Thesis Proposal:
A Software Approach to Global Optimization

by

Marina Schmidt

Abstract

Mathematical models are a gateway into understanding theoretical or experimental occurrences, however to understand these models certain parameters need to be optimized to obtain the optimal behaviour or value. Global optimization is a branch of optimization that takes a function and maximizes (or minimizes) with in a given search space. Researchers over the past decades have developed numerous global optimization algorithms for solving problems by using various designs. However, global optimizations can struggle when the search space yields multiple local minima, this can cause many solver to get stuck in the search and slow down finding the global minima value. Another challenge is sometimes the mathematical models can complex and long to calculate causing the solver to spend a lot of time evaluating the model. These are only a few problems that can occur as other challenges can arise. To aid the solver in surpassing these challenges two pieces of software were developed and studied on two particular applications: Computefarm and Checkpointing. Computefarm is a distributed system that parallelizes the iteration step of a solve by distributing function evaluations to farmed computers. Checkpointing is a robust database schema that ensures the safety of data from being lost in failure in the optimization and is used to also monitor the solver. This is used to manipulate solvers and function evaluations to speed up the search for the global value. One application that is studied in this thesis is designing quantum error correction circuits. Quantum computers cannot rely on software to correct errors because of the quantum mechanical properties of subatomic particles. Instead circuits are designed to correct for different type of errors however, to ensure a high fidelity of the circuit a simulation of a circuits fidelity is optimized. This is optimized to obtain a circuit design for the four qubit and three qubit case with a fidelity of 99.99% by using the checkpointing software.

Another application is crystal structure prediction, this is done by using an ab initio code called VASP that obtains the total energy of given lattice structure. This determines the stability of the structure, predicting a stable structure like Diamond or Graphite has researchers to study structures. These simultation however are very complex and can be long to run for more complex structures like Silicon Dioxide. By applying the Computefarm with a solver multiple simulations can be ran at the same time producing the result of

tetragonal Silicon dioxide structure. By using both pieces of software these applications were examples of the aid they present in optimizing problems a relative amount of time.

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CCCZ	Controlled controlled controlled Z gate
qubit	Quantum bit