Thesis Proposal: GLOBAL OPTIMIZATION: SOFTWARE, APPLICATIONS

by

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Abstract

In certain applications a single local optimal value will not be satisfying to most difficult problems, to do better a global search for a global to find a potential optimal solution is required. However, simplying looking for a solution on a global scale is not simple, in the context of combinatorial problems, global optimzations are NP-hard problems. Making it a challenge to find a single optimal solution or all feasible solutions in a single to multiple search space. To aid in finding a solution quickly and robostly, software appraoches can be applied to a global solver to aid in helping it solve the problem.

One piece of software used in aiding global solvers is distributed system send out function evaluations to multiple machines, this grants a form of parallelism to the solver, to evaluate multiple long calculations in period of one evalutions. One praticular software used with pythOPT, python enviroment for problem solving, is Computefarm, this software utilizes the server-client model to distribute function evaluations to farmed computers. By doing this a form of parallelism is created and decreases the time spent on each iteration of the solver. By applying this method to global solvers, like Particle Swarm Optimization, applications for example crystal prediction was optimized N times faster, where N is number of computers farmed by the software. The reason this application benefits from computefarm is that the objective function can take over ten minutes to determine the total energy of a crystal structure using the Vienna Ab Initio Simulation Package software.

Another software approach is implement a database to monitor the simulation and keep backups of the solver status at each several iterations, known as checkpointing. Though is commonly thought of method to apply to a solver in case of computer or solver failure, it is difficult to implement because external dependencies. However, because of the flexibility of pythOPT development a simple checkpointing schema is implemented to store values for monitoring purposes and solver statuses for robustness in case of failure. This becomes heavily desired when a specific result is known but the problem is difficult and convergence is not obtained quickly. One example is the qunatum error correction application, because of the desired fidelity value desired in simulated circuit the optimization can be long and difficult to find a single feasible point. Finding a feasible solution can take weeks to months for various

variations, because of this unkown length of time to solve a database is implemented in to the global solver to sore evaluations for monitoring the solver and in case simulations are stopped then a restart can be done.

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CCCZ	Controlled controlled controlled Z gate
qubit	Quantum bit

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Introduction

Global optimizations provides a promise to finding a single solution or multiple solutions to a problem.

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Software

Compute farm

Compute farm is software that farms computer resources to preform computational tasks.

Database

Chapter 4

Applications

Designing error control circuit for 4-qubit quantum computer

Quantum computers offer the promise of a spectral leap in performance for solving non-polynomial problems. Some examples of non-polynomial problems a quantum computer could solve are prime factoring, database searching and quantum simulations. Each problem requires a number qubits needed in a system to solve; prime factoring requires a three qubit system to factorize 15 but implementations have been made up to five-qubit systems[**?**]. Likewise quantum computers use logic gates to solve steps in a algorithm for these problems these operations can also require high number of qubit in a system. One operation that is focused on in the rest of this chapter is the encoding operation that requires a minimum of four qubits. A five-qubit system would take the next step and decode the encoded bit string. As operations and algorithms to solve non-polynomial problems using a quantum computer march forward higher number of qubit systems are needed to preform the needed operations to solve complex problems. However, with this promise to solve non-polynomial problems comes the obligation of increased error correction to guarantee sufficient robustness to fault tolerance. When dealing with security and encryption error correction becomes the up-most importance to ensure information is reliable and secure.

In a qubit system errors occur by two ways: decoherence and machine error; decoherence is caused when environmental sub-atomic particles, photons or neutrinos, interact externally with the qubit system. This minor interaction over time dampens the qubit oscillatory pulse, losing all information given to the system. This error is included in the gate fidelity that is optimized experimentally, in the qubit optimization shown in this chapter we only look at the intrinsic fidelity. The intrinsic fidelity only considers the machine error because of it being easier to simulate in a computer program. Machine error is caused by optical measurements of the qubit system. Because qubits are sub-atomic particles they have quantum mechanical properties that allow them to be in both states at the same time. When a measurement is taken at a single state it is measured but a system can be given probabilities for the qubit system to favour a specific state. These probability coefficients are combinations that give the qubit system the capability to take 2^N bits of information, where N is the number of qubits. When the qubits are measured between states, several measurements are taken to get a mean state that the qubit system favours however, machine error can occur here. If not enough measurements are taken, or an optical sensor error occurs and misreads a state then the final mean state can be wrong.

Therefore fault tolerance is needed in a qubit system to ensure the states that are measured are reliable for the given probabilities. This is also known as the stability of the qubit system and because of their entanglement property of creating superpositioned states, sensors have to have a high resolution to properly measure the N potential states in a N-qubit system. One can imagine this makes the optimization more difficult to solve as the number of qubits increase to guarantee the stability, thus the reason of quantum computer chips only using three-qubit systems.

For a qubit system to be used in a processor chip a guaranteed intrinsic fidelity of 99.99% needs to be promised in the error correction component. This value is lowest fidelity that has shown a strong enough stability for the system with correcting errors in gate fidelity, which is optimised experimentally. To ensure a high enough gate fidelity, the intrinsic fidelity is optimized in a simulation to find values of circuit parameters that reproduce 99.99% for machine errors, then tests are ran on the circuit design to obtain the overall best gate fidelity. Because the three qubit processor chip has been manufactured and has been optimized to meet the required intrinsic fidelity, the four qubit system is now the next system to be optimized.

The four-qubit system is an essential step in security as it will be used in creating an encoding gate. Because encoding is a form of encryption that potentially can be stronger than standard techniques used by a transistor computers it is strongly desired in security and quantum networks. The problem is with out a five-qubit system to decode the message without human knowledge, minimal errors cans be made such that human can decode with out too much time for testing. This drives to optimize the error correction circuit in the single-shot Tofoli gate, the primary gate used for measuring qubit states with minimal amount of machine error. Therefore when errors are observed the error correction circuit is used as a fault tolerance guard when the superior processor circuit fails.

The Toffoli gate is a universal gate set[?] for quantum computers that has the property to be in reversible circuits. Thus can be utilized in gate operations like encoding and decoding because the are the reversed operations of each other. Combined with a single shot measurement scheme allows the circuit to optimal in processing time, however this comes at cost with higher error by taking only one reading. Therefore by optimizing the circuit design to obtain an minimal processing time that obtains an intrinsic fidelity greater than 99.99%, these gates can then be utilized in encoding applications and other reversal logic gates.

To obtain this high intrinsic fidelity an error correction component needs to be placed in the circuit design, this is done by implementing a controlled Z gate that is known for its ability to flip any bit in the system. Primarily it can be used to flip any error bits. Therefore the error correction component is optimized to obtain a minimal processing time to produces a intrinsic fidelity greater than 99.99%[?].

To do this the following model is optimized using a hybrid global optimization solver, Global Search from MATLABs Global Optimization toolbox, to optimize the circuit constants for a given processing time that satisfies the constraint

$$0.9999 \leq f(x).$$

The model uses the excitation energy states to determine the qubit state. Because electrons do not like to be excited too long they release some of the energy over time this can then be read in to determine the qubit states. However, because of quantum mechanics there is no way to determine the qubit state as it can be in both states at the same time until it observed. The observation of an electron is the frequency it release from shifting energy states this is known as the shift frequency ($\Delta_k(t)$) and the anharmonicity (η_{jk}) of the shit in frequency for each qubit is measured. By knowing these two factors and using Planks constant, h, the qubit state with respect to the jth excitation level can be determined by

$$E = h(j\Delta_k(t) - \eta_{jk}). \tag{4.1}$$

One other factor that is considered when reading qubit states, is that they can interact with one another because their charge and energy being released by an electron this interactions is called entanglement. To measure how strong the interaction between two electrons is a couple strength,g_k, is determined, this is experimentally measured constant. The coupling strength is only determine between the X and Y axis because they are controlled in the controlled-controlled-controlled-Z (CCCZ) gate, which is for a four qubit system. The X and Y coupling operators [**?**] is represented as

$$X_k = \sum_{j=1}^{n} \sqrt{j}|j-1\rangle_k\langle j|_k + hc \tag{4.2}$$

$$Y_k = -\sum_{j=1}^{n} \sqrt{-j}|j-1\rangle_k\langle j|_k + hc. \tag{4.3}$$

By obtaining the excitation energy **??** and coupling operators **??**, a Hamiltonian of the qubit states can then be determined. The Hamiltonian that is first determined is the drift Hamiltonian that describes the system of states that cannot be controlled the CCCZ gate and show the natural energy transition of the system

$$\frac{\hat{H}^{dr}(t)}{h} = \sum_{k=1}^{n-1} \frac{g_k}{2}(X_k X_{k+1} + Y_k Y_{k+1}) \tag{4.4}$$

The next Hamiltonian that is constructed is the controlled Hamiltonian, this Hamiltonian represents the part of the system that is controlled by the CCCZ gate over time,t.

$$\frac{\hat{H}^{C}(t)}{h} = \sum_{k=1}^{n}\sum_{j=0}^{n}(j\Delta_k(t) - \eta_{jk})|j\rangle_k\langle j|_k \tag{4.5}$$

In **??** the parameters that are being optimized over is the shift frequency, $\Delta_k(t)$, at a given time. The predicted shift frequency is subtracted by the anharmocity, η_{jk}, of the qubit system to determine any error.

By adding both Hamiltonians **??** and **??**, the general Hamiltonian of qubit system [**?**] is determine to be

$$\hat{H}\big(\Delta_{k(t)}\big) = \hat{H}^{dr} + \sum_{k=1}^{n} \Delta_{k(t)} \hat{H}^{C(t)} \tag{4.6}$$

$$\frac{\hat{H}(t)}{h} = \sum_{k=1}^{n}\sum_{j=0}^{n} (j\Delta_k(t) - \eta_{jk}) |j\rangle_k \langle j|_k + \sum_{k=1}^{n-1} \frac{g_k}{2} (X_k X_{k+1} + Y_k Y_{k+1}). \tag{4.7}$$

By varying qubit Hamiltonian **??** over a duration of time to measure the qubit states, Θ, the unitary qubit state evolution for the whole system can be determined for a number of processing steps, T.

$$U\big(\Delta_k(\Theta)\big) = Te^{\left\{-i \int_0^{\Theta} \hat{H}\left(\Delta_k(\tau)\right) d\tau\right\}}. \tag{4.8}$$

Because electrons can be excited to higher energies that are not necessary to the gate computation, the unitary evolution matrix gets projected onto matrix that only utilizes the desired energy states,

$$U_{\mathscr{P}}\big(\Delta_k(\Theta)\big) = \mathscr{P} U\big(\Delta_k(\Theta)\big) \mathscr{P}. \tag{4.9}$$

With the projected unitary evolution matrix **??** the required information of the system is obtained and the intrinsic fidelity is determined

$$\mathscr{F}\big(\Delta_k(\Theta)\big) = \frac{1}{N} \left| \mathrm{Tr}\Big(CCCZ^{\dagger} U_{\mathscr{P}}\big(\Delta_k(\Theta)\big)\Big) \right|. \tag{4.10}$$

This model describes the general n-qubit system and applying the four qubit CCCZ gate to obtain the overall intrinsic fidelity. By approaching the problem as a feasibility problem, we have been success in obtaining processing times for the error correction gate up to 65 nano seconds. The following Table **??** show currently running time gates and their current status of highest fidelity.

T (ns)	Intrinsic fidelity	CPU time
150	1.0	1 week
120	0.999977	1 week
75	0.999908	1 week
74	0.9999546	13 days
70	0.9999795	3 months
65	0.9999785	3 months

T (ns)	Intrinsic fidelity	CPU time
27	0.999992	1 day
26	0.9999	1 month
25	0.994626	1 month
23	0.974143	1 month
20	0.935444	1 month
15	0.907205	1 month
10	0.843589	1 month

With success of this method of approaching this problem were proceeding to use a global optimization solver from pythOPT, a python problem solving environment, to solve this problem as well looking into to lower and higher qubit systems.

By optimizing this problem as a feasibility problem we are able to obtain solutions for three and four qubit system, bring a new approach to optimizing quantum error corrections simulations. These give a promising design to a circuit that will be place on quantum processor chip. These chips can then be dedicated to encoding bit strings for security purposes that are using quantum networks. Likewise, furthers our understanding of optimizing for quantum error correction simulation and pushing to solve the five-qubit system. Striving to solve the five-qubit system is the next step to design a stable decoding gate to match the four-qubit encoding gate.

T (ns)	Intrinsic fidelity	CPU time
500	0.305841	2 week
300	0.41861	2 week
250	0.295303	1 month
200	0.608859	1 month
200	0.868338	1 month

Rational Design, Crystal Structure Prediction

Chapter 5

Conclusion

I conclude that I have solved the problem!