

This methodology may be described as the *Decomposition/Recombination* strategy and in the following section we illustrate how a similar strategy may be utilised for the digital simulation of open quantum systems.

4. Digital simulation of open quantum systems

The problem considered in this section, to which we would like to apply the methodology illustrated in Section 3, is that of simulating the dynamics of Markovian open quantum systems. In particular, given a continuous one parameter semi-group of quantum channels $\{T_t\}$ [8], where $T_t : \mathcal{B}(\mathcal{H}_s) \to \mathcal{B}(\mathcal{H}_s)$ is a completely positive trace preserving map from and onto the bounded operators on the Hilbert space of the system $\mathcal{H}_s \cong \mathcal{C}^d$, we would like a digital simulation algorithm which provides the state of the system at time t, given by $\rho(t) = T_t[\rho(0)]$, where $\rho(0) \in \mathcal{B}(\mathcal{H}_s)$ is the initial state of the system [3]. Every such continuous one parameter semigroup of quantum channels $\{T_t\}$ has a unique generator

$$\mathcal{L} : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S) \tag{7}$$

such that

$$T_t = e^{t\mathcal{L}} = \sum_{k=0}^{\infty} \frac{t^k \mathcal{L}^k}{k!} \tag{8}$$

and $\mathcal{L}$ satisfies the differential equation

$$\frac{d}{dt}\rho(t) = \mathcal{L}(\rho(t)), \tag{9}$$

known as a master equation. Furthermore, a linear super-operator $\mathcal{L} : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S)$ is the generator of a continuous dynamical semigroup of quantum channels, if and only if it can be written in the form

$$\mathcal{L}(\rho) = i[\rho, H] + \sum_{k,l=1}^{d^2-1} A_{l,k}([F_k, \rho F_l^\dagger] + [F_k \rho, F_l^\dagger]), \tag{10}$$

where $H = H^\dagger \in \mathcal{M}_d(\mathcal{C})$ is Hermitian, $A \in \mathcal{M}_{d^2-1}(\mathcal{C})$ is positive semidefinite and $\{F_i\}$ is a basis for the space of traceless matrices in $\mathcal{M}_d(\mathcal{C})$. Eq. 10 is known as the Gorini, Kossakowsi, Sudarshan and Lindblad form of the quantum Markov master equation and we refer to A as the GKS matrix [8]. It is also crucial to note that for any quantum channel $T : \mathcal{B}(\mathcal{H}_s) \to \mathcal{B}(\mathcal{H}_s)$ it is always possible to introduce a dilation space $\mathcal{H}_E$ with $\dim(\mathcal{H}_E) = [\dim(\mathcal{H}_S)]^2$ such that there exists a unitary matrix $U \in \mathcal{M}_{d^3}(\mathcal{C})$, known as the Stinespring dilation [8], where

$$T(\rho) = \mathrm{tr}_E[U(|e_0\rangle\langle e_0| \otimes \rho)U^\dagger] \tag{11}$$

and $|e_0\rangle\langle e_0| \in \mathcal{H}_E$ is some initial state of the environment. In light of the above the Kliesch et. al. [9] have provided the following digital simulation algorithm for Markovian open quantum systems, which can be seen as a direct generalisation Lloyd's initial Hamiltonian simulation algorithm [7] discussed in the previous section:

(i) Assume that the system consists of N subsystems of Hilbert space dimension d. Furthermore, assume that the generator $\mathcal{L}$ is k-local in the sense that it can be written as the sum

$$\mathcal{L} = \sum_{\Lambda \subset [N]} \mathcal{L}_\Lambda \tag{12}$$

where $[N] := \{1, ..., N\}$ and $\mathcal{L}_\Lambda$ are *strictly* k-local, i.e. $\mathcal{L}_\Lambda$ act non-trivially on at most k-subsystems.

(ii) Simulate the total dynamics $T_t = \exp(t\mathcal{L})$ through recombination of the constituent channels $T_{t/m}^{(\Lambda)} = \exp(t/m\mathcal{L}_\Lambda)$. Each constituent channel may be simulated via the Stinespring dilation (whose unitary is guaranteed an efficient gate decomposition as a result of strict k-locality) and the error introduced by such time discretization is bounded by the Trotter decomposition theorem for Liouvillian dynamics [9], a direct generalisation of the Lie-Trotter theorem into the superoperator regime.

The algorithm described above can be seen as the direct analogue of Lloyd's initial Hamiltonian simulation algorithm in that it *assumes* the existence of a natural decomposition into constituent semi-groups which may be efficiently simulated, and then proves the efficiency of recombining these semi-groups. Given this fundamental platform and the success of similar strategies for digital simulation of Hamiltonian systems a general decomposition/recombination strategy is naturally suggested for Markovian evolutions, specified not by strictly k-local generators, but rather by generators with arbitrary GKS matrix A:

(i) Decompose the generator $\mathcal{L}$ into the sum of generators which may be efficiently simulated.

(ii) Simulate the entire evolution through recombination of the constituent semi-groups via a Lie-Trotter theorem for Liouvillian dynamics or some suitable generalisation.

One such generalised decomposition/recombination strategy, for the simulation of arbitrary Markovian dynamics of a qubit, has recently been presented in [10] and as in Hamiltonian simulation it is expected that the class of evolutions which may be simulated using this strategy can still be greatly broadened while the algorithmic costs are simultaneously reduced.

5. Conclusion

We have provided a brief introduction to the field of quantum simulation. In particular we have described the difference between analog and digital quantum simulations and provided a description of how the decomposition/recombination strategy for the simulation of Hamiltonian evolution may be generalised for the simulation of Markovian open quantum systems.

Acknowledgments

This work is based upon research supported by the South African Research Chair Initiative of the Department of Science and Technology and National Research Foundation. Ryan Sweke acknowledges the financial support of the National Research Foundation SARChI program.

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