SPS Chapter Research Award Proposal

Project Proposal Title	Data Analysis and Accuracy: Small Supercomputer Versus a Dell Dinosaur
Name of School	University of Kentucky
SPS Chapter Number	3511
Total Amount Requested	$1,157.20

Abstract

Computational methods provide powerful tools for solving problems in physics. We plan to build a mini-supercomputer from Raspberry Pis following the "Tiny Titan" build specifications available from Oak Ridge National Lab. Once built, the cluster can be used indefinitely for education, outreach, and community building.

Proposal Statement

Project Overview

There are several new technologies that have revolutionized the ways to approach physics. One of these technologies is accessible supercomputers. Many physicists work with enormous amounts of data that require sufficient computational power to analyze: national labs, NASA, and many industry jobs use supercomputers to handle large quantities of data. Today's physics students need to be trained in data analysis in order to interface with complex computing systems. This project will try to answer the most fundamental questions for students: How does a supercomputer work? How is parallel processing used in physics? Why is this useful for data analysis?

Physics research is already being shaped by the growing accessibility of parallel processing. Computational methods allow us to test theoretical models, and as these models increase in complexity, parallel processing is required to compute data in a realistic amount of time. We can already see an increasing demand for physicists with computational backgrounds; however, there are limited resources for this kind of experience in REUs and traditional physics classes. We hope to provide a resource for UK and local SPS chapters to give undergraduate physicists an opportunity to gain this experience.

We plan to build a mini-supercomputer based on the "Tiny Titan" Raspberry Pi cluster, then use three programs to demonstrate important physical concepts such as mathematical approximations, complex modeling, and interactive systems. The Ising Model is a standard problem in many core physics classes, and there exist many ways to simulate this mathematical model and can include a visual representation. Additionally, we hope to assemble a π approximation model and a molecular dynamics simulation. We think that this will provide a well-rounded introduction for people without computer backgrounds, and the molecular dynamics simulation would model a previous UK SPS project: a self-modulating whirlpool.

By offering multiple research goals, we hope to introduce students of all backgrounds to the process of writing code for parallel processing and explain why this data would not be achievable on a typical desktop. We will compare the results of the Tiny Titan to a desktop computer to examine the increase in accuracy and data handling of a supercomputer. This project will demonstrate the uses for parallel processing in an accessible manner for undergraduate students. These three programs will give students an appreciation for the importance of accuracy in data analysis, as well as a hands-on introduction to computational physics.

The Tiny Titan build with our three interactive programs fulfills several goals of the SPS program as well as strengthening the school's community and our chapter connections. There has been an initiative at UK to strengthen the network of physics undergraduates through team building games and competitions. We will construct a server for SPS games and hold our own physics competitions with the Tiny Titan. We will also invite local SPS chapters to our friendly game nights and use the mini-supercomputer to stay connected through our gaming server and competitions. We will place the SPS logo on the cluster case, as a recruitment and advertising tool.

This mini-supercomputer will also serve as an excellent demonstration tool for outreach events. It will be a centerpiece for the SPS-sponsored Open Lab Day at UK, where we invite other SPS chapters in our state to visit UK for lab tours and display cutting-edge physics research. We will have a gaming system controller wired to the Tiny Titan to make the demonstrations user-friendly and accessible, as we often have high school students attend as well.

At UK, there are two core physics classes that are centered on computational physics, and many of our SPS members are also enrolled in mathematics, computer science, and computer engineering programs.The Tiny Titan would provide a chance for physics undergraduates to receive hands-on experience in data analysis and parallel processing.These classes expose students to Monte Carlo simulations and give rise to deeper questions about data analysis in research applications, but there are currently limited avenues of exploration for physics students at UK. This mini-supercomputer would be a resource for any undergraduate student interested in learning outside of the classroom.

We think that this project is highly valuable because of our experiences in physics classes that can be expanded upon by creating a resource like this, as well as the more creative question of "what can a physicist do with a supercomputer?" The field of physics is becoming increasingly technical, experience in computer engineering and data analysis is a skill set in high demand for physicists. Many of our undergraduate members are involved in research projects that would greatly benefit from access to a more powerful data processing system, and we plan to invite local SPS chapters to use this great resource as well. Access to a mini-supercomputer would allow more students to propose their own projects and encourage networking with our peers in mathematics, computer science, engineering, and more. This will not only be an outreach tool for SPS but a recruitment tool, as we can encourage other students to join SPS and take introductory physics classes.

Project Background

The Ising Model is a representation of ferromagnetic behavior of materials at different temperatures, which is a common problem in computational physics and gives students exposure to modeling physical effects using mathematical representation. We will examine the effects of temperature variation on magnetism, specifically the Curie temperature at which ferromagnetic materials can become magnetized or unmagnetized due to the behavior of individual particles in the material. Expected behavior of this model would be that a larger model with more data points will be more accurate and approximate the Curie temperature more closely.

The molecular dynamics simulation is the second proposed program, students will participate in the creation of a complex system and will be able to relate the model to a demonstration that our SPS previously built, a self-modulating whirlpool. This will be an interactive simulation that can be modulated with a game system controller, performing actions on the system such as increasing or decreasing particle size to explore the effect on viscosity, introducing outside elements to disrupt the stability of the system, and time-dependent models of sedimentation and precipitation with variable starting parameters. The expected behavior of this model will be a more responsive environment and the ability to model more complex interactions with a more powerful system.

Pi is one of the fundamental constants of the universe. Estimating π using the Monte Carlo method will teach students the importance of mathematical approximations in physics, and we will test how many digits of π that a Tiny Titan can calculate with reasonable accuracy. Irrational numbers like π are notoriously hard to calculate because of their non-algebraic nature, the methods of calculation require subtle approximations that have effects in the overall accuracy of the result. This estimation and loss of accuracy are crucial to many experiments as π is a constant in many equations across physics. Expected behavior of this model would be that a more powerful system could more accurately compute the value of π.

The results of these three programs will be compared on the Tiny Titan and a Dell desktop that is currently owned by UK SPS. We take for granted the computing power of this older desktop, but comparing its results to a small supercomputer would show how it stands against the future of computing.

Expected Results

The expected increased efficiency on the Tiny Titan will be measured and quantified as accuracy and model size/data points. The expected increase in accuracy of program results on the Tiny Titan will be compared to program results from the Dell and measured against known values of π and Curie temperature. The Tiny Titan's ability to run complex models will be demonstrated by comparing model size and time responsiveness of models to the models run on the Dell, and the number of data points that each machine is capable of generating in a model will be recorded as a function of computing power.

To demonstrate the efficiency of parallel processing, the cluster can be confined to one Raspberry Pi, or "node" in the Tiny Titan build, then additional nodes can be added to see the increase in computational productivity. This can be quantified by accuracy and data size and graphed as a function of node number. We expect the accuracy and model size to increase with each node addition up to a point where these values will plateau and additional nodes will have less effect.

Description of Proposed Research - Methods, Design, and Procedures

The first step will be building the Tiny Titan and running a simple exercise to test the result of increasing "nodes" by adding Raspberry Pis. This will establish our baseline for analysis on the Tiny Titan. While this build is being completed, our three teams of SPS members will begin assembling the interactive programs. These teams will first run their programs on the Dell workstation and establish their baseline data points on the Dell. Once we have the Tiny Titan completed, our teams will test their programs on the supercomputer.

The first team will work on a C++ version of the Ising Model, which students in the advanced computational physics class have worked on in the past. Python will be used to create visualizations for the Ising Model, the output will be a small video file that will model how magnetized particles acts when the temperature is raised or lowered. For reference, we will be using Schroeder's "Introduction of Thermal Physics" and Simon's "The Oxford Solid State Basics" for references.

The second team will use ORNL GitHub resources for the water simulation from the Tiny Titan repository. This simulation repository will be the beginning of our molecular dynamics simulation, we will modify this code to include an interactive viscosity parameter. This simulation will be styled like a video game with interactive features for viscosity, particle mixing, and displacement elements. This will pair with a previous project, the self-modulating whirlpool, for a demonstration of virtual systems versus direct application.

For the estimation of π using the Monte Carlo method, we will decide between a Mathematica or C++ approach, based on the success of the C++ Ising Model. For further reading and reference we will use Bevington's "Data Reduction and Error Analysis for Physical Sciences."

We plan on having weekly meetings formatted as a research or lab meeting, where people will present their progress and help each other with any problems. Students who have already had the upper division computational physics course will work with students in the introductory data analysis class, and students with computer science and engineering experience will lead workshops at these weekly meetings to strengthen skills with other members. Our SPS advisor can also provide advice and assistance since he has computational physics research experience, as well as lend his copy of Press' "Numerical Recipes in C."

Project Logistics and Support

All SPS officers will be involved in the planning and execution of the Tiny Titan build, as well as the SPS members who volunteer for the three programming groups. There are approximately a dozen SPS members who have experience in computer science and engineering, and eight SPS members have previously done research at Oak Ridge National Laboratory and Los Alamos National Laboratory involving parallel processing and computational analysis. These members will be team leaders for the programming teams, and an undergraduate who is a dual program student in computer engineering has volunteered to oversee the build itself.

Our SPS faculty advisor is a condensed matter physicist who teaches one of the computational methods and analysis classes at UK, he will be available for questions and mentoring students. SPS is a student organization, so we have a dedicated club room in the Chemistry-Physics building on campus. We already have a desktop computer in our club room that will be used as a comparison for all of the programs on the Tiny Titan. We have access to hardware such as monitors, surge protectors, and adaptors, and access to University-licensed programming software with plenty of documentation. The logistics for hosting a mini-supercomputer will be supported by our department.

Project Timeline

1) Parts will be ordered by the end of January.
2) Programming teams will form and begin weekly meetings by February.

3) Teams will assemble and test programs on the Dell desktop by the end of April.
4) The Tiny Titan build will be finished by the end of April.
5) Interim report with established data baselines and documentation of the Tiny Titan build will be submitted on May 31st.
6) The Ising Model program will be running on the Tiny Titan by July, and the Tiny Titan will be used as a recruitment tool during freshman orientation of Fall 2019.
7) The water simulation program with additional features will be running on the Tiny Titan by the end of August.
8) The Tiny Titan will be presented at Open Lab Day 2019 on the decided date in September, the chapter will present documentation of this to SPS.
9) The estimation of π program will be running on the Tiny Titan by the end of November.
10) The final report will be prepared with a fully documented Tiny Titan build (descriptive essay with pictures), pictures and reports from all outreach events (UK freshman orientation or "K-week," Open Lab Day, game nights and physics competitions), and a GitHub repository where all programs will be stored for future use.

Budget Justification

The Raspberry Pis are the majority of the budget as they form the basis for the entire Tiny Titan cluster, but we will purchase them in a kit that comes with other necessary components to cut down on cost. The ethernet cables are necessary to link the cluster together and to the monitor, and the ethernet cable switch will allow each Pi to be connected and disconnected independently. Each Raspberry Pi requires an SD card that will function as memory for the cluster, and we plan on purchasing a manual to accompany these kits. We will be using our own computer, keyboard, and mouse to write the programs.

An Xbox controller will allow us to interface with the Tiny Titan in an accessible manner and create simulations that are interactive for students. We already have access to USB cables and adaptors for this accessory, and we will be using surge protectors and speakers that we already own. The final item we are requesting in the budget is a monitor. We would like a quality monitor for demonstration purposes and will be asking our department for financial assistance with this accessory item.

Bibliography

Bevington, P. R., & Robinson, D. K. (2010). *Data Reduction and Error Analysis for the Physical Sciences*. Boston: McGraw-Hill.
Schroeder, D. V. (2000). *An Introduction to Thermal Physics*. United States: Robin J. Heyden.
Simon, S. H. (2017). *The Oxford Solid State Basics*. Oxford: Oxford Univ. Press.
Press, W. H. (2002). *Numerical Recipes in C*. Cambridge: Cambridge Univ. Press.
Tiny Titan Build Guide. (2015). Retrieved from http://tinytitan.github.io/downloads/TinyTitanBuildGuide.pdf

Links to webpages selling the items we will need to build the cluster.

- A guide book on using the Raspberry-Pi and different associated projects
- The Raspberry-Pi model which we plan to use
- Additional parts for working with Raspberry-Pi
- The connectivity port to connect all nodes in the cluster
- Cords to make the connections with
- Controller for use with the Oak Ridge National Lab outreach simulation
- Monitor to display the user interface