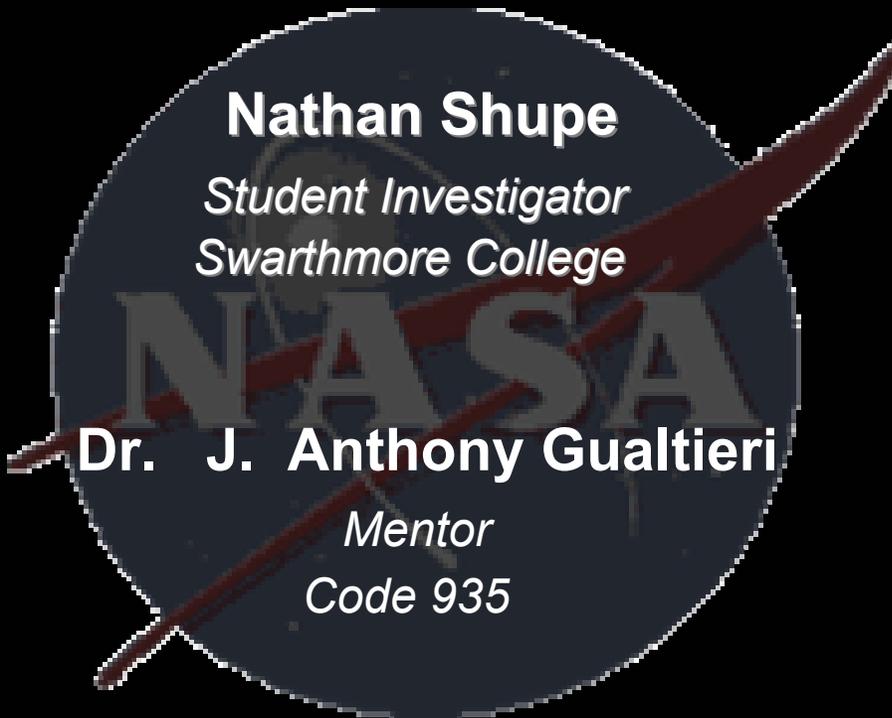


Quantum Mechanical Simulations on a Beowulf Cluster



VSEP

VISITING **S**TUDENT **E**NRICHMENT **P**ROGRAM

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.

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- D. Importance of Research

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- B. Beowulf Cluster
- C. Simulation Code Development

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Quantum History



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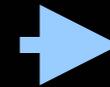
- Conventional quantum mechanics has the wave-function which allows us to **decode** information about nature.
- In this respect, quantum mechanics is well-defined in that we can precisely **predict** information about physical systems.
- The question remains, however, of how nature can **encode** the information in the wave-function.
- Conventionally, the answer to this question has been we do not and cannot know.

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The choice at hand:

The **wave-function**¹ is simply an **algorithm** which describes our **knowledge** of the universe.

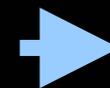


Quantum Mechanics is an **epistemological** model.

(or)

(or)

The **wave-function** corresponds to something **physical** in reality.



Quantum Mechanics is an **ontological** model.

¹ We shall define the wave-function as the probability amplitude of finding a particle at a certain position and time.

Feynman Paths

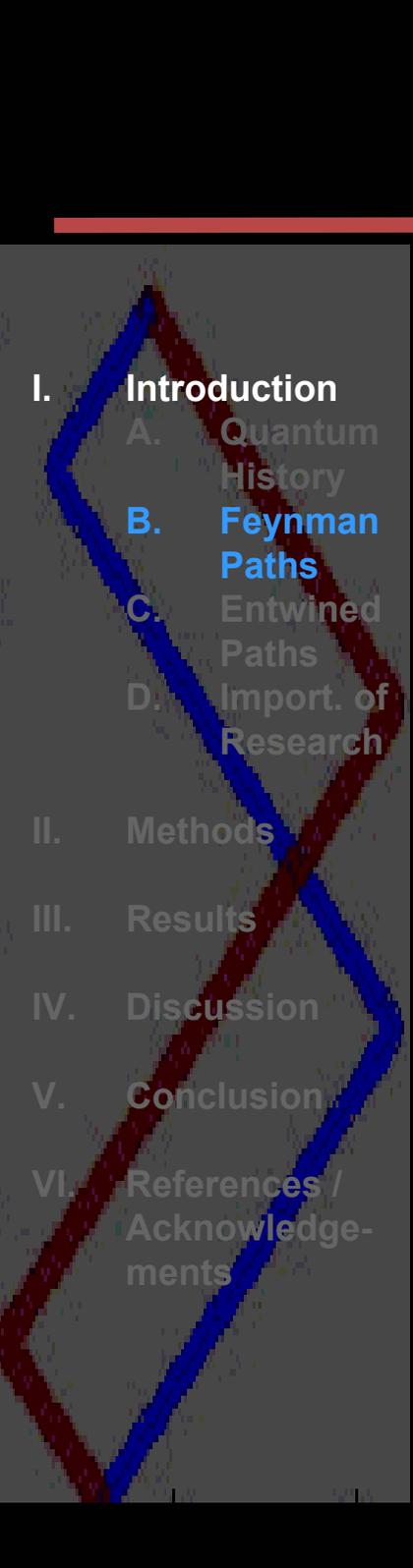
The Problem:

At initial time t_a a particle starts from the point x_a and moves to a final destination x_b at time t_b .

The probability amplitude, or kernel, to get from a to b is given by:

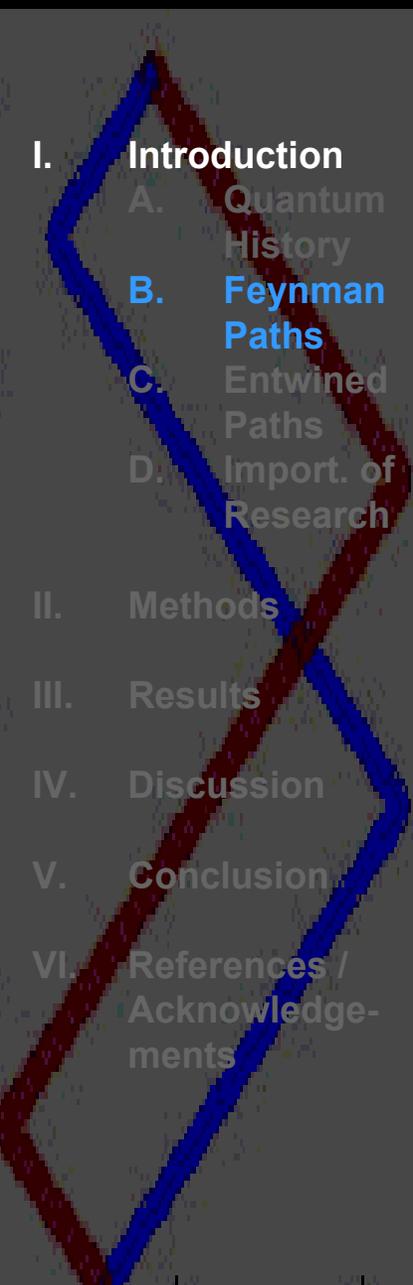
$$K(b, a) = \sum_{paths} \phi[x(t)] \quad (1)$$

where $K(b, a)$ is the kernel, $x(t)$ is a path, and $\phi[x(t)]$ is the probability amplitude of that path.



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Feynman Paths



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- Thus, according to Feynman's formulation, the **probability amplitude** or **kernel** of a particle moving from one point to another in space-time is the **sum of all of the amplitudes of all of the possible paths** from the initial position to the final destination.
- One way to define paths between points in space-time is to apply a **lattice structure** to space-time. In order to consider relativistic particles, we will use the **chessboard or checkerboard model**.

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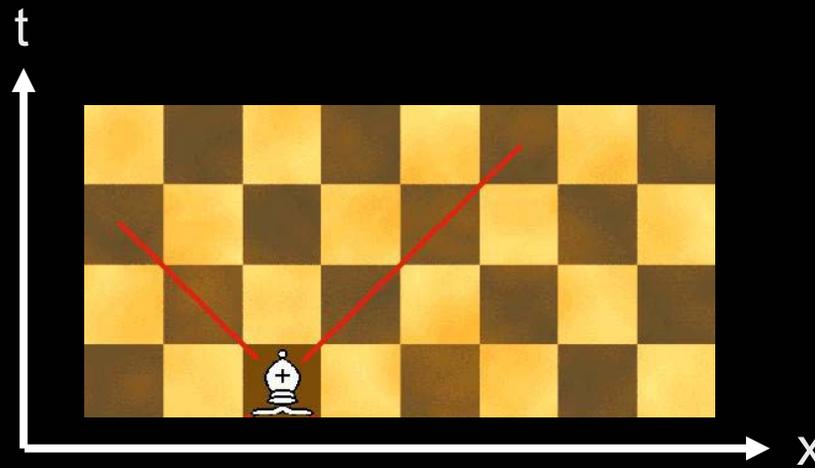


FIG. 1: Chessboard Model.

An example of a space-time trajectory of a relativistic particle is shown in Fig. 2.

If the time and space axes are in the right units², then relativistic particles will move on diagonals, similar to the moves of a bishop.

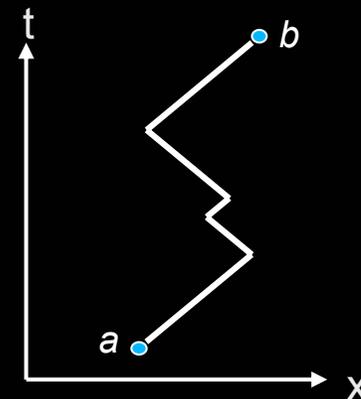


Fig. 2:
Path of a Relativistic Particle from a to b .

² The velocity of light, the mass of the particle, and Planck's constant are all unity.

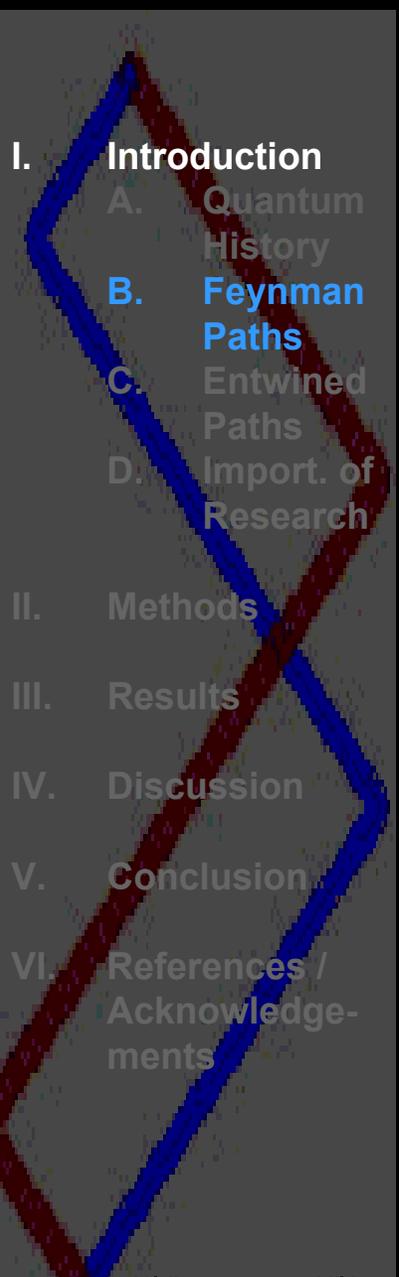
Feynman Paths

If we assign ε to be the magnitude of time steps on the lattice, and that the path direction can only change at the boundaries of the time steps, then the probability amplitude of traversing a path is given by:

$$\phi = (i\varepsilon)^R \quad (2)$$

where R is the number of corners, or direction changes of the path, and i is $\sqrt{-1}$.

This definition of the path probability amplitude changes the expression of the kernel.



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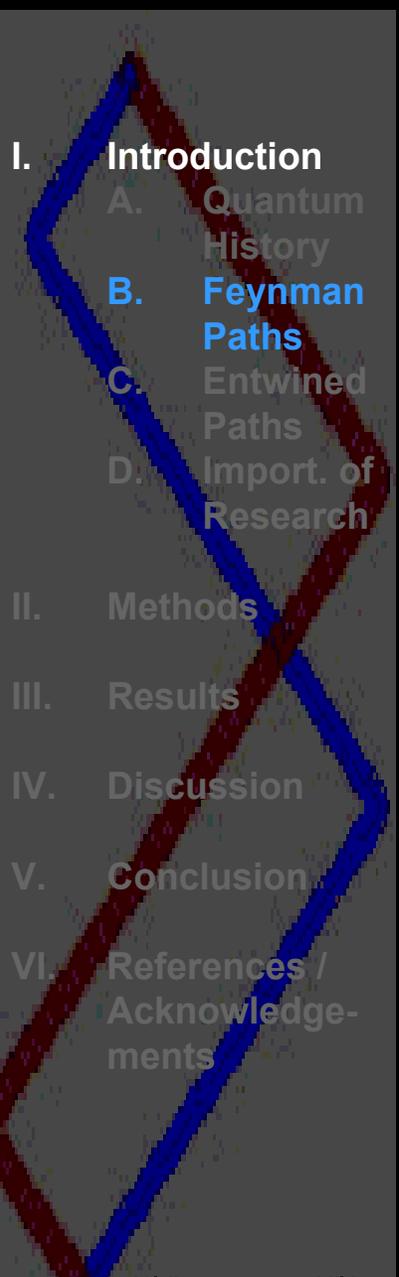
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The kernel can be calculated by adding up the contributions for the paths with R corners.

$$K(b, a) = \sum_R N(R) (i\varepsilon)^R \quad (3)$$

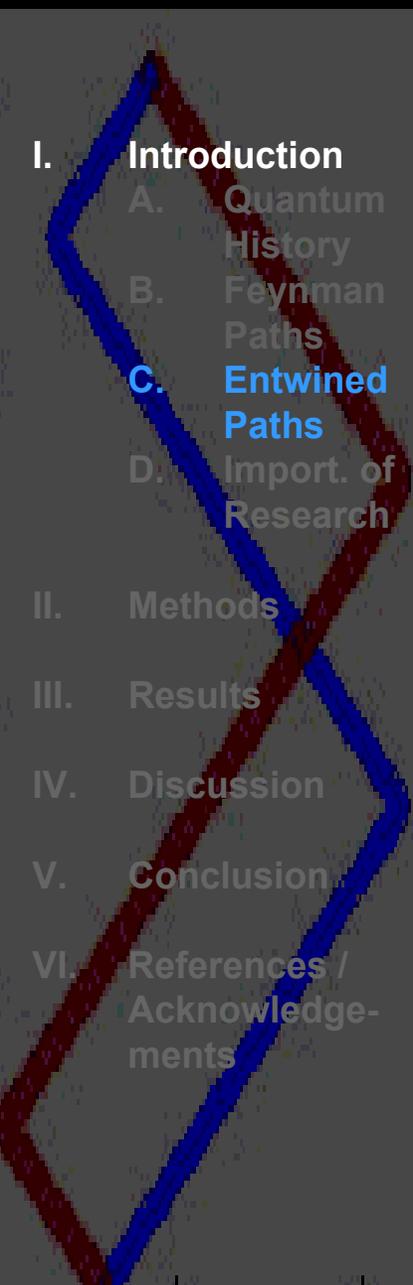
$N(R)$ is the number of paths possible with R corners.

As a result of our chessboard formulation, the **probability amplitude** and **kernel** are now valid for a free particle moving at **relativistic speeds in one dimension**. Therefore, the **kernel** should be equivalent to the **Dirac propagator**.



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Entwined Paths

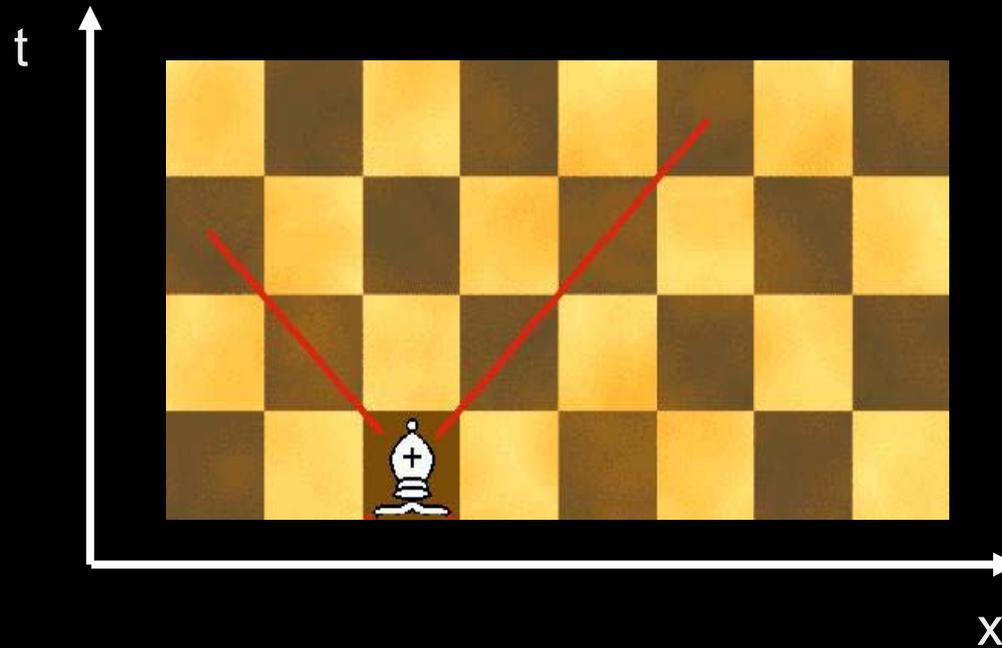


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- Recall that relativistic particles move on diagonals in the chessboard model, similar to the moves of a bishop.
- Note that once a bishop moves from its initial position, it can always return to that position, provided that there are no other pieces in the way.
- As a result, a **single bishop** could trace out **every possible path** on the chessboard from its initial square to another, simply by moving forward to the desired square, returning to its original, and then repeating the process for a different path.

Entwined Paths

FIG. 4: Chessboard Model for a Feynman Path.

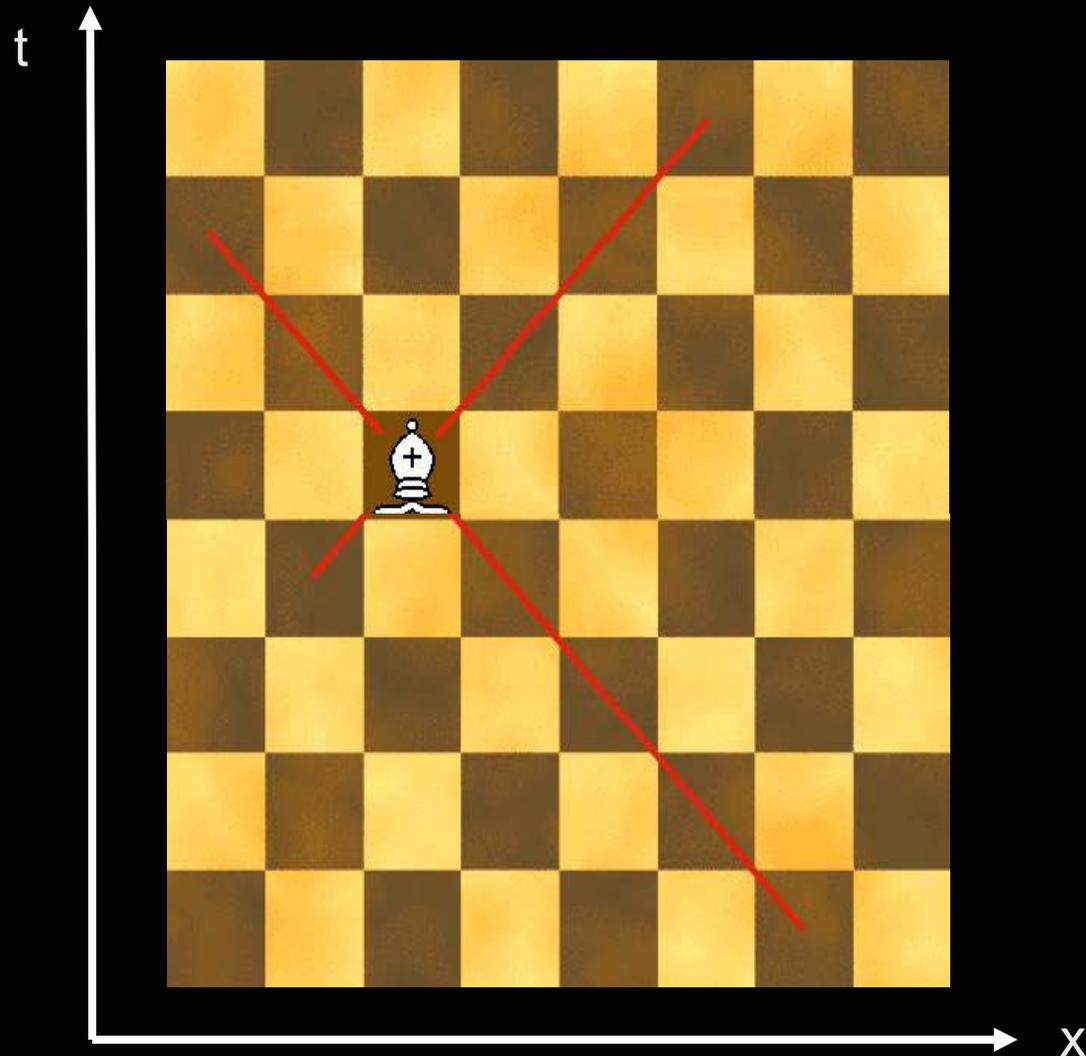


Feynman paths restrict the moves of the bishop to a forward direction...

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Entwined Paths

FIG. 5: Chessboard Model for an Entwined Path.



whereas entwined paths permit backward moves as well.

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Entwined Paths

For entwined paths, a **blue line** denotes a path moving **forward in time** (electron), and a **red line** denotes a path moving **backward in time** (positron).

The path is constructed as follows:

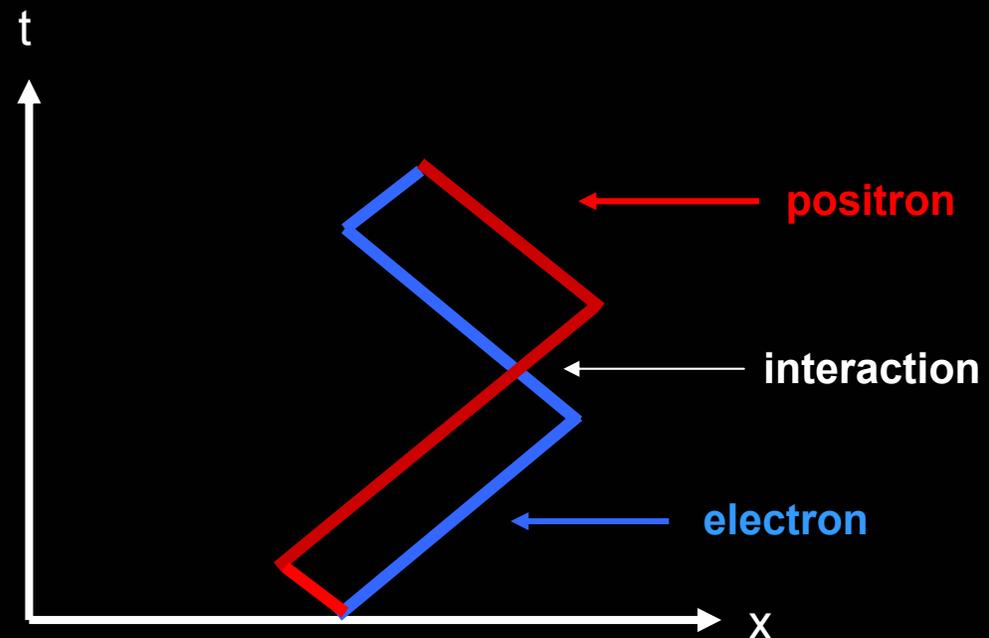


FIG. 6: Entwined Path Construction.

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The simulation code generates entwined paths somewhat differently, since half of the entwined path holds all of the information necessary to generate the entire path.

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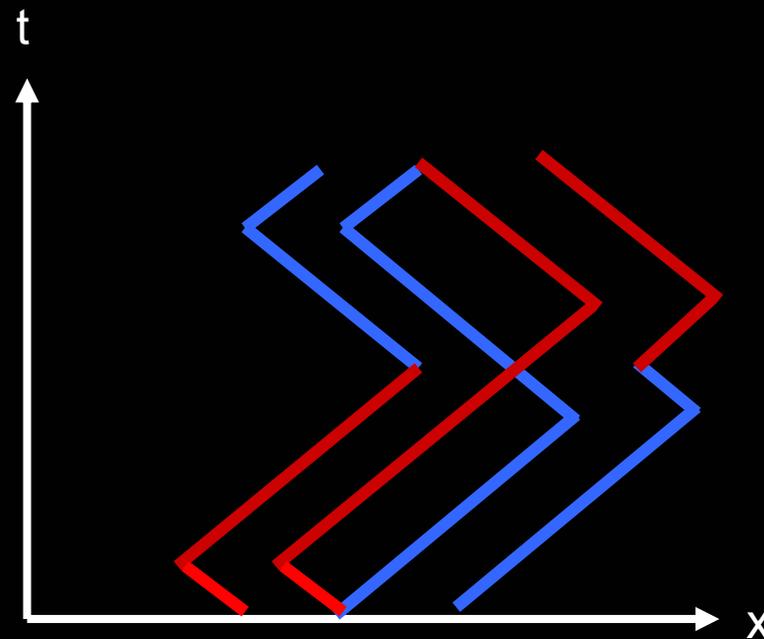
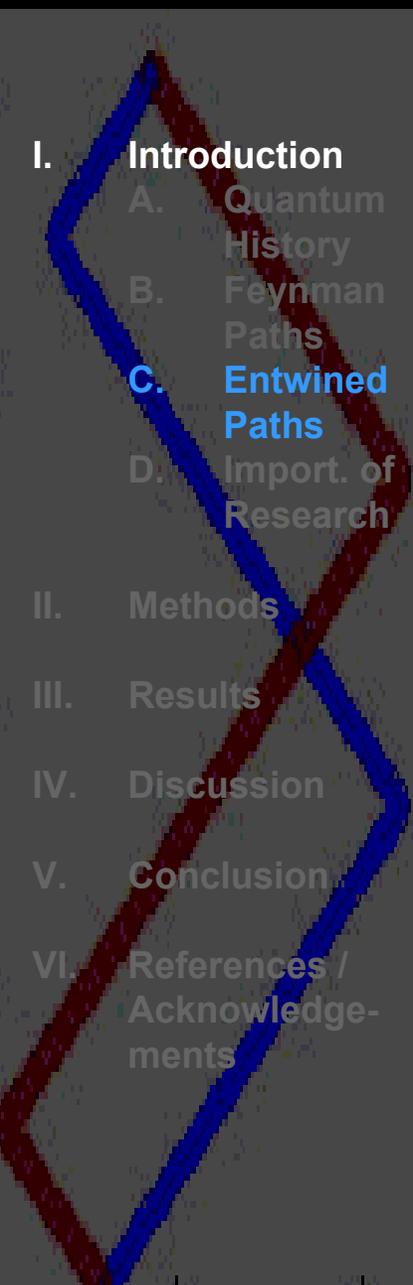


FIG. 7: Right Envelope of an Entwined Path.

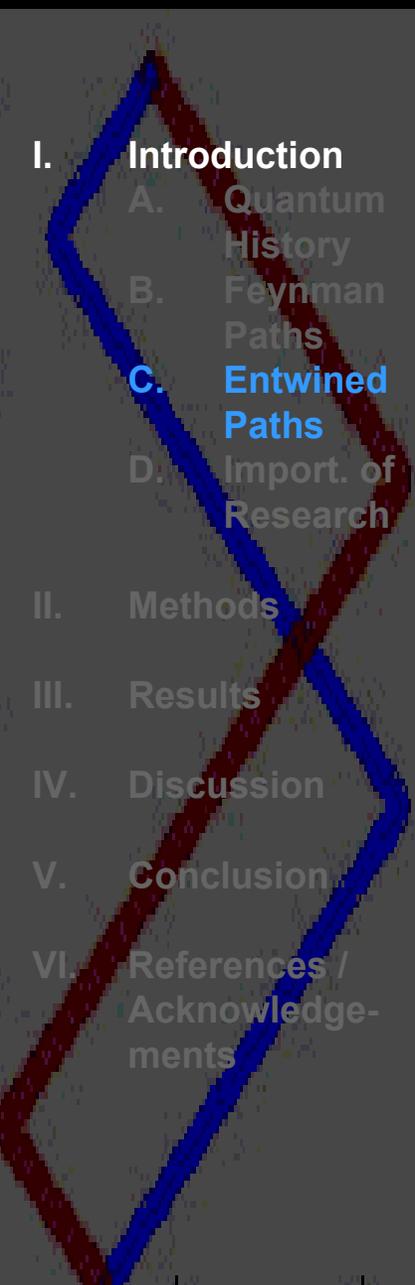
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- **Feynman paths** have a **many-to-one** correspondence with the particle they are describing (i.e., many paths must be generated in order to complete the ensemble and extract the propagator).
- **Entwined paths**, on the other hand, have a **one-to-one** correspondence with the particles they describe, since our method of constructing entwined paths starting and ending at the **same point** in space-time creates a **single path**.
- Therefore, **entwined paths** can more easily be associated with **physical trajectories**.

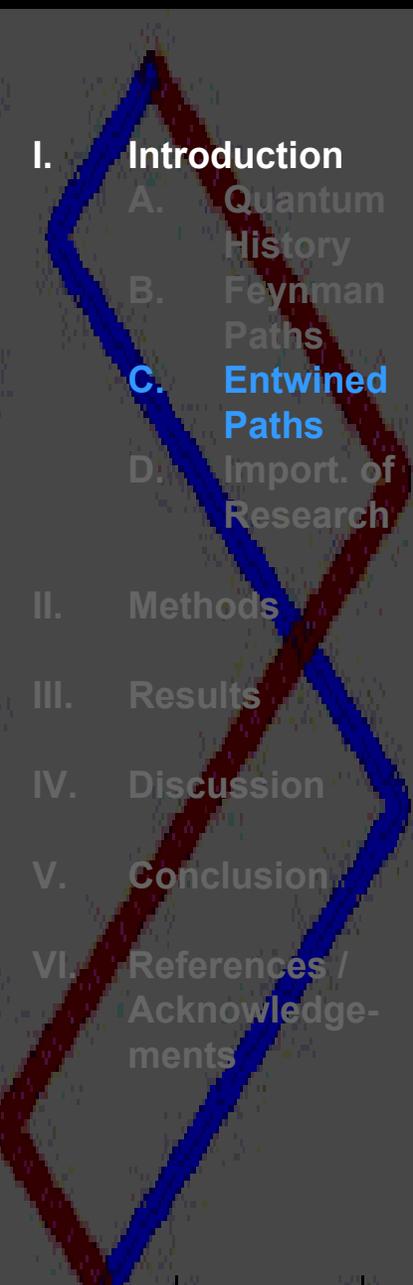
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- Another advantage of entwined paths is that they create the **phase** of the wave-function **without invoking** an **analytic continuation**.
- That is, the **phase** of the wave-function does not have to be artificially created by making the probability amplitudes complex, but rather comes about naturally as the result of the **space-time geometries** of the **entwined paths**.

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- Essentially, with **entwined paths** we are trying to do for **quantum mechanics** what **Weiner paths** did for **diffusion**.
- That is, we are trying to show that these **paths** actually correspond to **physical trajectories**, and in so doing show that the **mechanics of propagation** and the **measurement postulates** are the result of an **underlying stochastic process**³.

³ A process governed by probabilities, like the flipping of a coin.

Importance of Research

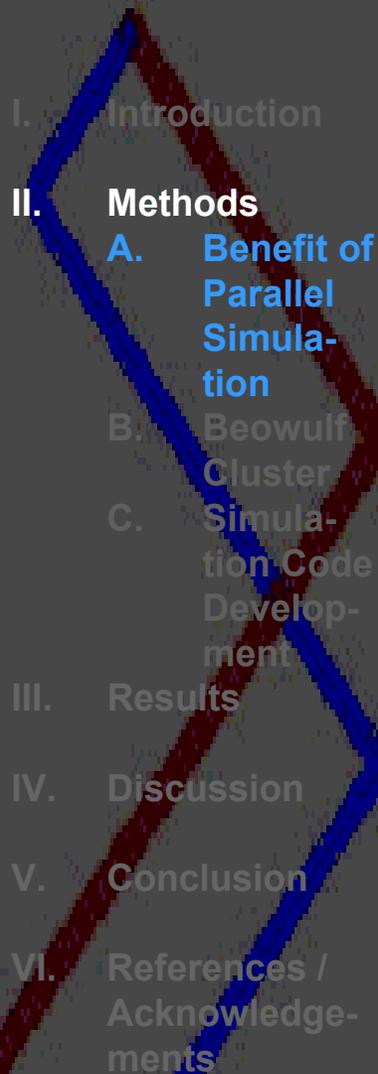


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- By running the code on *Medusa*⁴, and confirming our results from simulations on a single processor, we have shown that this parallel environment is an **effective tool** for computations which **simulate simple quantum mechanical systems**.
- A model of this kind may lead to **further insights** into **quantum mechanics**, thereby allowing more effective **application** of our **understanding** of **quantum mechanics** (e.g., **quantum computing**.)

⁴ A 64 node Beowulf cluster machine. The nodes have 2 processors (AMD Athlon 1.2 GHz, 512K of cache) each and are connected by a MYRINET (Myricom) network.

Benefit of Parallel Simulation



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- Since our model is based on an underlying stochastic process, simulations with better statistics will produce better results.
- One way to increase the statistics of a simulation is to run the code on many processors at once, such as in a parallel computing environment, and then compile the results from all of the processors in order to produce a result.
- For this project, we used *Medusa*, a Beowulf cluster machine environment.

Beowulf Cluster

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- A Beowulf Cluster, having a **distributed memory system**, is well suited to run **many copies** of the simulation code simultaneously.
- Essentially, we ran **identical copies** of the code on all of the processors, with **different parameters** (origin, probability of state change) for each processor. Thus, each processor simulated a **single particle** in a box.
- After the simulations had completed, we recompiled the information into an output file on a single processor machine, and used a graphing utility to visualize the results.

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- Initially, the simulation code was developed in a **single processor** environment, which allowed for easier coding and testing.
- Once 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.

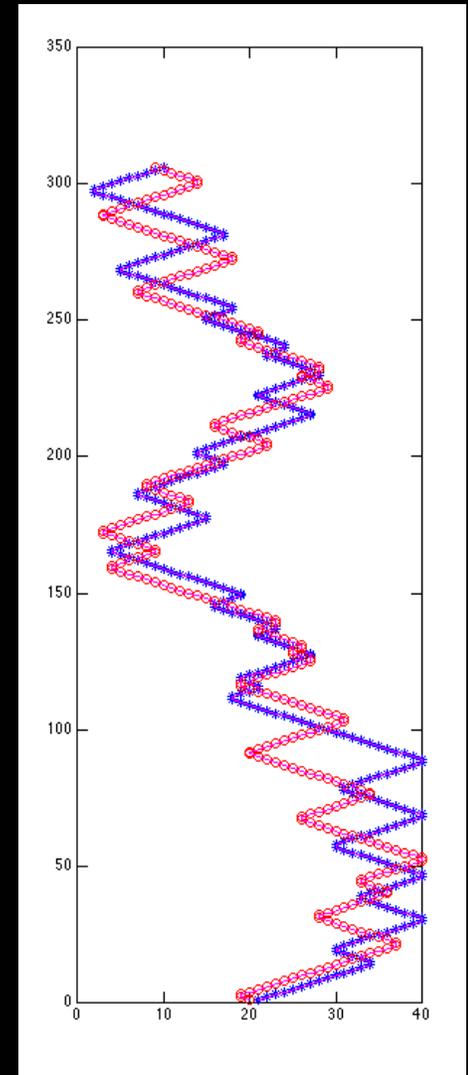


FIG. 8: Entwined Path in a Box.

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The criteria of our code assessment were:

(1) the code successfully stored the projection of each particle's **space-time history** and when necessary referenced this history to produce a **state change**, and

(2) that if given initial conditions for the energy **eigenfunctions**, the **eigenfunctions** of the particle were shown to **persist**.

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- 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 manually, but later elected to instead use the **MATLAB C Compiler**.

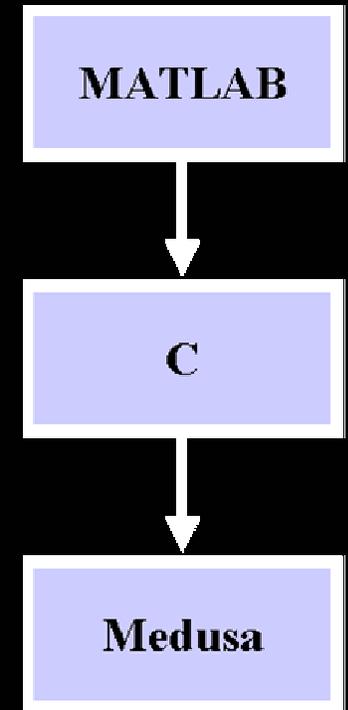


FIG. 9: Simulation Code Development.

Dirac Propagator for a Free Particle

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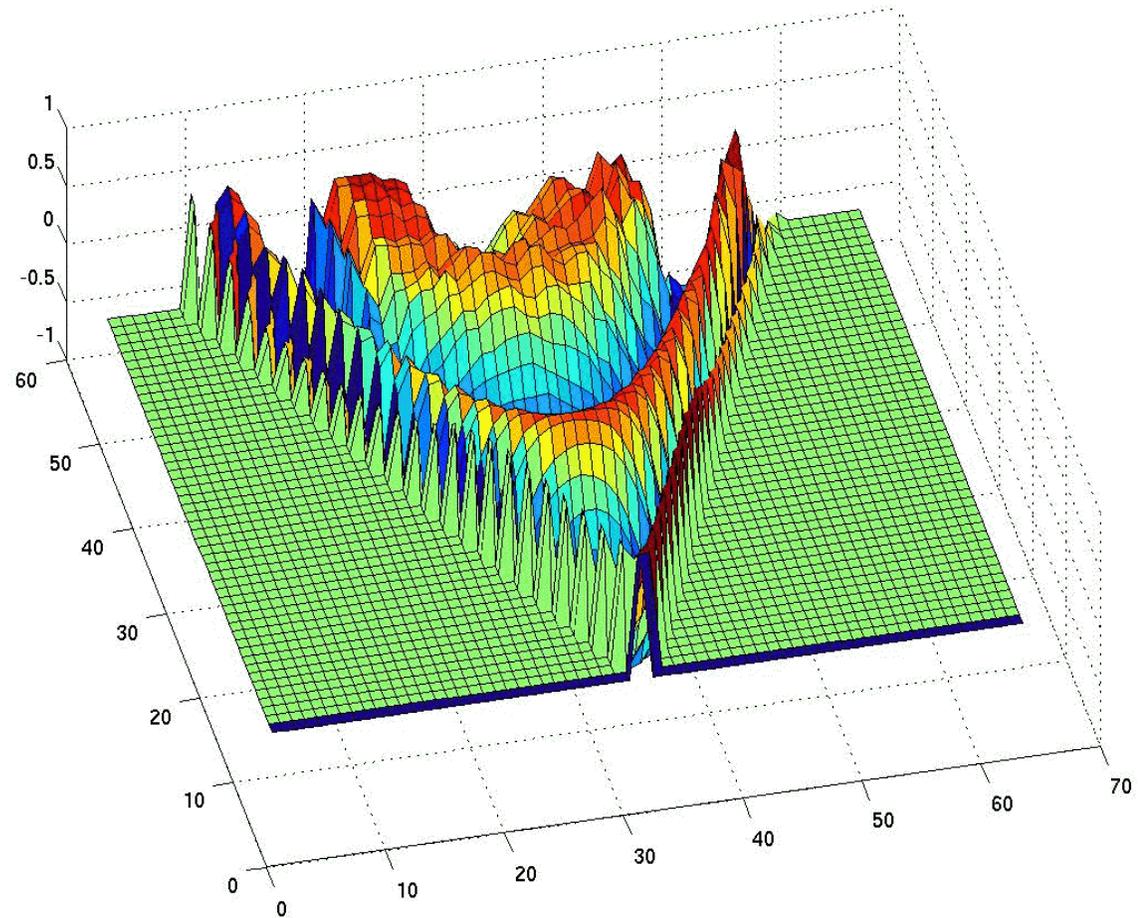


FIG. 10: Dirac Propagator for a Free Particle. This result came from a simulation code which did not retain the space-time history, and was run on Medusa, a Beowulf cluster.

Time Evolution of the Ground State of a Particle in a Box

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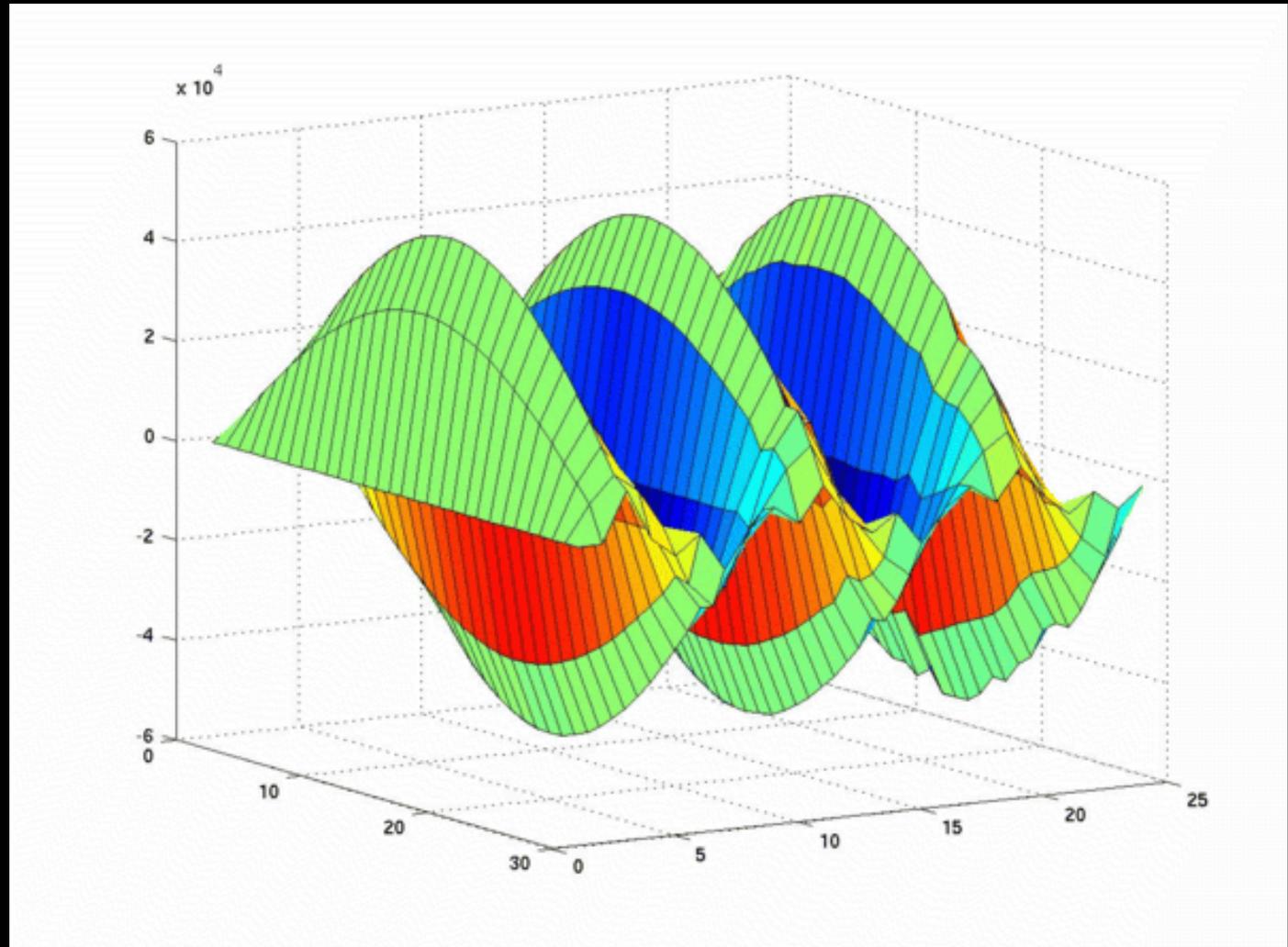
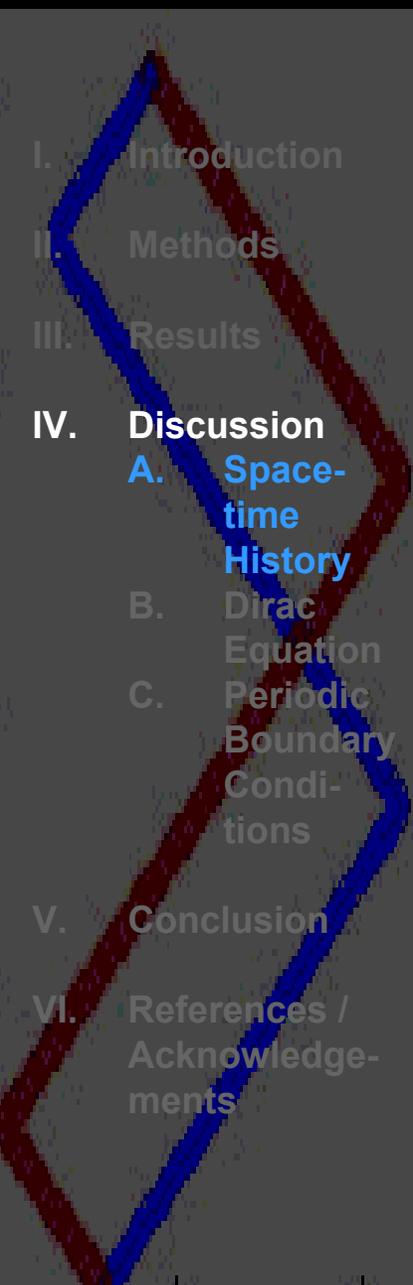


FIG. 11: Time evolution of the ground state of a particle in a box. This result came from a simulation code which did not retain the space-time history, and was run on a single processor machine.

Space-time History



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- Thus far, our results are limited to MATLAB simulate 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 to **accelerate the convergence** of the code (from $1/n$ to $1/\sqrt{n}$, where n is the number of time steps).
- Preserving the space-time history speeds up convergence because particles can look at the **eigenspace** and **minimize fluctuations** if necessary.

Dirac Equation

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- In Fig. 11, notice that the wave-function has jagged edges at the **boundaries** of the box, and becomes worse as time progresses.
- Initially, we thought these rough edges were a problem with the code, but recently found that the problem arises from a property common to all discrete models of the Dirac equation for a particle in the box.
- Given an **initial trigonometric condition** for the wave-function, the Dirac equation is **not separable**.

Periodic Boundary Conditions

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- One way to avoid the problems with the Dirac equation for a box is to set up **periodic boundary conditions**.
- Fig. 12 shows the output of the newest version of the simulation code.
- Periodic boundary conditions allow the Dirac equation to **separate** given **trigonometric initial conditions**.

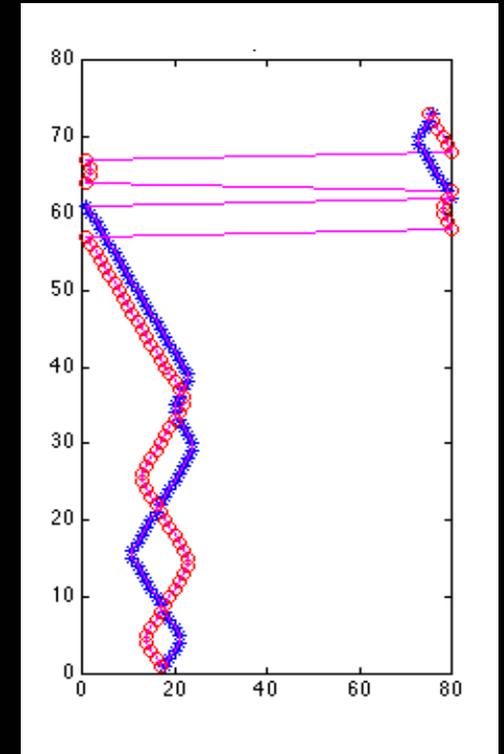


FIG. 12: Entwined path in a box with periodic boundary conditions.

Accomplishments

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- The entwined path model preserves the propagator for the particle in a box and retains the energy eigenfunctions given initial conditions.
- 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.

Future Work

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- In the near future we hope to show that the **Born Postulate**⁵ holds under a **simple measurement scheme** for our simulation of a particle in a box.
- Also, we plan to rewrite the simulation code so that both the **right and left envelope** of the entwined paths check the eigenspace in order to **determine state change**.
- Lastly, we also plan to further parallelize the code so that processors can **share their space-time histories**.

⁵ The postulate states that the probability of measurement of a particle in a certain state is the square of the modulus of the wavefunction.

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Acknowledgements

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