Acquisition of a Distributed Computation and Immersive Visualization Environment for Complex Systems -Scientific Applications on Arrays of MultiProcessors (SCAAMP)

Final Report

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This grant supported the acquisition of equipment to support work in several fields, with an emphasis on simultaneously advancing research in applications areas and in making high-end computing and visualization resources more accessible to users. Significant progress was made in each of the targeted application areas, and breakthroughs in software systems and methodologies have been made which greatly enhance the ability of users to access and make effective use of high-performance systems.

I. Summary of accomplishments

This project focused on usability of, and application development in distributed high performance computing environments. To adequately represent the range of computational problems facing science today, challenge problems in astronomy, chemistry, computer science, mathematics, physics, and visualization were selected for participation in the SCAAMP (Scientific Applications on Arrays of MultiProcessors) distributed computing testbed. Important developments from this award are listed below and selected publications are included in Section IV.

Computer Science

The critical question addressed by the computer science research under this grant was how to make high-end computing and visualization resources efficiently accessible to users. We expressed this as achieving scalability in a different sense: achieving high performance and geographically distributed computing with a linear scaling of the application user's effort as well as parallel speedups.

The methods we proposed introducing relied on problem-solving environments (PSEs). A PSE provides a set of tools for users to carry out research in their area, while hiding complexity of the underlying computer software and hardware architecture. When PSEs are introduced to a computational research area such as numerical linear algebra (Matlab), mathematical derivations (Maple), or fluid dynamics (FIDAP) they greatly increase productivity and free the researcher from becoming a computer science expert. The shortcoming of PSEs is that they are specialized for a single application area and require major programming effort. Our approach was to create instead a set of reusable software tools for common PSE features: graphical user interfaces, inter-program communications, visualization, etc. This toolkit (called PSEware) allows applications users to rapidly build their own PSEs, rather than requiring the combined efforts of teams of computer scientists, numerical analysts, and others.

This research led to the creation of "component architectures" for scientific computing. This model presents a user with a set of reusable software components which can be quickly connected together (typically with a visual programming interface) to create complete solutions. Components differ from standard software pieces such as subroutines, libraries, or objects. Component composition involves modifying and linking binaries, rather than source code which must then be re-compiled. Components interact on a peer-to-peer basis; no component is designated as a "main" program which controls the others. Component systems are a natural environment for multi-language and heterogeneous computing systems, unlike object-oriented systems built using C++ We built a prototype component architecture toolkit called the LSA which encapsulates software from many sources for manipulating, analyzing, and solving large sparse linear systems of equations. Those components can be arbitrarily distributed across the Internet, and at the NCSA Alliance 98 meeting it was demonstrated seamlessly connecting components in California, Illinois, Indiana, and Minnesota. Currently we are building a presentation for the SC98 High Performance Computing Challenge, which will tie together internationally distributed software and hardware components to carry out the largest simulation ever attempted for industrial mold-filling applications.

Astronomy

Rotating gaseous disks similar to the one which presumably formed our own Solar System are now known to be common around young stars. The SCAAMP protostellar disk project is devoted to studying the spiral instabilities which occur in these disks due to disk self-gravity. Such instabilities can radically alter the structure of the disks, possibly even producing planets or other companion objects. The interest in this mechanism has been heightened by the discovery, over recent years, that gas giant planets are often found orbiting close to their parent stars. The approach of the IU group is to perform 3D hydrodynamic simulations which determine the nature and consequences of gravitational instabilities in numerical models of circumstellar disks. These star/disk simulations are unique in that they are fully three dimensional and include the star and the star/disk boundary. The SCAAMP machine makes it possible to use grids of up to half a million cells in order to resolve the physics of both the star and the disk accurately. The most important result since the arrival of the SCAAMP machine at IU has been a comparison among unstable disks evolved under different assumptions concerning disk energetics. The effect is extreme, ranging from complete fragmentation of the disk for high effective cooling rates to heating and modest puffing of the disk but no fragmentation for modest cooling. Some of the results are in press; others are still being analyzed. Future plans include increasingly realistic treatments of heating and cooling. The nonlinear hydrodynamic calculations are supplemented by linear analyses to verify the nature of the unstable modes detected. Additional work in progress includes an investigation of the circumterrestrial gas and debris belt which may have been ejected into orbit around the proto-Earth by a giant impact. It is possible that gravitational instabilities in the belt played an important role in facilitating the origin of the Moon.

Physics

The work of S. M. Girvin's group has focussed on numerical studies of strongly correlated quantum and classical systems, including superconductors and two-dimensional electron gases in the quantum Hall regime. The primary techniques used are classical and quantum Monte Carlo. We have developed a particular implementation of the stochastic series expansion quantum Monte Carlo method which has proved very useful in the study of quantum ferromagnets. In addition we performed a study of the importance of winding number equilibration in quantum Monte Carlo simulations. For large system sizes it is very difficult to equilibrate different winding number sectors, but we were able to prove that the correct answer can be obtained without doing this.

Kharen Tevosyan completed a Ph.D. research project motivated by recent experimental and theoretical studies of the quantum Hall effect in quasi-one-dimensional organic metals of the TMTSF2X family. The quantum Hall effect occurs in two-dimensional metals in the presence of strong perpendicular magnetic fields and is a consequence of the peculiar quantum mechanics of charged particles in this circumstance. The metals studied are called quasi-one-dimensional because their electrons move freely along chains present in these structures, but do not move easily from chain to chain. It was known experimentally that these materials show the quantum Hall effect only when they have a spin-density-wave type of magnetic order, and that this order only occurs when the materials are placed in an external magnetic field. The object of this research was to contribute to the improve understanding of quantum Hall behavor in these materials by numerically exploring the properties of several different models for these materials. Using the SCAAMP 02000 he was able to explore a wider variety of models than in earlier work and make solid conclusions on the importance for physical properties of different types of disorder which can be present in these materials and on the importance of the details of electronic inter-chain tunneling properties. His work succeeded in shedding light particularly on the influence of disorder on the quantum Hall effect in these materials which is quite different from its influence in conventional quantum Hall systems.

Steve Gottlieb conducted seven dynamical quark runs on the 64 processor Origin2000 at three different couplings. The calculations were done to study the spectrum of light hadrons and (when combined with results done elsewhere, e.g., PSC, ORNL, IU Paragon) show an extremely interesting difference from calculations done within the quenched approximation. For dynamical quarks we find that the nucleon to rho mass ratio is higher than within the quenched approximation.

Chemistry

Considerable progress was made in several areas of computational chemistry, including density functional code extensions to the MELD electronic structure computation program, and work with Gaussian, Inc. to get Gaussian94 running on the Origin2000. A number of novel electronic structure calculations (listed in the publication section below) were carried out.

Mathematics

Jolly and Simmonet developed an application for the integration of a set of six nonlinear coupled partial differential equations describing the dynamic of the mid-latitude oceanic circulation, in order to compare the low-frequency variability of this model with the variability of the North Atlantic basin. They used an explicit temporal scheme in order to achieve integration in time of the system. In almost every experiment they integrated over a very long time (between 100 and 150 years of time integration) and the results were compared according to the shape of the basin, the grid resolution and some physical parameters. The calculations used up to 32 processors and ran for several hours for each experiment.

Visualization and computer graphics

Shakespeare is concerned with photoaccurate lighting models for large structures and has developed a set of parallel rendering codes based on Radiance by R. Ward. Radiance has been extended to include media effects, calibrated lighting instruments, psychologically correct low-light rendering and many other physically based techniques. Because of the large size of the models and the large number of lighting instruments, the Origin2000's parallel shared memory architecture was well suited to the computations.

In support of the computational science described above, several CAVE VR applications were developed. These include codes for the visualization of hadron spectra, X-ray crystallographic data and structures, n-body astrophysics computations, approximate rendering techniques for photoaccurate lighting models, and support for real-time visualization and computational steering via a CAVE rendering module for NAG Explorer.

II. Equipment purchased

The acquisition process was considerably more difficult and lengthy than we originally planned, because the during the time between the writing of the grant proposal and the actual purchase, several new high-performance architectures (the SGI Origin 2000, the newer HP Exemplars, and Sun's Ultrafire servers) were announced. In addition, the Office of the Vice-President for Information Technology at Indiana University provided significant funds over the promised match, allowing us to upgrade the visualization equipment from two ImmersaDesks to a CAVE and an Immersadesk, as well as two FTE's to support the 3D immersive visualization equipment and two FTEs for programming support and system administration for this project.

A set of benchmarks consisting of application codes and architecture-probing codes from Indiana University (IU) were used and specified in the RFP. The equipment finally acquired includes:

- An SGI Origin 2000 with 64 processors, 15 Gbyte of memory, and 43 Gbyte of disk space. This is the primary computational server.
- An SGI Origin 2000 with 4 processors and 500 Mbyte of memory. This machine is used for compilation, development work, and as a hardware test stand for the larger machine. Supporting software, including the SGI Varsity Pack, Parallel development tools, NQE batch submission, AVS and NAG Explorer
- A StorageTek 9710 tape robot for archival storage
- A 8x8 CAVE 3D immersive visualization environment from Pyramid Systems, Inc..
- A four processor SGI Onyx2 with 1GB memory, 18GB disk, and ATM NIC
- A Pyramid Systems ImmersaDesk
- A two processor SGI Onyx2 with 500MB memory, 9GB disk, and ATM NIC
- Two Cisco LS1010 ATM switches

III. Students Supported Under this Award

Three M.S. students and three Ph.D.s were graduated under this award. Currently nine Ph.D. students, two M.S. students, one post-doc and one undergraduate are supported by this award.

IV. Selected Publications Resulting from Award

E. Houstis, E. Gallopoulos, R.Bramley and J. Rice, "Problem-Solving Environments for Computational Science", IEEE Computational Science And Engineering, v.4, #3, 1997, pp. 18-21.

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P. Henelius and S. M. Girvin, "A Numerical study of the random dimerized XX spin-1/2 chain", Phys. Rev. B57, 11457 (1998).

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C. Timm, S. M. Girvin, and H. Fertig, "Skyrmion lattice melting in the quantum Hall system", Phys. Rev. B, (in press, October 15, 1998).

C. Bernard, T. Blum, T.A. DeGrand, C. DeTar, S. Gottlieb, U.M. Heller, J. Hetrick, C. McNeile, K. Rummukainen, R.L. Sugar, D. Toussaint, and M. Wingate, "Update on the hadron spectrum with two flavors of staggered quarks", to be published in Nucl. Phys. B, (Proc. Suppl.).

C. Bernard, C. DeTar, S. Gottlieb, Urs M. Heller, J. E. Hetrick, C. McNeile, K. Rummukainen, R. Sugar, and D. Toussaint, "Light Hadron Spectrum with Kogut-Susskind Quarks", presented at Lattice '98, Boulder, Colorado July 14-18, 1998, to appear in the proceedings.

A.J. Hanson and E. Wernert, "Constrained 3D Navigation with 2D Controllers," in Proceedings of IEEE Visualization '97, Phoenix, AZ, Oct 22-24, 1997. pp. 175-182 (IEEE Computer Society Press, Los Alamitos, CA, 1997).

R. Shakespeare, SIGGRAPH'98 Course 33: Rendering with Radiance: A Practical Tool for Global Illumination.- Instructor. Orlando, July 1998

R. Shakespeare, Digillusions: International Seminar on Digital and Virtual TV and Film Design. "Digital visualization: its impact on the theatre design process and art., Presenter. Helsinki, Finland. September 25, 1998.

R. Shakespeare, United States Institute for Theatre Technology 1998 National Conference, "Computer Visualization: Lighting Design in Virtual Reality?", Long Beach, California. March 1998

R. Shakespeare, USITT 1997 National Conference, "Computer Visualization and Lighting Complex Environments", Pittsburgh, Penn. March 1997.

R. Shakespeare, 6th Biennial Foundations in Art: Theory and Education National Conf., "Light and Color in Three and Four Dimensions", Richmond, Virginia. March 1997.

M. Papakhian, "Comparing Job-Management Systems: The User's Perspective", April-June 1998, IEEE's Computational Science and Engineering