Quantum Mechanical Simulations on a Beowulf Cluster

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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.

Summary

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 [2, 3].

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 (a distributed memory parallel environment) 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.

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 algorithm that generates an entwined path in a box [1] 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.

Thus far, we have been able to use our simulation of entwined paths to produce the Dirac propagator for a free particle, and the time evolution of the ground state of a particle in a box. Our initial findings indicate that 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.

References

[1] G. N. Ord. box-path-generate.m, 2003.
[2] G.N. Ord and J. A. Gualtieri. The Feynman Propagator from a Single Path. *Physical Review Letters*, **89**(25):1-4, 2002.