Numerical Studies of the Klein-Gordon Equation in a Periodic Setting

Brian Leu, Albert Liu, Parth Sheth

Abstract

Our focus is to understand three dimensional solutions of the Klein-Gordon equation produced with initial conditions that tend to zero at infinity. We utilize an existing program simulating various solutions of the equation, and produce high resolution simulations using the XSEDE parallel computing resources. When simulated on a large grid, it can be seen that solutions "blow up", a result that is still the subject of much study. We also perform a scaling study of the code to analyze the optimization effects of parallel computing, such as the relationship between number of cores and processing speed as well as overall speed increase in comparison to traditional simulation methods. The methods used in this study can be applied to modeling other wave-form equations as well.

Background

In modern physics, there is significant interest in studying and modeling quantum-scale interactions and forces. The Klein-Gordon equation is useful in modeling interactions such as the interactional energy in an aggregate of nucleons [3]. The focusing/defocusing nonlinear equation describes the evolution of a possible complex scalar field u:

$$\frac{\partial^2 u}{\partial t^2} - \Delta u + u = \pm|u|^2 u \qquad (1)$$

Where + is the focusing case and - is the defocusing case. Interest has been generated in analyzing the equation on an infinite three-dimensional space with various initial conditions and observing the solution behavior. Specifically, the solutions produced with initial conditions that tend to zero at infinity are of special interest. Because short term simulations of nonzero solutions on a finite domain and infinite solutions are similar, as time goes on the solution behaves differently for both domains. This poses an interesting study of the interactions of the Klein-Gordon equation in a periodic setting. Thus, scaling results to a large grid with numerous time-steps is necessary to accurately observe the difference between nonzero solutions on a finite domain and infinite solutions in a long-term setting.

Methods

An existing programs simulating various solutions of the equation were used [1], in which we varied the initial conditions, including grid size and time-step number. First Matlab and Python programs were used to identify interesting initial conditions. Then the Trestles site at SDSC was used to conduct high quality simulations, and the visualizations were processed using Visit. Trestles was chosen due to its efficiency running small to medium size jobs. Most of our jobs were conducted with a 512^3 grid with 5000 timesteps.

An Undergraduate Perspective

In addition to investigating the Klein-Gordon equation, another goal of this project is to provide an undergraduate perspective on supercomputing. When considering students studying both STEM and other areas, disappointingly few are excited about supercomputing. This is a problem that should concern all areas of the academic community, as research moves towards an increasingly large-scale, large-data direction. It is our firm belief that improving the user interface as well as lowering cost of entry will result in richer engagement from newcomers.

Methods for improving usability

- Integrate existing file management service (Globus etc.) or develop portal file service
- Inclusive precompiled software provides advantages over scattered packages to compile

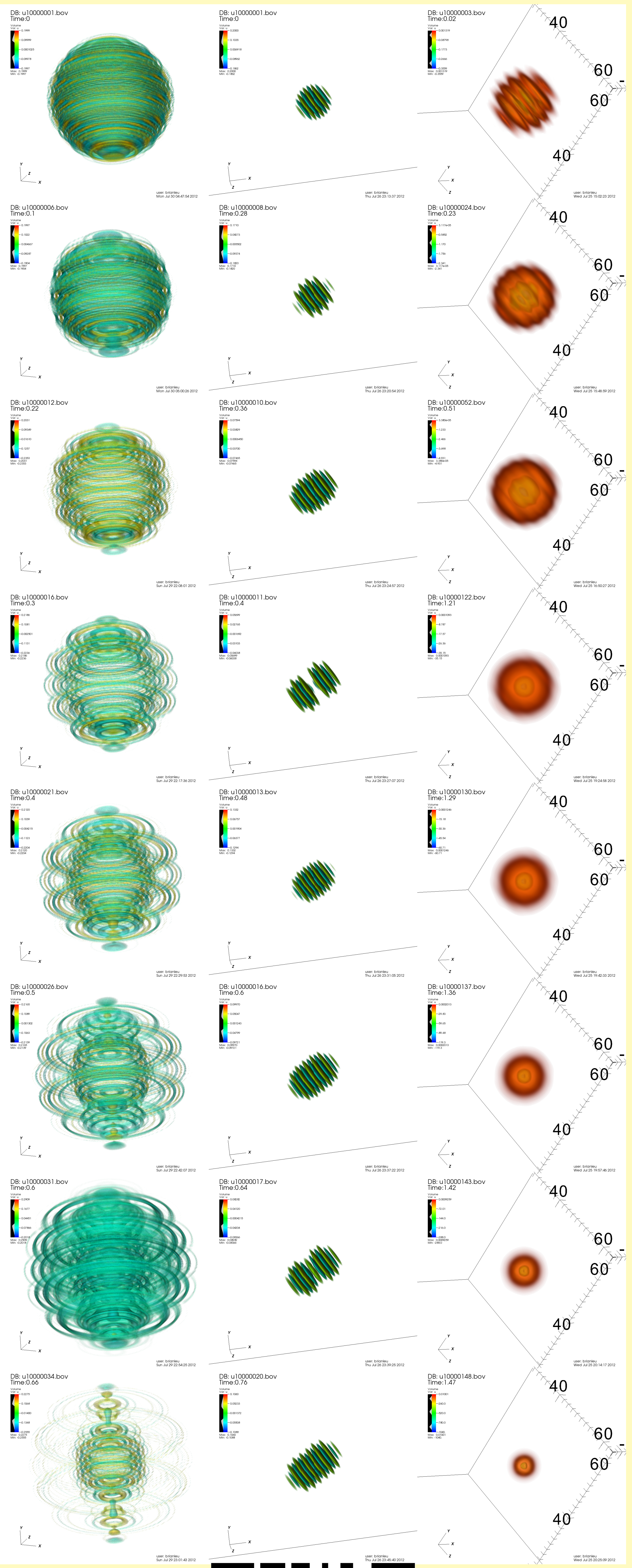
Postive Experiences

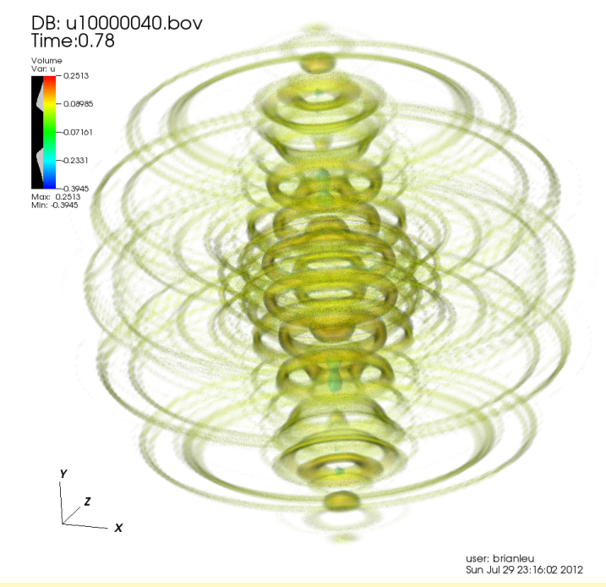
- Templates for submission scripts etc.
- Command line examples for interactive jobs, job reservations and other cluster functions

Ways to increase student engagement

- Focus on faculty-student interaction
- Increase availability of education resources (tutorials, literature etc.)

Simulation Results

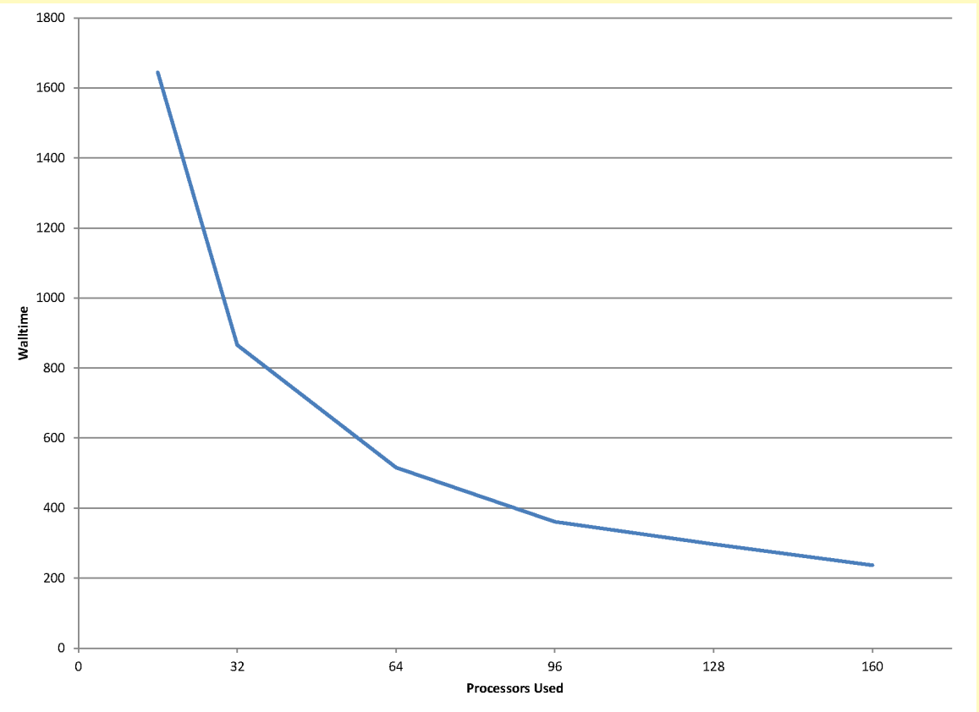




Scan the QR code to the left to view some of our simulations in motion.

Scaling Results

In order to demonstrate the performance increase supercomputing provides, we conducted the same job using a variety of core numbers to chart the results. Each test was conducted on a 64^3 grid with 2000 0.001 second timesteps. It is important to note that a linear relationship between core number and performance increase was not observed, due to overhead communication cost between nodes.



Conclusions

From our study, it is evident that to simulate such behavior accurately, models must be created in a large grid with fine point precision. Our work thus demonstrates the necessity of supercomputing in the field of visualization and beyond. In addition, our group represents the diversity of fields supercomputing can be applied to, as we all plan to apply high performance computing to our future work in electrical/computer engineering, computational biology, and applied physics. It is our hope that the success of our work will disprove the belief that high performance computing is an area isolated only to fields concerning technology.

Acknowledgements

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References

[1] G. Chen, B. Cloutier, N. Li, B. Muite, and P. Rigge, Parallel Spectral Numerical Methods, Blue Waters Undergraduate Petascale Module, (2012).

[2] L. Yang, Numerical Methods of the Klein-Gordon Equation Masters The- sis, National University of Singapore, (2006).

[3] L. I. Schiff, Nonlinear Meson Theory of Nuclear Forces II. Nonlinearity in the Meson-Nucleon Coupling, Physical Review, (1951).

[4] R. Donninger and W. Schlag. Numerical Study of the Blowup/Global Ex- istence Dichotomy for the Focusing Cubic Nonlinear Klein-Gordon Equation, Nonlinearity 24, 2547-2562, (2011).