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MRI: Acquisition of a High Performance Cluster for the University of Maine Scientific Grid Portal

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Final Report for Period: 08/2008 - 07/2009 Principal Investigator: Dickens, Phillip M. Organization: University of Maine Submitted By: Dickens, Phillip - Principal Investigator

Submitted on: 12/07/2009 Award ID: 0723093

Title: MRI: Acquisition of a High Performance Cluster for the University of Maine Scientific Grid Portal

Project Participants

Senior Personnel

Name: Dickens, Phillip

Worked for more than 160 Hours: Yes Contribution to Project:

Name: Fastook, James

Worked for more than 160 Hours: No

Contribution to Project:

The supercomputing system has been purchased and will be installed on July 14th. The CoPrincipal Investigators will become significantly more involved in the project once the infrastructure is in place.

Name: Segee, Bruce

Worked for more than 160 Hours: No

Contribution to Project:

The supercomputing system has been purchased and will be installed on July 14th. The CoPrincipal Investigators will become significantly more involved in the project once the infrastructure is in place.

Name: Chawathe, Sudarshan

Worked for more than 160 Hours: No

Contribution to Project:

The supercomputing system has been purchased and will be installed on July 14th. The CoPrincipal Investigators will become significantly more involved in the project once the infrastructure is in place.

Name: Zhu, Yifeng

Worked for more than 160 Hours: No

Contribution to Project:

The supercomputing system has been purchased and will be installed on July 14th. The CoPrincipal Investigators will become significantly more involved in the project once the infrastructure is in place.

Post-doc

Graduate Student

Name: Campbell, James

Worked for more than 160 Hours: Yes

Contribution to Project:

This student is supported by the department as a Teaching Assistant. His Masters project is to parallelize one of the climate models and to develop the infrastructure to support multiple models running concurrently for the University of Maine Scientific Grid Portal (UMSGP). He also was a student in my Grid computing course that designed and prototyped some of the

Undergraduate Student

Name: Henderson, Julius

Worked for more than 160 Hours: Yes

Contribution to Project:

This student was in my Grid computing class that prototyped components of the software infrastructure for the University of Maine Scientific Grid Portal. He is currently working in another NSF-funded project and is supported through an REU supplemental grant for Award No. 0702748.

Name: West, Kara

Worked for more than 160 Hours: Yes

Contribution to Project:

Kara is developing the graphics system that will visualize the data (in real time) resulting from the execution of the climate models. She is currently supported by the University of Maine REU Site program under Grant No. 0754951.

Name: Farouk, Sherief

Worked for more than 160 Hours: Yes

Contribution to Project:

This student was interested in joining the project and is investigating the use of GPUs to execute components of the climate models. He is self-supported.

Name: Deane, Tristan

Worked for more than 160 Hours: Yes

Contribution to Project:

This student is working on the web portal and the communication infrastructure for the University of Maine Scientific Grid Portal for his senior capstone project.

Name: Murphy, Joshua Worked for more than 160 Hours: Yes Contribution to Project:

Joshua developed on the 'green supercomputer' a prototype version of the distributed lock manager for object-based I/O.

Technician, Programmer

Other Participant

Research Experience for Undergraduates

Name: Doan, Sara

Worked for more than 160 Hours: Yes Contribution to Project: Sara worked on the real time visualization component of the Grid Portal.

Years of schooling completed:JuniorHome Institution:Other than Research SiteHome Institution if Other:Allegheny CollegeHome Institution Highest Degree Granted(in fields supported by NSF):Bachelor's DegreeFiscal year(s) REU Participant supported:2009REU Funding:REU supplement

Organizational Partners

Other Collaborators or Contacts

We have collaborated with researchers from the University of Maine Climate Change Institute. Such collaborations have focused on their expertise in the physics of climate change models, and our expertise in the parallelization of such models and the real time remote visualization of simulation output data.

Activities and Findings

Research and Education Activities: (See PDF version submitted by PI at the end of the report)

Findings:

The findings (or products) of this project are the development of the prototype University of Maine Scientific Grid Portal, the development of high-resolution climate change models, providing interactive access to such models, and providing outreach to the state?s K-12 schools.

Training and Development:

This project has provided the first real computer science research experience for all of the students involved. These students are gaining (and have gained) valuable experience in high-performance computing, an area in which they had no prior knowledge. They are developing an understanding of the need for high-performance computing, the technical challenges that come with designing and implementing parallel/distributed software systems, and are learning how to function as a member of a research team. They are also seeing how their individual contributions fit into the larger context, and are feeling the excitement that comes from developing a system that is significantly more powerful than anything they could build on their own. The graduate student is also gaining valuable skills in working with large-scale simulation models and in mentoring undergraduate students.

Outreach Activities:

Outreach to K-12 Schools

We are developing a special interface to the University of Maine Scientific Grid Portal (UMSGP) for the state?s middle and high school students. It will provide, via the Internet using an ordinary Web browser, student access to important climate change models being developed at the University of Maine. One such accessible model is the University of Maine Ice Sheet Model (UMISM), which was developed by Jim Fastook (Department of Computer Science) to study the behavior of the world?s glacial systems in response to climate change. This special interface will, among other things, allow students to interact with UMISM as it executes on a ?green supercomputer?, which is an ultra energy-efficient supercomputer with 648 processors obtained through this MRI award. The supercomputer generates high-resolution animation showing how the glacier evolves over time, and streams the animation over the state?s high-speed optical network (MaineREN) to the student?s laptops. By providing interactive access to the simulation model, students will be able to modify environmental parameters, such as the ambient temperature or level of carbon dioxide in the atmosphere, and receive immediate visual feedback on how such changes impact the ice sheet being studied.

The educational goals of this project are to (1), make students aware of the impact of climate change on the earth?s ecology, (2), to expose students to the process of scientific discovery in an interesting and friendly environment, (3), to spur student interest in

careers in the sciences, and (4), to entice students to stay in the state of Maine for their undergraduate (and hopefully graduate) studies.

Journal Publications

Jianhui Yue, Yifeng Zhu, and Zhao Cai, "An Energy-Oriented Evaluation of Buffer Cache Algorithms Using Parallel I/O Workloads", IEEE Transactions on Parallel and Distributed Systems, p. , vol. 19, (2008). Published,

Yifeng Zhu, Hong Jiang, Jun Wang, and Feng Xian, "HBA: Distributed Metadata Management for Large Cluster-Based Storage Systems", IEEE Transactions on Parallel and Distributed Systems, p., vol. 19, (2008). Published,

Books or Other One-time Publications

Dickens, Phillip M., "Computing Climate Change: Just the Tip of the Iceberg", (2009). Magazine, Published Bibliography: Scientific Computing

Jianhui Yue, Yifeng Zhu and Zhao Cai, "Energy Efficient Buffer Cache Replacement", (2008). Conference not found in database, Published Bibliography: Proceedings of 16th Annual Meeting of the IEEE International Symposium on Modeling, Analysis, and Simulation of Computer and Telecommunication Systems (MASCOTS'08) (short p

Jianhui Yue, Yifeng Zhu, Cai Zhao, "Impacts of Indirect Blocks on Buffer Cache Energy Efficiency", (2008). Conference not found in database, Published Bibliography: Proceedings of the 37th International Conference on Parallel Processing (ICPP 2008)

Web/Internet Site

Other Specific Products

Product Type: Software (or netware)

Product Description:

The University of Maine Scientific Grid Portal is a significant software system that provides worldwide access to important climate change models via the Internet. It supports real-time, remote visualization of simulation output, and interactive access to executing models. These features provide excellent support for both research educational outreach activities.

Sharing Information:

We currently have a prototype implementation of the Grid Portal. It provides access over the Internet to important climate change models, interactive access to such models, and the remote visualization of simulation output. We are currently testing and evaluating the system, and plan to place it in the public domain by May of 2010.

Contributions

Contributions within Discipline:

We have made two primary contributions to the field of computer science. First, our approach to parallelizing important climate change models can serve as a roadmap for other efforts in this area. Second, our work with parallel I/O has significantly increased the performance of ROMIO, which is the most widely used implementation of the MPI-IO standard. Our work in extreme-scale meta-data management represents another important contribution in the area of high-performance I/O.

Contributions to Other Disciplines:

This work benefits the climate change research community in two significant ways. First, applying high-performance computing technologies to otherwise sequential simulation models both increases the resolution of the model and decreases its execution time. This is critically important to climate change researchers because the higher the resolution of the model the higher the level of scientific knowledge that can be gleaned from its execution. Second, the University of Maine Scientific Grid Portal will make important climate change models available to the larger climate change research community.

Contributions to Human Resource Development:

This project has provided significant training in high-performance technologies for six undergraduate students and one graduate student. This includes the mentoring of two female undergrads.

Contributions to Resources for Research and Education:

This proposal has enabled the purchase of a 648-core low-energy supercomputer.

Contributions Beyond Science and Engineering:

This project addresses a critical need for very high-resolution climate models that can provide deeper insight into the phenomenon of global climate change, increase our understanding of the impact of climate change on the world's population, and provide a window into the future of climate change. Development of the University of Maine Scientific Grid Portal further expands research productivity by making the models available to the larger climate change research community via the Internet using an ordinary Web browser. Increasing the number of researchers that can access and utilize this important research infrastructure will further increase the collective knowledge about the impact of global climate change. Presenting the models is such a way that captures the imagination of our K-12 students, and gets them excited about the scientific process, will help attract the next generation of scientists that will address climate change and other critical scientific problems.

Conference Proceedings

Categories for which nothing is reported:

Organizational Partners Any Web/Internet Site Any Conference

Final Project Report for Award 0723093 Dr. Phillip M. Dickens, Principal Investigator

Project Activities

The primary focus of this project has been the development of the University of Maine Scientific Grid Portal (the Grid Portal), which is anchored by a 648-processor "green supercomputer" purchased through this MRI award. The Grid Portal is a multi-faceted project with three key components:

- Working with University of Maine domain scientists to parallelize their simulation models for execution on the "green supercomputer". This enables the development of high-resolution model that, in turn, increases the scientific knowledge that can be gained from their execution.
- Taking these enhanced models and making them available to the larger community over the Internet using an ordinary Web browser. The Grid Portal is designed such that Ph.D. climate change researchers and K-12 students alike can profit from its utilization.
- Providing real time, remote visualization of simulation models.

Our work in this project has attracted funding from the University of Maine FY2010 Strategic Investment Fund. This is a highly prestigious award within the University of Maine System, and, even though the funding level is modest (\$20,000), it is nonetheless quite impressive given the dire funding situation in the state of Maine. The FY2010 award will fund the acquisition of a cluster of four Nvidia Tesla C1060s (for both computation and rendering), and two 4x4 high-resolution display walls (one for the University of Maine campus and one for the University of Southern Maine). The high-resolution display walls provided through the FY2010 award significantly enhance our research in the area of real-time remote visualization, and provide an excellent test-bed for the K-12 outreach activities.

University of Maine Scientific Grid Portal

The University of Maine Scientific Grid Portal is anchored by the 648-processor low-power supercomputer (SiCortex SC-648) purchased through this MRI award. A traditional supercomputer of this size requires vast amounts of electricity to run and to keep the system from overheating. In fact, the electrical load is so high that such systems must be housed in a special facility with three-phase electrical power. In contrast, the supercomputer purchased for the Grid Portal requires only a single 115-volt outlet (with a 30-amp fuse) to power it, and a traditional window air conditioner to cool it. Because of the tremendously reduced power consumption, this system is referred to as a "green supercomputer".

The Grid Portal can be thought of as a gateway to a collection of computing resources, scientific applications and data, tools for research and education, and graphics and animations of important physical processes. It provides a simple, user-friendly interface based on Web Services and Grid technologies, and is accessible via the Internet using a standard Web browser. The Grid Portal will allow researchers from around the world to access some of the important research infrastructure developed at the University of Maine including, for example, the widely used University of Maine Ice Sheet Model (UMISM) discussed above. Other important models and tools, which have been developed by our collaborators at the University's world-renowned Climate Change Institute, will also be made available through the Portal.

Development of the Grid Portal Infrastructure

One of the key activities of this project has been the development of the Grid Portal infrastructure itself. We currently have a highly successful prototype implementation of the system, which consists of four main components: the "green supercomputer" that executes the climate change simulation models, a rendering cluster that takes simulation output data (at the end of each time step) and generates images of simulation state, a Grid Portal Web server, and a client Web browser.

Figure 1 depicts the initialization of a new session on the Grid Portal. The client accesses the Portal through the Grid Portal Web server via the Internet using an ordinary Web browser. Once connected, the user is presented with a list of available climate change simulation models. A simulation controller for the selected model is then initiated on the "green supercomputer" (there is one controller per simulation model). The controller then establishes a connection with the controller of the rendering cluster (note that there is a single controller for the rendering cluster), and both controllers obtain the IP address of the client browser from the Web server. Next, the simulation and rendering controllers each establish connections directly with the client browser. Once these final connections are made, the Grid Portal Web server has no further involvement in that simulation session.

The connections established during the initiation of the session are used as follows. The connection between the simulation controller and the rendering cluster is used to send simulation output data at the end of each time step. Once the rendering cluster generates a high-resolution graphical image representing the current state of the simulation, it uses the connection between it and the client to stream the images directly to the client. The connection between the client and the simulation controller is allows the client to modify parameters to the simulation model as the simulation is executing (i.e., interactive access to the model). This is shown in Figure 2.

Developing this infrastructure involved significant testing and evaluation of various design and implementation options. For example, we investigated the use of the "green supercomputer" for both model execution and the rendering of system state. We decided to utilize an external rendering cluster primarily because of the lack of available PCI Express slots on the supercomputer. We also looked at the issue of performing server-side or client-side rendering of the simulation output data. We finally settled on performing all rendering on the server-side because of the lack of processing power in the laptops that are provided to the K-12 students. We are still investigating issues associated with image compression, which will become increasingly important as we increase the resolution of simulation models.

University of Maine Ice Sheet Model

The University of Maine Ice Sheet Model (UMISM) is a mathematical model that predicts the formation and disappearance of glacial ice sheets. It is an important and widely used model that has been applied to the Antarctic, Greenland, Scandinavian, and Laurentide ice sheets. The model predicts ice thickness, velocity, and temperature of glaciers as functions of position and time.

The resolution of a model such as UMISM determines the amount of scientific knowledge that can be gleaned from its execution. Modeling ice sheets at a resolution of 20 km requires on the order of 80,000 nodes and is taxing the capabilities of current sequential computers. Recently, new data has become available that maps the Antarctic Ice Sheet at a resolution of 5 km. However, modeling ice sheets at a resolution of 5 km requires 1.3 million nodes, and, in the worst case, results in a 16,000-

fold increase in runtime compared to models executing at a resolution of 20 km. Thus significantly increasing the resolution of ice sheet models requires the parallelization of UMISM and its execution on a supercomputing platform.

We performed a large number of benchmarking experiments to determine the most compute intensive modules in the code. UMISM forms partial differential equations (PDE) to describe ice sheet thickness and velocity, which are solved numerically using the finite element method (FEM). Our benchmarking studies showed that solving the resulting systems of simultaneous linear equations represents 80% of the computational costs of the model. We are taking two approaches to reducing the costs of this computation. First, we are integrating PETSc¹, which was developed at Argonne National Laboratory and provides a scalable, parallel solution for applications modeled by partial differential equations, into UMISM. Second, we are developing a parallel matrix solver on Graphics Processing Units (GPUs) to take advantage of the tremendous parallelism such devices provide. We have largely finished the integration of PETSc into UMISM, and have just recently begun our work with GPUs.

Thus far, we have increased the performance of UMISM from one time step every two seconds to nine time steps per second. However, we are at the point where increasing the number of cores beyond 20 does not result in further performance gains, the reasons for which are a focus of current research. Thus while we have not yet reached our goal of 30 - 60 time steps per second, we have made excellent progress, and look forward to even more significant speedups once these issues are resolved.

Real Time Remote Visualization

As noted, important climate change models, such as the widely used University of Maine Ice Sheet Model (UMISM)², generate output data at the end of each time step depicting the current state of the ice-sheet being studied. Currently, such output data is stored while the model is executing, and high-resolution graphical images, representing the state of the ice-sheet at the end of each time step, are generated only after the simulation has completed. This project is focused on creating such images as the simulation is running, one high-resolution image per time step, creating animation showing how the ice-sheet evolves over time in response to climatic changes. This allows researchers to *interact* with the simulation model as it is executing, providing powerful new capabilities such as changing model parameters as the simulation is executing (e.g., ambient temperature), and receiving immediate (visual) feedback on how such changes impact the behavior of the ice-sheet being studied. It also enables powerful new techniques, such as computational steering, where the researcher can guide the simulation to focus in on areas that seem particularly interesting at any given time.

Utilization of the Supercomputer

In addition to the development of the University of Maine Scientific Grid Portal and high-resolution climate change models, the supercomputer has served as an important test bed for our work in high-performance I/O. This includes development of our object-based caching system, energy-aware buffer cache algorithms, and meta-data management.

¹ http://www.mcs.anl.gov/petsc/petsc-as/

² Developed by co-PI Dr. Jim Fastook, Computer Science Department

Presentations

The Computer Science Department and SiCortex (the manufacturer of the "green supercomputer" purchased with this MRI award) jointly presented a "green supercomputing" demonstration on October 14, 2008, showing that ten bicyclists could power a 648-processor supercomputer. The impact of this feat was magnified by the fact that the supercomputer was executing UMISM to model the Greenland Ice Sheet, and was creating real time animation showing how the ice sheet responded to changes in model parameters.

This demonstration sparked international attention. The PI was interviewed by all three local television stations and the Bangor Daily News after the demonstration, and has given fifteen interviews since then that have appeared in various media outlets. This work in this area has been featured on the home page of the National Science Foundation (1/14/09), the cover page of Scientific Computing (July, 2009, subscription base of 95,000), Campus Technology (1/22/09), HPCWire.com (1/15/09), SupercomputingOnline.com (4/8/08), O'Reilly (1/14/09), Government Technology (11/12/08), and SearchDataCenter.com (4/28/09). The "green supercomputing" event was covered by 75 additional news and industry publications.

Figures

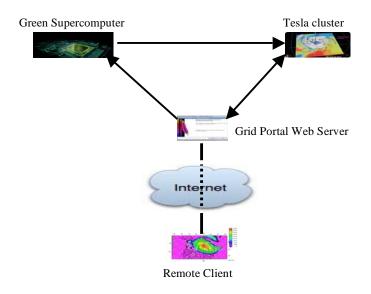


Figure 1. First, the client connects to the Grid Portal over the Internet using an ordinary Web browser. The server then initiates the chosen model on the supercomputer, which subsequently opens a connection to the client browser and the rendering engine. The rendering cluster then contacts the Web server to obtain the IP address of the client.

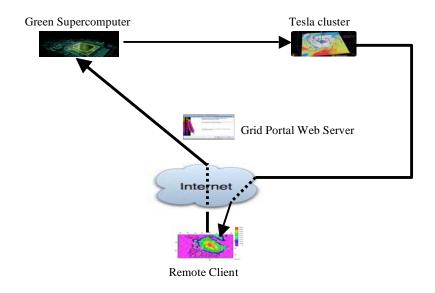


Figure 2. Once the new session is initialized, the client communicates directly with the supercomputer and the rendering engine. Both are one-way communications only, with the client sending commands to the simulation controller and the rendering cluster controller sending images of system state to the client (at the end of each time-step).