Quantum Mechanical Simulations on a Beowulf Cluster

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I. ABSTRACT

The objective of this project was to develop a parallel simulation code from a similar single processor code, and then run the parallel simulation code on a Beowulf cluster machine. The code studied utilizes a random path model using entwined paths that can be shown to model the quantum mechanical properties of a particle in a box. By running the code on *Medusa*, a Beowulf cluster machine environment, and confirming our results from simulations on a single processor, it has been shown that this parallel environment is an effective tool for computations which simulate quantum mechanical systems. In addition, significant progress has been made in showing that the equations of quantum mechanics are governed by an underlying stochastic process.

II. INTRODUCTION

Conventionally, quantum mechanics has been an epistemological rather than an ontological model of the universe. That is, with quantum mechanics we have an algorithm (the wave function) which describes our knowledge of the universe, but there is no guarantee that our algorithm actually corresponds to anything physical in reality. One way to guarantee this correspondence is to show that the equations of quantum mechanics can be derived from a model describing the reality of space-time. We are trying to develop a candidate for such an ontological model using fractal trajectories called entwined paths (Figure 1).

Since our model is based on an underlying stochastic process (a process governed by probabilities, such as the flipping of a coin), simulations with better statistics will produce better results. One way to increase the statistics of a simulation is to run it on many processors at once, such as in a parallel computing environment.

Successful simulation of this entwined path model on a Beowulf cluster would show that this parallel environment is an effective tool for simulating quantum mechanical systems. In addition, a model of this kind might also lead to further insights into quantum mechanics, thereby allowing more effective application of our understanding of the processes underlying the equations of quantum mechanics. Specifically, a better understanding of the processes underlying the equations of quantum mechanics may facilitate the design and implementation of quantum computation.

III. METHODS

Initially, the simulation code was developed in a single processor environment, which allowed for easier coding and testing. Once we were satisfied with the single processor code, we ported the code to a parallel environment in order to produce better statistics and to more vigorously test the validity of our model. The criteria of our code assessment were:

(1) The code successfully stores the past statistics of the entwined paths for each point in the space-time grid and when necessary references this history to produce a state change;

(2) If given initial conditions for the energy eigenfunctions, the eigenfunctions of the particle are shown to persist.

The algorithm that generates an entwined path in a box (Ord, 2003) was originally written in MATLAB (MathWorks, version 6.5), which meant that before the code could be ported to a parallel environment it would have to be rewritten in another language, such as C or Fortran (we chose to rewrite in C). At first, we tried to do this conversion manually, but due to time constraints and translation difficulties we elected to instead use the MATLAB C compiler to convert the code to C (Figure 2).
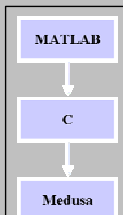
MATLAB → C → Medusa

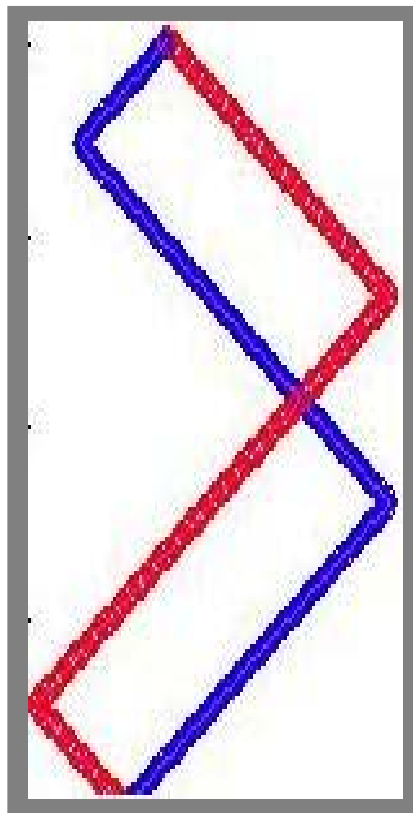**FIG. 2: Simulation code development.**

FIG. 1: Entwined path in a box.
In this model, entwined paths are confined to a two-dimensional discrete space. In the above figure, the y-axis is time, and the x-axis is space. The axes are scaled by the speed of light, such that objects traveling at the speed of light will move on diagonal paths, similar to the moves of a bishop on a chessboard. In the figure, the blue line can be thought of as representing the path of an electron (moving forward in time) and the red line of a positron (moving backward in time). The box has a width of L and a height of t_ret (return time of one cycle).
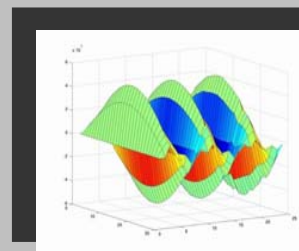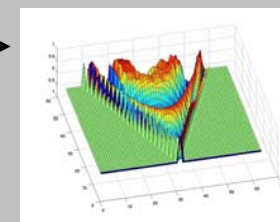
IV. RESULTS

FIG. 3: Time evolution of the ground state for a particle in a box.
This result came from a simulation code which did not retain a space-time history, and was run on a single processor machine. (Ord, 2003)

FIG. 4: Dirac propagator for a free particle.
This result also came from a simulation code that did not retain a space-time history, and was run on Medusa, a Beowulf Cluster. (Ord, Gualtieri, 2003)

V. DISCUSSION

(See Figures 3 and 4)

- Thus far, our results are limited to a MATLAB simulation code that does not retain a history of past events for each point in the space-time grid. The newest versions of the simulation code do meet this criterion, which is in place in order to accelerate the convergence of the code.

- In Figure 3, the wave-function is jagged at the boundaries of the box, and becomes worse as time progresses. Initially, these rough edges at the boundary were thought to be a problem with the code, but later we found that the problem arises from a property common to all discrete models of the Dirac equation for a particle in a box. That is, given initial trigonometric conditions for the wave-function, the Dirac equation is not separable.

- The statistics of Figure 4 are much better than Figure 3 because more processors allow us to simulate more entwined paths, thereby allowing the result to better resolve from the underlying stochastic process.

VI. CONCLUSION

The entwined path model preserves the propagator for the particle in a box and retains the energy eigenfunctions given initial conditions. Since the entwined path model is based on a stochastic process, the model better approximates the equations of quantum mechanics when it has better statistics. We have shown that running the simulation code on a Beowulf cluster is a simple and efficient way to get better statistics for the simulation, and have therefore demonstrated the effectiveness for simulating quantum mechanical systems of this kind using this type of parallel environment. In the near future we hope to show that the Born Postulate, which states that the probability of measurement of a particle in a certain state is the square of the modulus of the wave function, also holds under a simple measurement scheme for our simulation of a particle in a box.

VII. REFERENCES / ACKNOWLEDGMENTS

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