High Performance Computing In Physics Education

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Abstract— We envision a future where computation is an integral part of the education of every physics student. We are working toward that future by creating a vibrant community of educators, a forum for open discussion, a collection of educational resources, and a set of strategies and tactics that support the development and improvement of all aspects of computational physics education. This paper discusses our motivations, goals, and the role we see for High Performance Computing in the physics curriculum.

Index Terms—High performance computing, physics education.

1 INTRODUCTION

Our mission is to increase the utilization of computing technology to improve the physics curriculum. From programs used to acquire and analyze data and simulations used to illustrate concepts in the classroom to applications that solve complicated physics problems on supercomputers, computer software plays a vital role in enhancing physics education and serves as an essential tool for the physicist of the twenty-first century.

We realize that it will take time and a focused effort to create an environment that is supportive of a strong computational presence in the classroom. We are confident that by creating and sustaining a community to work together and to share ideas and experiences we will achieve this goal.

The addition of a thoughtful national computational physics program will improve and transform physics education and provide students the skills they need to solve the problems they will encounter in today's world. Computer simulations and visualizations often illustrate concepts far more clearly than drawings on blackboards or in textbooks. Interactive computer programs that allow student involvement enhance student understanding. Whether using existing programs or writing code from scratch, the art of scientific computing is commonplace in today's workplace. Thus, graduates who have the skills to create and use scientific code are more marketable. Students develop a more complete understanding of physical systems by studying computational physics because the algorithms used in programs and the traditional equations of physics are the products of fundamentally different and complimentary modes of thought. Equations are statements of fact, while algorithms are the embodiments of processes. Students benefit by employing a variety of computational models to represent a single physical system and comparing their relative merits. This variety of alternative models is frequently not apparent in the simplified systems that are traditionally presented to the physics student. Numerical methods will make it possible to study systems that are not amenable to analytical solution, including complicated systems exhibiting emergent and chaotic behavior. Knowledge of the unique challenges of scientific computing (such as step and grid size, roundoff error, stability, and program validation and verification) equips the student to develop solutions to a much broader range of systems. Finally, the physics curriculum must include instruction in the art of using computers and microcontrollers to acquire and analyze observational and experimental data. These are essential skills for those who decide to pursue a career in experimental physics. Data analysis and mining techniques are also essential tools for extracting useful information from the large amounts of data generated by some computer simulations.

In order to bring these benefits to the student we will provide the physics educator with assistance. We will develop a variety of approaches to integrating computation into the student's educational experience. We will develop strategies and tactics to overcome institutional and cultural barriers. We will identify sources of funding. We will consider changes to the traditional curriculum. We will identify or create software and teaching materials. This is only a partial list of our endeavors. By working together we will provide solutions for challenges and create a future in which computer technology plays an essential role in all aspects of physics education.

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2 THE ROLE OF HIGH PERFORMANCE COMPUTING

We are exploring the application of High Performance Computing (HPC) in the classroom and working to increase its role in physics education.

In fact, with the dual-core and quad-core CPUs available in the current crop of personal computers and with 8-, 16-, 32-, and even 64- core machines expected in the next few years, the challenges and opportunities of HPC are rapidly coming to the desktop. And cluster and grid computing make even more computational power available to those who know how to exploit their capabilities. It is even possible to utilize the MIMD and SIMD power of modern CPUs and the GPUs in modern graphics cards to harness the power of parallel architectures that were once only the province of supercomputers.

The same is true of digital storage capabilities. Affordable desktop systems can currently contain more than a terabyte of storage and TeraGrid users have access to petabytes of storage.

In order to apply the rapid increases in computational capabilities to the area of physics education we must broaden our horizons and think beyond the simple systems normally studied in the physics classroom. In this respect, HPC can be considered an enabling technology that allows us to consider a much broader range of systems.

One important area of potential application of HPC is the handling of large datasets. A classical model of the state of one billionth of a mole of a substance (only 12 nanograms of carbon) would require more than a billion petabytes of storage. A brute force calculation of the mutual interactions of the gravitating bodies in a dwarf galaxy would require on the order of 10^{18} calculations per time step. Compare this to the ~10^{14} flop speed of today's fastest supercomputers. Climate models, nanoscale physics, ocean modeling, fluid dynamics, protein folding, and numerous other problems contain interesting physics that can only be revealed by simulations on HPC platforms.

There are also problems that don't require exceptionally large data sets, but do require a great deal of processing power. For example, a straightforward simulation of some biomolecular processes requires more than 10^{10} time steps [1]. A realistic simulation of protein folding is beyond the capabilities of today's fastest supercomputers and even simulations of highly simplified hydrophobic-hydrophilic lattice protein models are NP-complete [2], but protein folding is an interesting real-world process that can be used in the classroom to illustrate important thermodynamic principles.

A host of issues arises when developing code for HPC systems. Multithreading, message passing, fault tolerance, bandwidth between stored data and compute nodes, and more sophisticated algorithms (such as adaptive mesh refinement, iterative linear equation solvers, and Barnes-Hut N-body solvers) are just a few of the issues that confront the HPC user, but are of little or no concern to those who develop code to simulate simple systems. Writing low-level HPC code can be a very difficult task that may only be appropriate for physics students in a research setting or as a special project, but reuse of the code written by others could play a significant role in physics education. Whether using an existing program, writing a program that calls routines from an open-source library, or simply examining the results of simulations performed by researchers, HPC simulations enable students to explore the physics of more complicated and realistic physical systems.

3 PLANS FOR THE FUTURE

We are using a recent study published in Computing in Science and Engineering [3] as our guide to the current state of the computational physics curriculum. In May 2007 we will have a planning meeting that will assess the gaps between the current state and our vision of the future, gauge the effort required to close some of those gaps, begin the development of software and teaching materials, develop a roadmap for future efforts, and result in a White Paper. We will be getting input from physics educators and increasing awareness of our efforts at a satellite meeting that will be held in conjunction with the 2007 AAPT Summer Meeting. We will also present our work at the 2008 Gordon Research Conference on Physics Research and Education. For further information please visit our website at CompPhysEd.shodor.org.

6 CONCLUSIONS

We are working to realize a future in which computational technology plays an essential role in the education of every physics student. As we look to the future we see an increasingly important role for High Performance Computing. We are only beginning to explore HPC's potential to enhance physics education and we are interested in input from the HPC community to help us further our goals.

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