

Report on article *Universal Quantum Simulator* by Seth Lloyd, 1996

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Contents

1	Context and motivations	1
1.1	Quantum computer	2
1.2	Quantum simulation	2
1.3	Discrete quantum simulation	2
2	Results and contributions	3
2.1	Isolated systems	3
2.2	Other systems	4
2.3	Preparation and measurement	4
3	Limits and further work	5
3.1	Qubit stability	5
3.2	Universal set of quantum gates	5
3.3	Efficiency with respect to sparsity	6

Universal Quantum Simulators is an article about both computer science and physics by Seth Lloyd. It was published in *Science*, vol. 273 in 1996 [Llo96]. Its main goal is to give a proof of Feynman’s conjecture in 1982 that quantum computers might be more efficient than classical ones in simulating quantum systems. To do so, he describes a methodology to simulate any kind of quantum dynamic using a limited set of controlable interactions on a known quantum system (the quantum computer). I will first present the context, and the motivations of such a work, before explaining more in detail his results and finally I will try to highlight the directions that are left open for further work.

1 Context and motivations

This article lies at the intersection of two different approach of quantum dynamics : quantum computation, and quantum simulation. The first one is of interest for computer scientist, who aim at finding the computational power of qubits with respect to classical bits, while the second one is a physicist issue, of

understanding how quantum systems that we cannot manipulate in laboratory may work. Both issues are brought together by discrete quantum simulation (DQS), which consists in the simulation of an unknown quantum system using qubits and controllable interactions between them, that is a quantum computer.

1.1 Quantum computer

A quantum computer is the quantum counterpart of a classical computer. Instead of using bits that can have values 0 or 1, it uses qubits whose value is a probability distribution on $\{0, 1\}$. To manipulate them, instead of using logical gates $AND(x, y)$, $OR(x, y)$, $NO(x)$ which rely on electric devices (usually transistors), it uses quantum gates that can be seen as linear transformation of the probability vector of qubits and which would be implemented using quantum interactions between qubits. These differences may give to quantum computers a computing power larger than classical ones, because they can store more information : the state of X qubits would require 2^X numbers to be stored on a classical computer, and because they can perform linear transformations on this information using one gate, while a classical computer would need to perform a whole matrix - vector product. The problem is to understand exactly what kind of computations could be solved faster using a quantum computer than a classical one.

1.2 Quantum simulation

On the other hand, quantum simulation is the problem of simulating quantum systems which cannot be reproduced and manipulated in laboratory. This can be for various reason, either because it exists only at temperatures or pressure that we are not able to create, because it too unstable, or too big, etc. What physicists can do in such a case, if they know the theoretical expression of the dynamic of the system is to find another system, manipulable, that behaves similarly. Then, if they are able to find a logical correspondence between the initial states of the simulated and simulating systems, they could retrieve information about the final state of the simulated system observing the final state of the simulating one. Those simulating systems can be designed ad-hoc, but it would be very useful to have a kind of universal quantum simulator, that is a quantum system whose initial state and dynamics could be set to mimic a large variety of other quantum systems.

1.3 Discrete quantum simulation

One way to design such a universal simulator is to use a quantum computer, that is a set of qubits and universal quantum gates $\{G_i\}$. The possible states of the simulated system are encoded as binary bit strings, and the dynamic to

go from one state to another is reproduced using quantum gates:

$$U_{sys} \sim U_{sim} = G_n \circ G_{n-1} \circ \dots \circ G_0 \quad (1)$$

$$|\phi(0)\rangle \rightarrow U_{sys} \rightarrow |\phi(t)\rangle \quad (2)$$

$$|00011011\rangle \rightarrow U_{sim} \rightarrow |10100001\rangle \quad (3)$$

Then, quantum mechanics allow to perform such a computation on superposition of these states [GAN14]. From there, three questions arise : what kind of system dynamic U_{sim} could be reproduced using a polynomial number of gates ? How could we efficiently set the qubits to reproduce the desired initial state ? How could we efficiently measure the qubits to retrieve information about the system's final state ?

These are the issues that the article *Universal Quantum Simulator* tries to adress.

2 Results and contributions

The main thesis of the article is that a quantum computer can efficiently simulate quantum systems as long as they evolve according to local interactions. To be clearer, a system of N particles that interact only with their neighbours (and not at long range) can be simulated on a quantum computer, using a number of qubits and an amount of time polynomial in N . To demonstrate this, the author first shows how to decompose the global dynamic into a sequence of local ones when the system is isolated (*i.e. doesn't exchange energy with its environment*), then how to deal with a system which is not isolated, and finally how initial state can be properly set and final state measured.

2.1 Isolated systems

An isolated system has a constant energy, and the evolution along time of its wave function $|\phi(t)\rangle$ can be described by a Hamiltonian H , which is a $N * N$ matrix such that:

$$|\phi(t)\rangle = \exp(-ihHt) * |\phi(0)\rangle \quad (4)$$

where h is the Planck constant. Then, as we consider a system evolving according to local interactions, the hamiltonian can be decomposed as $H = \sum_{i=1}^l H_i$ where each H_i acts only on k particles, and the time evolution can be approximated as:

$$\exp(-ihHt) = \left(\exp\left(\frac{-ihH_1t}{n}\right) \cdots \exp\left(\frac{-ihH_l t}{n}\right) \right)^n + \epsilon \quad (5)$$

where the approximation error ϵ can be made as small as desired by taking n sufficiently large. This means that instead of simulating all H_i together over duration t , we simulate them one after another n times, over duration $\frac{t}{n}$. From

there, the problem boils down to simulating each H_i using the quantum gates of the computer. This has been shown to be doable in m_i^2 operations, where m_i is the dimensionality of the space on which H_i acts, here 2^k (because H_i acts on k particles represented by vectors of dimension 2) [Llo96]. Thus, the total number of gates to apply to simulate H to a precision ϵ is:

$$C(H) = n \left(\sum_{i=1}^l m_i^2 \right) \leq n * 2^{2k} l \quad (6)$$

Once ϵ is fixed, so is n , and thus the complexity is proportional to 2^{2k} and to l . For local hamiltonians, typically nearest neighbour or next-nearest neighbour, k is constant, and l is proportional to N . Thus the overall complexity is proportional to N .

2.2 Other systems

Now, the quantum system we want to simulate may not be isolated. This means that it interacts with its environment, exchanging energy with it. The consequence for our simulation, is that the evolution of the system doesn't follow anymore an Hamiltonian H . Instead, it is the joint time evolution of the system and its environment $\rho_{SE}(t)$ that can be described by an Hamiltonian:

$$U(t) = \exp(-ihHt) \quad (7)$$

$$\rho_S(t) = \text{tr}_E(\rho_{SE}(t)) \quad (8)$$

$$= \text{tr}_E[U(t)\rho_{SE}(0)U^\dagger(t)] \quad (9)$$

$$= \text{tr}_E[U(t)(\rho_S(0) \otimes \rho_E(0))U^\dagger(t)] \quad (10)$$

where ρ denotes the joint density matrix. We could simulate everything at once, but the environment may be huge, involving a number of particle exponential in N . Actually we do not need to simulate the whole behavior of the environment, we just need to simulate its effect on the system of interest, and to do that we need at most as many variable as required for the system. This is because the environment has only N ways to act on the system: one for each particle. Thus, we finally need to consider the isolated time evolution of a simulated system - environment with just $2N$ variable, as we did before, and its complexity will still be polynomial in N .

2.3 Preparation and measurement

The only issues that are left open are now how to correctly setup the initial simulator state and how to extract the desired information of the final simulator state using a polynomial number of variables and operations. To do this, we consider preparation and measurement as kinds of interactions of the system with its environment. Preparing a given qubit in a given state corresponds to the environment performing a operation on the system that decreases its entropy

by 1. By building up a sequence of environment operations that would bring the system to the desired initial state, we can find the corresponding sequence of gates to apply in our computer to obtain the desired initial simulator state. Symmetrically, performing a measurement that gives us 1 bit of information about the simulator may be understood as the environment performing an operation on the system that increases its entropy by 1. And the same reasoning can be applied. Using this method, we only need 2 more variables to correctly prepare and measure our simulator, and both operation can be performed in polynomial time because of what was described before.

3 Limits and further work

Although this general methodology gives a useful framework to design universal quantum simulators using quantum computers, there is still some work to do before being able to actually perform such simulations and first of all to construct quantum computers that would be able to perform them. Also, even if local Hamiltonian decomposition has been solved in the general case in this article, it would be interesting to know if there are more efficient technics, in general or for particular ones.

3.1 Qubit stability

The first issue in order to construct quantum computers is to be able to manipulate and control quantum bits. For the moment, several technologies to implement them have been proposed, but none of them fully satisfies all the requirements of a quantum computer. Many of them exhibit poor scaling, meaning that we are not able to manipulate more than a few qubits, which dramatically limits the number of computations that the computer can perform. Another limit is the ability to have individual control on each qubit, without affecting the other [GAN14].

3.2 Universal set of quantum gates

Also, another theoretical and practical issue which is related to the previous one is to design and implement a universal set of quantum gates, that is a set of gates that can be combined to reproduce any $m * m$ unitary operator. It should also be efficient, in the sense that this reproduction should be feasible with just m^2 operations. Also much theoretical work has been spent on this issue, implementing such a set depends on the implementation of the qubits it should work with.

3.3 Efficiency with respect to sparsity

Finally, one should note that many physical systems' Hamiltonian are actually very sparse, and do not involve as much interactions as the ones described here.

Using this particularity may lead to more efficient technics to simulate them. It would also be of interest to know how the simulation's complexity decreases with respect to the sparsity of system's Hamiltonian[BCK15].

In conclusion, this article provides a proof of Feynman's 1982 conjecture that quantum computers are more efficient than classical ones to simulate quantum systems that evolve according to local interactions. It describes a methodology to prepare the initial state of the simulator, to decompose system's dynamic into smaller ones and simulate them, to simulate the interactions of the system with its environment, and to measure the final state of the simulator in order to retrieve the information of interest. All this is done in polynomial time and space with respect to the number N of particles of the system. It opens the way to universal quantum simulations as soon as quantum computers can be constructed, and raises new questions about the complexity of simulating various classes of Hamiltonians.

References

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