

2005/2006 REPORT



INNOVATIVE COMPUTING
LABORATORY

THE UNIVERSITY of TENNESSEE
Computer Science Department

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OVERVIEW

The Innovative Computing Laboratory's mission is a simple one, but one that requires both creativity and expertise. We aspire to be a world leader in enabling technologies and software for scientific computing. Our vision is to provide high performance tools to tackle science's most challenging problems and to play a major role in the development of standards for scientific computing in general.

Background

Sixteen years ago in 1989, ICL was started by Dr. Jack Dongarra when he was lured away from Chicago's Argonne National Laboratory. Dr. Dongarra was given a dual appointment as Distinguished Professor in the Computer Science Department at the University of Tennessee and as Distinguished Scientist at Oak Ridge National Laboratory (ORNL). This dual position was established by the UT/ORNL Science Alliance, Tennessee's oldest and largest Center of Excellence, as a means for attracting top research scientists from around the country and the world to visit the university and collaborate. Dr. Dongarra's arrival at UT signaled the beginning of a new era in enabling technology research as he built a strong foundation for collaboration and growth. As a result, many post-doctoral researchers and professors from multi-disciplines such as mathematics, geology, chemistry, etc. found their way to UT. Many of these scientists remained as post-doctoral researchers and worked with Dr. Dongarra, which helped him attract other researchers and top graduate students. Below is a list of some of the researchers who have helped Dr. Dongarra along the way and made ICL the respected organization it has become.

Zhaojun Bai

The University of California, Davis

Richard Barrett

Oak Ridge National Laboratory

Adam Beguelin

Turveo

Susan Blackford

Myricom

Henri Casanova

University of Hawaii

Jaeyoung Choi

Soongsil University, Korea

Andy Cleary

Lawrence Livermore National Laboratory

Frederic Desprez

ENS-Lyon

Edgar Gabriel

University of Houston

Robert van de Geijn

The University of Texas, Austin

Antoine Petit

Sun Microsystems France

Roldan Pozo

NIST

Erich Strohmaier

Lawrence Berkeley National Laboratory

Françoise Tisseur

Manchester University, England

Bernard Tourancheau

University of Lyon, France

Sathish Vadhiyar

Indian Institute of Science (IISc), India

Clint Whaley

University of Texas, San Antonio

Victor Eijkhout

University of Texas, Austin

During our early growth, many new exciting collaborations were created with other institutions including Rice University. Through interactions with colleagues at Rice, ICL became an integral part of the Center for Research on Parallel Computation (CRPC), a National Science Foundation (NSF) Science and Technology Center established in 1989 and lead by Rice University. CRPC worked to make parallel computation accessible to industry, government, and academia and to educate a new generation of technical professionals. During the 1990s, our collaborations increased and we have worked on a number of efforts that have since become part of the basic fabric of scientific computing around the world. The basic technologies that our research has produced include ATLAS, BLAS, FT-MPI, HARNESS, LAPACK, MPI, LAPACK, Netlib, NetSolve, PAPI, PVM, RIB, ScaLAPACK, and Top500 just to name a few. These

successes are continuing along with current ICL efforts such as Active Netlib, FT Linear Algebra, HPC Challenge benchmark suite, LFC, KOJAK, NetBuild, NetSolve/GridSolve, OPEN-MPI, PAPI, SANS-Effort including SALSA, and vGrADS. Many of these efforts have been recognized nationally and internationally, including four R&D 100 awards; PVM in 1994, ATLAS and NetSolve in 1999, and then PAPI in 2001.



Profile

Located at the heart of the University of Tennessee campus in Knoxville, ICL continues to lead the way as one of the most respected academic, enabling technology research laboratories in the world. Our many contributions to technological discovery in the HPC community, as well as at UT, underscore our commitment to remain at the forefront of enabling technology research.

Recognition for our efforts and the impact our efforts have had, and continue to have, on the goals of the University of Tennessee are reflected by the Chancellor of the Knoxville campus, Dr. Loren Crabtree: "Dr. Jack Dongarra and the researchers of his Innovative Computing Laboratory have been worldwide leaders in research in the high performance computing community for more than a decade. Thanks to the dedicated efforts of this outstanding group of faculty, staff and students, ICL has greatly enhanced the stature of the University of Tennessee, helping to make it one of the finest public academic research institutions in the United States, as recognized recently by *US News & World Report* and other sources. As the University continues to build new alliances and collaborations between national and international research communities, especially in conjunction with its strategic partnership with Oak Ridge National Laboratory, we will rely heavily on the expertise of ICL to help strengthen these relationships and address the challenging research complexities that the future undoubtedly holds for us. On behalf of the University, I commend Dr. Dongarra and his stellar group for their tremendous achievements over the years and for their role in elevating the standards for success in academic research here at UT."



From the Director

We are building from a firm foundation. Over the past 16 years, we have developed robust research programs, attracted some of the best and brightest students and researchers, and created leading-edge research programs. The ICL staff's ongoing ability to apply the latest technologies to provide advanced services and solutions for the scientific computing community underscores the ICL's leadership role.

The life of Computational Science revolves around a multifaceted software ecosystem. But today there is (and should be) a real concern that this ecosystem of Computational Science, with all its complexities, is not ready for the major challenges that will soon confront the field. Domain scientists now want to create much larger, multi-dimensional applications in which a variety of previously independent models are coupled together, or even fully integrated. They hope to be able to run these applications on Petascale systems with tens of thousands of processors, to extract all performance that these platforms can deliver, to recover automatically from the processor failures that regularly occur at this scale, and to do all this without sacrificing good programmability. This vision of what Computational Science wants to become contains numerous unsolved and exciting problems for the software research community. Unfortunately, it also highlights aspects of the current software environment that are either immature, under funded or both.

Advancing to the next stage of growth for computational simulation and modeling will require us to solve basic research problems in Computer Science and Applied Mathematics at the same time as we create and promulgate a new paradigm for the development of scientific software. To make progress on both fronts simultaneously will require a level of sustained, interdisciplinary collaboration among the core research communities that, in the past, has only been achieved by forming and supporting research centers dedicated to such a common purpose. I believe that the time has come for the leaders of the Computational Science movement to focus their energies on creating such software research centers to carry out this indispensable part of the mission. I have every confidence that our community stands ready to step up again to this momentous new effort.

Our plans for the future are founded on our accomplishments as well as our vision. That vision challenges us to be a world leader in enabling technologies and software for scientific computing. We are helping to maintain the balanced software ecosystem. We have been and will continue to be providers of high performance tools to tackle science's most challenging problems and to play a major role in the development of standards for scientific computing in general. As the pace of change accelerates in the coming years, we expect our innovative, pioneering research efforts to match that pace.

During these exciting times, I am grateful to our sponsors for their continued endorsement of our efforts as we continue to evolve and strengthen our organization. My special thanks and congratulations go to the ICL staff and students for their skill, dedication, and tireless efforts in making the ICL one of the best centers for enabling technology in the world.

Jack Dongarra
Director, ICL

ICL RESEARCH

Computational challenges in the 21st century are placing steep demands on the development of adaptable computing applications and tools for the scientific community. We have been successful at embracing these challenges and appropriately adapting our research over the years.

In addition, such challenges and demands have presented our group with incredible opportunities to continue participation in the national research agenda. These demands have not only allowed ICL to grow but have also allowed us to demonstrate the range and diversity of the research performed by our staff and students. Our large and wide-ranging portfolio of research efforts has evolved consistently since 1989 and in 2005-2006, we will support or participate in more than 17 significant projects.

Numerical linear algebra, specifically the numerical libraries that encode its use in software, has been the foundation of our work since the beginning. But because of the unique demands for enabling technology in the computational science community over the past decade, we expanded our research to include work in high performance and distributed computing. Our efforts in these areas fostered the need for expertise in performance analysis and benchmarking for high-end computers. The enormous investments by both government and private industry in high performance computing have made our ability to do research in this area correspondingly important. Finally, as a by-product of a long tradition of delivering high quality software produced from our research, we have helped to lead the movement to build robust, comprehensive, and well-organized asset management tools.

As the world learns to harness enormous computing power to efficiently perform such tasks as graphical simulations and analysis of massive data sets, ICL faces increasing pressure to stretch the boundaries of discovery. Incredible growth and change in parallel computing technology and the demands placed on such technology by government and private business consistently challenge us to apply expert-level understanding to each of our research endeavors.

On the following pages, we provide brief summaries of the research in each of our four main areas of focus - numerical libraries, high performance distributed computing, performance analysis and benchmarking, and asset management.

Acknowledgement Our success over the years has been due to many factors, not the least of which are those organizations that provide physical and financial resources. Without the support of the many agencies and organizations that have funded, and continue to fund, our efforts we simply would not be able to conduct leading edge research. The main source of support has been federal agencies that are charged with investing the nation's computational research funding: the National Science Foundation (NSF), Department of Energy (DOE), Department of Defense (DoD), the Defense Advanced Research Projects Agency (DARPA), the Office of Naval Research (ONR), and the National Institute of Health (NIH). However, strong support from private industry has also played a significant role. Some organizations have targeted specific ICL projects. But others have made contributions to our work that are more general and open-ended. We gratefully acknowledge the following for their generosity and their significance to our success:



ICL has long been a leader in producing standards, algorithms, and software for numerical linear algebra – a quintessential ingredient of computational science.

Sparse linear systems and eigenvalue calculations come from, among others, applications that involve partial differential equations, and dense operations arise from boundary element methods, quantum scattering, etc. Answering this demand, we have teamed up in the past with other researchers and industry to lead efforts like the BLAS Technical Forum and various linear algebra packages: LINPACK, LAPACK, ScaLAPACK – all of which standardized programming interfaces and made performance portable across the plethora of modern hardware.

Our contributions to this community have drawn heavily on our expertise in high performance numerical linear algebra. Most of our on-going projects relate in one way or another to the concept of **Self Adapting Numerical Software (SANS)**. The **ATLAS** project may be considered the bridge between the old style kernel computation optimization and SANS-style poly-algorithm approach. The latter is applied extensively in ICL's current projects such as Accels, LFC, and SALSAs.

Members of the ICL team continue to address the issue of fault-tolerance in linear algebra codes – a growing concern for systems with ever increasing numbers of processors and hardware heterogeneity. A combination of both new theoretical results as well as middleware solutions is being developed to address this problem.

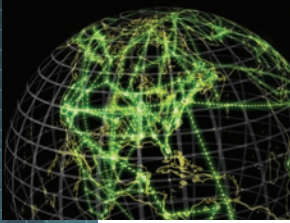
Considerable progress has been made in the development of the **SALSAs** system for heuristic decision making in the context of linear and nonlinear system solving. The software functions as an increasingly powerful testbed for iterative linear system solvers, using the available methods from the PETSc library, and attached packages such as Hypre. For internal use in the system, as well as for external use in matrix libraries or generally for communication between numerical software components, we have extended our metadata standard for matrix data that formalizes the matrix characteristics we analyze. We have released a library that defines this standard through an API and an XML file format. A collection of analysis modules for generating characteristics of user input data was released in 2005. We also are continuing research on identifying statistical techniques and tools for building heuristics.

As Supercomputer systems grow larger the possibilities of system and software failures increase, thus we are investing considerable effort into designing and implementing new custom fault tolerant numerical kernels through the **FT-LA** project. We believe successful approaches to fault tolerance in next generation high end computing environments, where thousands of processors will be the norm, must leverage intimate knowledge of the application and its underlying numeric algorithms in order to achieve the efficiencies necessary in terms of adequate failure recovery times and system resource usage such as for additional disk and memory storage that is normally required. But the demands of this approach can be steep when compared to simpler, slower, resource hungry methods such as system wide coordinated disk based checkpointing. We have therefore recently begun to focus on algorithm based disk-free fault tolerance that uses various in-memory encodings to allow for scalable recovery of parallel codes.

The **LFC** project draws on the conceptual underpinnings of the SANS software by choosing the best algorithm in a given context and tuning based on input data characteristics. The publicly available code includes all of ScaLAPACK's decompositional linear solvers. The in-development code adds computational server capabilities that add data persistence and all of ScaLAPACK's solvers including singular value and eigenvalue. LFC's ease of deployment has been proven time and time again while delivering the best possible performance levels across multiple architectures.

Recently, we have begun a major overhaul of the **LAPACK** and **ScaLAPACK** software collection. With renewed funding, new development is supplanting prior work done only by volunteers, which had fallen behind the theoretical and algorithmic advances that have been published or implemented elsewhere. Software and hardware landscapes continue to evolve requiring different techniques to make a successful programming library.

For the nano-physics community, we are studying certain eigenvalue problems where interior eigenvalues are needed, which are degenerate and close to a gap in the spectrum with known location (the gap separates energy levels of interest). This problem poses a considerable challenge to traditional methods, and we are investigating different solution approaches.



ICL RESEARCH

Distributed Computing

ICL's commitment to distributed computing spans more than a decade and has included involvement in a wide range of successful projects such as the Parallel Virtual Machine (PVM) and the Message Passing Interface (MPI) standard. Distributed computing provides a fundamental platform for building efficient modern high performance applications. Currently, we are involved in multiple levels of distributed computing from high-level problem solving environments such as GridSolve/NetSolve and VGrADS, through middleware technologies such as GridRPC and various MPI implementations such as FT-MPI (Fault Tolerant MPI) and the open source community Open MPI project as well as advanced Grid computing research through the **Scalable Intracampus Research Grid (SInRG)**. SInRG is described in more detail in the Hardware section (p. 21).

GridSolve is an RPC style Grid middleware that allows the domain scientist to combine the power of distributed hardware and software and utilize them from within familiar general purpose Scientific Computing Environments (SCEs) such as Matlab and Mathematica. The latest release of the GridSolve system is based on the emerging GridRPC standard API and will be included in a future NSF Middleware Initiative (NMI) release. GridSolve has evolved from the NetSolve system but includes many enhancements. Communications in GridSolve have been improved over NetSolve by transparently handling NATs (network address translators) using 'receiver makes right' protocols and allowing background data transfers for nonblocking operations. Additional improvements in the system software include faster matrix transpose routines for C to Fortran calling (and vice versa) and support for very long running jobs via the option to disconnect from servers and access results later, even from a different client machine. To simplify writing client code we provide a new code generator that automatically generates client examples in C showing the GridRPC calling sequence. Services are compiled to statically-linked executables, so there are no issues with library paths or various flags for different linkers. The services are not linked in with the server binary itself, so to add a new service simply requires building the new service and placing it in the proper directory which are then detected dynamically, eliminating the need to restart the server to enable the new problem.

We will soon begin extending GridSolve to reduce client complexity for the execution of parallel jobs. This will involve sophisticated scheduling, data management, and heuristics for selecting the appropriate number of processors. We will also develop a workflow system to allow for scheduling of entire task graphs onto available GridSolve resources. Meanwhile, development is underway to add a flexible authentication layer based on the Simple Authentication and Security Layer (SASL).

The complexity, unreliability, and overhead of low-level operations in today's systems obscure the Grid's potential. The **Virtual Grid Application Development Software (VGrADS)** project lead by Rice University, to which we contribute, attacks a fundamental part of this problem - how to more effectively program and use these highly complex and dynamic systems. The VGrADS Execution System (vgES) has been developed to provide fast, scalable resource selection and application management, and an experimental fork of GridSolve has been modified to use vgES as its execution system. Experimental proof-of-concept work has demonstrated a Matlab GridSolve client that can transparently launch a fault tolerant, parallel linear algebra application (based on FT-MPI) running as a GridSolve service on a dynamically selected set of Grid resources (managed by vgES). Other institutions involved in the VGrADS project are also conducting research on topics as varied as application monitoring, workflow applications, generalized fault tolerance frameworks, and resource characterization.

Message Passing has become the dominant programming paradigm for distributed memory high performance applications. ICL's expertise in this area has led to the development of a leading edge MPI 1.2 implementation; **FT-MPI**. This MPI implementation allows for flexible new models of fault tolerance and recovery that were previously impossible. Since the release of the FT-MPI runtime library at SuperComputing 2003, system level software and environment management have both been enhanced and improved to allow for higher performance, robustness and scalability. The FT-MPI runtime has undergone a number of major performance improvements recently. The buffer management system has been altered so that it is now driven by the capabilities of the underlying communications driver allowing for better overlap of data conversion and communication. Current research in FT-MPI is mainly centered on improving the robustness, speed and scalability of the fault recovery algorithms and further extending the optimization of collective communications. This research covers diverse topics from as self-healing network topologies to the fundamental understanding and modeling of group communications.

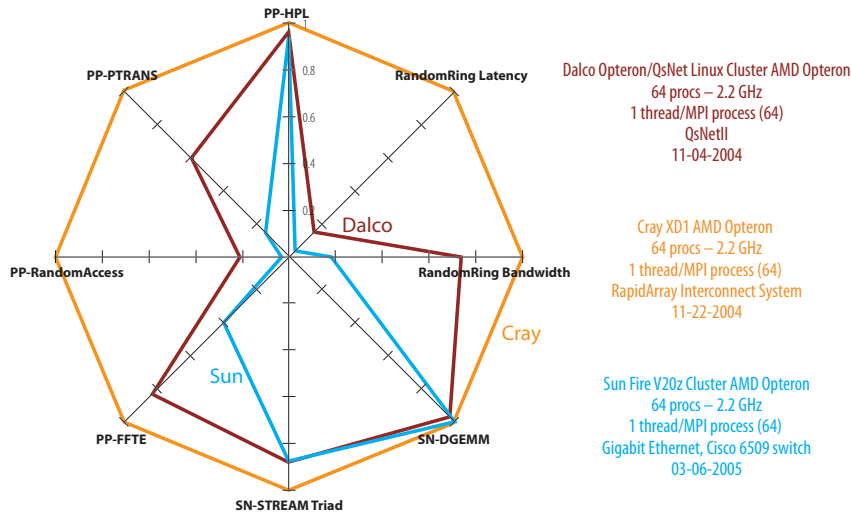
Many features of FT-MPI such as runtime design, point-to-point RDMA messaging, buffer management and tuned collective communication algorithms are currently being applied to a new open source MPI implementation known as **Open MPI**. This is a collaborative project between LANL, Indiana University, ICL, and HLRS Stuttgart, Germany. In a later stage of integration, the fault tolerant mechanisms of FT-MPI will also be added to Open MPI as a runtime user selectable module.

ICL continues to play a leadership role in benchmarking and performance analysis efforts that measure and report performance on high performance computing (HPC) machines.

The **LINPACK benchmark** is a numerically intensive test for solving a dense system of linear equations and has been used for years to measure the floating-point performance of computers. Performance on this benchmark is the basis of the semi-annual **TOP500** list that ranks the fastest 500 computers in the world. Our research staff has also led the development of a portable high-performance implementation of the LINPACK benchmark for distributed memory parallel computers, called **High Performance LINPACK**, or **HPL**. HPL contains many possible variants for the various operations, in order to provide the user with the opportunity of experimentally determining an optimal set of parameters for a given machine configuration. To examine the performance of HPC architectures using kernels with more challenging memory access patterns than HPL, the **HPC Challenge (HPCC)** project has developed a suite of benchmarks that bound the performance of many real applications as a function of memory access characteristics. HPCC provides a single program to download and run with a simple input file, similar to HPL. However, in addition to HPL, HPCC currently includes several other benchmarks for measuring sustainable memory bandwidth, the rate of random memory updates, and the latency and bandwidth of a number of communication patterns.

In addition to developing benchmarks, our research staff is actively involved in the development of performance evaluation tools and methodologies. As a basis for the collection of accurate and relevant performance data, we have developed a portable library interface for access to hardware performance counters on most modern microprocessors. The interface, called the **Performance API**, or **PAPI**, not only provides a standard set of routines for accessing counter data, but also defines a common set of performance metrics considered relevant and useful for application performance tuning. PAPI provides two interfaces to the underlying counter hardware; a simple, high level interface for the acquisition of simple measurements and a fully programmable, low level interface directed towards application and tool developers with more sophisticated needs. **KOJAK**, a joint project with the Central Institute for Applied Mathematics at the Research Centre Jülich, is an automatic end-user performance tool aimed at providing high-level feedback on the performance behavior of HPC applications written in OpenMP and/or MPI. Mechanisms are provided to automatically collect event traces at runtime and supplement the trace data with hardware counter values using PAPI. The analysis component uses pattern recognition to convert the traces into information about performance bottlenecks relevant to developers.

An extensive web interface to the HPC Challenge results database has been created where results have been submitted for as many as 60 systems. Results can be exported to an Excel database or to an XML



Sample kiviati diagram of HPC Challenge results for three platforms based on the same AMD Oteron processor.

file. Kiviat diagrams can be easily generated at the website to allow comparative analysis of multi-dimensional results. A sample kiviati diagram is shown in the figure above.

Recent work on PAPI has extended the API to provide access to network counters and temperature sensors. In order to allow access to both on-processor and off-processor counters and sensors simultaneously, multiple platform-dependent substrates may now be used together during the same application execution. For example, this capability has allowed us to collect both hardware counter data and temperature data during a single program run and look for correlations between these two types of data. Because power consumption and fault tolerance are increasingly becoming issues for large-scale machines, system and application-level performance analysis tools will need temperature and power consumption data from the hardware in order to tune the system and map the application in a balanced manner. PAPI has also been ported to new platforms such as Cray XT3 and IBM BG/L.

A recent extension to map performance data onto process topologies (virtual and physical) has raised the semantic quality of the feedback returned and significantly increased KOJAK's suitability for large-scale applications. Also, KOJAK's new ability to organize hardware counters in custom hierarchies provides the user with a truly holistic picture of the hardware-software interface. To support platforms with efficient remote-memory access hardware, KOJAK now also measures and analyzes one-sided communications based on either MPI-2 or SHMEM. Finally, a new filter utility accounts for and removes perturbation errors from trace files. A new version of KOJAK incorporating these and other new features has recently been released for a number of HPC platforms including Cray X1 and XD1 and IBM BlueGene/L. To meet the scalability requirements imposed by the tremendous increase in the number of processing elements that will characterize future generations of HPC platforms, we are developing entirely new concepts that will radically change the way trace data are collected, analyzed, and visualized.



ICL RESEARCH

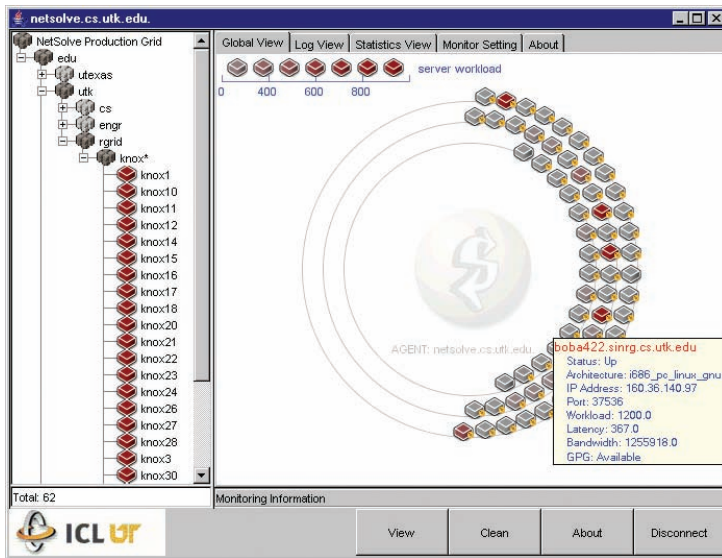
Asset Management

The creation and development in the 1980s of the Netlib repository for mathematical software and other related resources represents the cornerstone of ICL's repository and asset management efforts. Netlib's enormous past success and benefits to HPC have been well established. As a result of such success and the ever increasing demands for software reuse generated by the proliferation of scientific computing and simulation in the US, the National High-performance Software Exchange (NHSE) was formed in the mid 1990s by several academic institutions and government agencies with the primary goal of establishing discipline-oriented software repositories that could be contributed to and maintained by experts in their respective fields. ICL was one of the academic partners called upon to participate in this national effort.

One result of the NHSE effort was the development of the **Repository in a Box (RIB)** toolkit, which was developed to enable the creation and interoperability of discipline-oriented, web-based software repositories, specifically for the tools and applications generated by the HPC community. RIB development and enhancement continues here at ICL and has evolved to support the creation of repositories to store and share any type of digital object. The progression of our repository efforts also continues with our work on **NetBuild**, which is a project to make it easier for authors and installers of application software to utilize standard computational software libraries. NetBuild intercepts calls to compilers and/or linkers, identifies which libraries are needed for an application, locates those libraries, downloads them, installs them, and links them into the executable. NetBuild thus eliminates the need for those libraries to be installed manually. NetBuild can also choose the "best" among several candidate libraries for a particular platform – for instance, using a BLAS that is optimized for the user's CPU instruction set extensions and cache sizes.

RIB has been completely rewritten in Java to become more streamlined and flexible. By removing the built-in web server and database along with the scripts to manage both, the new incarnation of RIB decreases install time and leverages an object-oriented data model while still providing flexibility for catalog building and robust metadata interoperation. Many new features have also been added, such as the ability to navigate through all object components in a tree-like structure from the catalog view and new intuitive interfaces to database operations that allow selective retrieving and displaying of information from multiple classes in an easy-to-read table format. New utilities have also been developed for interfacing RIB with the performance data management framework in the TAU project so that metadata from RIB about applications can be linked with performance studies of those applications.

There are ongoing discussions among the **Netlib** developers/administrators to overhaul the entire repository resource, from aesthetic and interface improvements to redefining the scope and type of



Screenshot of the ReST Monitor displaying software activity in a cluster environment.

the collection. While still very useful, the Netlib collection and the interface to it have remained largely unchanged over the past several years. One approach that has received considerable attention is to re-engage the mathematical community to create a more robust, dynamic repository with the ultimate goal of increasing contributions to the collection.

A new NetBuild client has been released with the ability to handle many more libraries, including the netBSD package collection. NetBuild can now support packages that use threads and multiple CPUs. Metadata support for representing compiler dependencies and data-format dependencies has also been added. Other recent changes include pre-loading support, include file support and cross-compiling support. NetBuild is currently being extended to support additional platforms, “include” files needed during source compilation, and the ability to utilize other library package formats and other repositories. NetBuild libraries are also now cryptographically signed and the signatures verified as the libraries are downloaded in order to deter “Trojan horse” attacks.

Another management application that has been developed recently is the **Remote Software Toolkit (ReST)**, which was started after observing the difficulties involved in distributing, maintaining, and monitoring software in distributed environments. It is not uncommon for the effort needed to distribute a piece of software across a large, heterogeneous environment to outweigh the benefit of having the software in such an environment. ReST aims to provide a framework for application developers to make use of a suite of applications for users of distributed environments. The three primary parts of the ReST project are the ReST Installer, Explorer, and Monitor. Each component is designed to be modular and easily extended for use in a wide range of other projects.

PEOPLE

Perhaps the most important component of our success is our people. Having an exceptional staff enables us to apply the necessary skills to perform challenging and rewarding research. The diversity of our full and part-time staff of 32, which comprises individuals from all over the world including Great Britain, Poland, France, Russia, China, and Korea, allows us to approach research problems from many directions.

Being a part of a Computer Science (CS) department at a large research university, we have a responsibility to combine teaching and research. With a CS program consisting of nearly 200 students, additional help with our projects is readily available and we have been very proactive in securing graduate and undergraduate internships and assistantships for those students who are motivated, hard working, and willing to learn. Currently, we support more than a dozen students.



ICL Group, Fall 2005

ICL Staff and Students



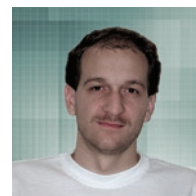
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Research Associate



Bivek Agrawal
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Thara Angskun
Graduate Research Assistant



George Bosilca
Research Scientist



Ramkrishna Chakrabarty
Graduate Research Assistant



Zizhong Chen
Graduate Research Assistant



Tom Cortese
Research Scientist - CE Onsite Lead



David Cronk
Research Director



Jack Dongarra
University Distinguished Professor



Peng Du
Graduate Research Assistant



Graham Fagg
Research Associate Professor



Don Fike
Research Assistant



Teresa Finchum
Administrative Services Assistant



Erika Fuentes
Graduate Research Assistant



Nathan Garner
Research Consultant

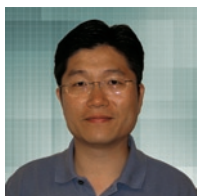


Alice Gregory
Administrative Support Assistant

ICL Staff and Students Continued



Jan Jones
Publications Coordinator



Myung Ho Kim
Visiting Scholar



Julien Langou
Research Scientist



Julie Langou
Research Associate



Tracy Lee
Accounting Specialist II



Daniel Lucio
Graduate Research Assistant



Piotr Luszczek
Research Scientist



Eric Meek
Consultant



Shirley Moore
Associate Director



Keith Moore
Senior Research Associate



Terry Moore
Associate Director



Phil Mucci
Research Consultant



Paul Peltz
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Jelena Pjesivac-Grbovic
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Farzona Pulatova
Graduate Research Assistant



Tracy Rafferty
Business Manager



David Rogers
Graphic Designer



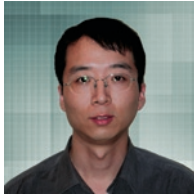
Keith Seymour
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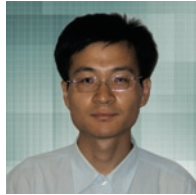
Zhiao Shi
Graduate Research Assistant



Sergei Shinkarev
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Fengguang Song
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Yuan Tang
Senior Research Associate



Dan Terpstra
Research Leader



Joe Thomas
IT Analyst III



Stanimire Tomov
Senior Research Associate



Scott Wells
Assistant Director



Jiayi Wu
Graduate Research Assistant



Qiu Xia
Graduate Research Assistant



Asim Yarkhan
Senior Research Associate



Haihang You
Research Associate



Yuanlei Zhang
Graduate Research Assistant

Since our group was founded, we also routinely host numerous visitors from around the globe. Some of our visitors stay briefly to give seminars or presentations while many remain with us for as long as a year collaborating, teaching, and learning. Though many of our visitors are professors from various international universities, we also host researchers and administrators from many research institutions. In addition, it is not uncommon to have students (undergraduate as well as graduate) from various universities study with us for months on end, learning about our approaches and solutions to computing problems. The experience shared between our visitors and ourselves has been extremely beneficial to us, and we will continue providing opportunities for visits from our international colleagues in research.

We are proud to boast that most of our students have gone on to apply the experience and knowledge gained while working at ICL to careers with many of the largest companies in the computing industry including Hewlett-Packard, Hitachi, IBM, Inktomi, Intel, Microsoft, Myricom, NEC, SGI, Sun Microsystems, and many others.

Recent Visitors

Ed Anderson

EPA National Environmental Scientific Computing Center

Aurelien Bouteiller

INRIA, The French National Institute for Research in Computer Science and Control, France

Eduardo Echavarria

Université Claude Bernard Lyon, France

Serge Gratton

CERFACS, The European Centre for Research and Advanced Training in Scientific Computation, France

Fred Gustavson

IBM

Myhung Ho Kim

Soongsil University, South Korea

Kamil Iskra

Universiteit van Amsterdam, The Netherlands

Wesley Jones

NREL, National Renewable Energy Laboratory

Sanjay Kale

University of Illinois at Urbana Champaign

Daniel Kressner

Umeå University, Sweden

John Levesque

Cray

Alan Malony

University of Oregon

Yves Robert

Laboratoire de l'Informatique du Parallélisme École Normale Supérieure de Lyon, France

Luis Sarmenta

Ateneo de Manila University, Philippines

Olaf Storaasli

ORNL

Alan Sussman

University of Maryland

Christof Vömel

University of California, Berkeley

Reed Wade

CADRES

Jerzy Wasniewski

Technical University of Denmark

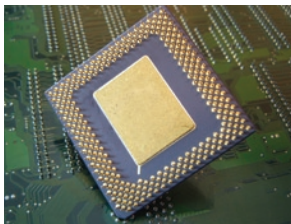
ICL Alumni

Carolyn Aebischer	1990-1993	Ed Anderson	1989-1991	Papa Arkhurst	2003
Dorian Arnold	1999-2001	Zhaojun Bai	1990-1992	Ashwin Balakrishnan	2001-2002
Richard Barrett	1992-1994	Alex Bassi	2000-2001	Micah Beck	2000-2001
Adam Beguelin	1991	Annamaria Benzoni	1991	Scott Betts	1997-1998
Nikhil Bhatia	2003-2005	Noel Black	2002-2003	Susan Blackford	1989-2001
Fernando Bond	1999-2000	Randy Brown	1997-1999	Murray Browne	1998-1999
Cynthia Browne	2005	Antonin Bukovsky	1998-2003	Greg Bunch	1995
Henri Casanova	1995-1998	Sharon Chambers	1998-2000	Jaeyoung Choi	1994-1995

ICL Alumni
Continued

Eric Clarkson	1998	Andy Cleary	1995-1997	Jason Cox	1993-1997
Cricket Deane	1998-1999	Frederic Desprez	1994-1995	Jun Ding	2001-2003
Jin Ding	2003	Martin Do	1993-1994	Leon Dong	2000-2001
David Doolin	1997	Andrew Downey	1998 - 2003	Mary Drake	1989-1992
Julio Driggs	2002-2004	Brian Drum	2001-2004	Victor Eijkhout	1992-2005
Brett Ellis	1995-2005	Shawn Ericson	2004	Zachary Eyler-Walker	1997-1998
Lisa Ezzell	2003-2004	Markus Fischer	1997-1998	Xiaoquan Fu	2003-2004
Edgar Gabriel	2003-2004	Lynn Gangwer	2000-2001	Tracy Gangwer	1992-1993
Kelley Garner	1998	Jonathan Gettler	1996	Eric Greaser	1993
Stan Green	1992-1996	Hunter Hagewood	2000-2001	Christian Halloy	1996-1997
Sven Hammarling	1996-1997	Hidehiko Hasegawa	1995-1996	Satomi Hasegawa	1995-1996
Chris Hastings	1996	David Henderson	1999-2001	Greg Henry	1996
Sid Hill	1996-1998	George Ho	1998-2000	Jeff Horner	1995-1999
Yan Huang	2000-2001	Chris Hurt	2002	Paul Jacobs	1992-1995
Weizhong Ji	1999-2000	Weicheng Jiang	1992-1995	Song Jin	1997-1998
Balajee Kannan	2001	David Katz	2002	Youngbae Kim	1992-1996
Michael Kolatis	1993-1996	Coire Kyle	2005	Amanda Laake	2003-2004
Jeff Larkin	2003-2005	DongWoo Lee	2000-2002	Todd Letsche	1993-1994
Sharon Lewis	1992-1995	Xiang Li	2001	Weiran Li	2002
Chaoyang Liu	2000	Kevin London	1996-2005	Matt Longley	1999
Richard Luczak	2000-2001	Robert Manchek	1990-1996	Tushti Marwah	2004
Paul McMahan	1994-2000	Jeremy Millar	1998-2002	Michelle Miller	1999-2003
Cindy Mitchell	2001-2002	Steven Moulton	1991-1993	Shankar Narasimhaswami	2004-2005
Peter Newton	1994-1995	Caroline Papadopoulos	1997-1998	Leelinda Parker	2002
Antoine Petitet	1993-2001	James S. Plank	1991-1992	Roldan Pozo	1992-1994
Tammy Race	1999-2001	Ganapathy Raman	1998-2000	Kamesh Ramani	2003
Mei Ran	1999-2004	Yves Robert	1996-1997	Ken Roche	1999-2004
Tom Rothrock	1997-1998	Tom Rowan	1993-1997	Kiran Sagi	2003-2005
Evelyn Sams	1998-1999	Farial Shahnaz	2001	Majed Sidani	1991-1992
Shilpa Singhal	1996-1998	Thomas Spencer	1999-2001	Erich Strohmaier	1995-2001
Martin Swany	1996-1999	Daisuke Takahashi	2002	Judi Talley	1993-1999
Keita Teranishi	1998	John Thurman	1998-1999	Francoise Tisseur	1997
Bernard Tourancheau	1993-1994	Lauren Vaca	2004	Sathish Vadhiyar	1999-2003
Robert van de Geijn	1990-1991	Scott Venckus	1993-1995	Reed Wade	1990-1996
Michael Walters	2001-2005	R. Clint Whaley	1991-2001	Susan Wo	2000-2001
Felix Wolf	2003-2005	Tinghua Xu	1998-2000	Tao Yang	1999
Yong Zheng	2001	Luke Zhou	2000-2001	Min Zhou	2002-2004

HARDWARE RESOURCES



Crucial to our efforts are the hardware resources on which we conduct our research. Not only do we have multiple, heterogeneous systems in-house, we also have access to multiple architectures around the country due in large part to our many collaborators and partners. Locally, we maintain systems ranging from individual desktops to large, networked clusters. Below is a summary of the many computing resources used by ICL.

The following are the local systems that we use on a daily basis to test our work:

- 32 node Intel P4 cluster connected with Dolphin Networks
- IBM Power 3s
- Commodity-based Itanium clusters
- SGI Octane
- 64 node Intel EM64T cluster connected with Myrinet 2000
- 64 node AMD Opteron cluster connected with Myrinet 2000

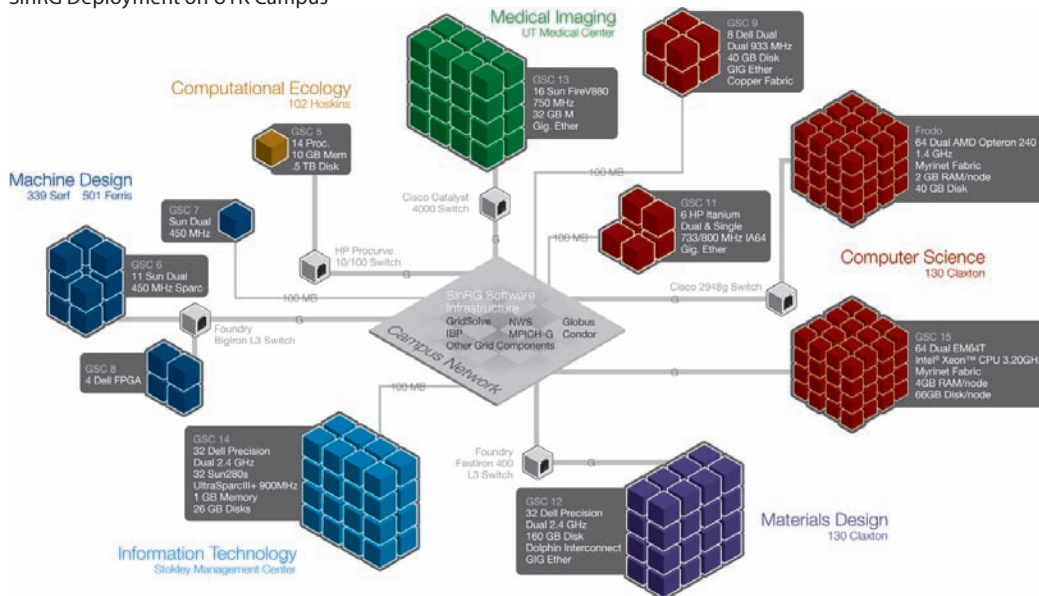
Being part of a large Computer Science department allows us to leverage additional resources including several server class machines and several HPC clusters. These clusters consist of multiple architectures including Itaniums, Itanium2s, Pentium 4s, and AMD processors that comprise over 100 machines with various architectures. All of our clusters are arranged in the classic Beowulf configuration in which machines are connected by low latency, high-speed network switches. Soon we will be adding a 22 node AMD Dual Core Opteron Cluster connected with Infiniband and Myrinet.

In addition, exclusive access to many remote resources, some that are regularly found in the Top500 list of the world's fastest supercomputers, help keep us at the forefront of enabling technology research. The recent modernization of the DOE's Center for Computational Sciences, just 30 minutes away at the Oak Ridge National Laboratory (ORNL), has enabled us to leverage our ORNL collaborations to take advantage of what is becoming the world's fastest scientific computing facility. Below are some of the systems that we currently utilize around the country:

- Cray X1, XT3, and XD1
- IBM SP, Power 3, 4 and 4+, Cluster 1600, and BlueGene/L
- Several large Linux Clusters
- SGI Origin 2000, 3000, 3800, 3900, and Altix

For our Grid computing research, we utilize and help maintain a campuswide grid architecture known as the Scalable Intracampus Research Grid (SinRG), an NSF funded research infrastructure established by the Computer Science department under ICL leadership. This infrastructure provides hardware computing resources within the boundaries of the Knoxville campus for interdisciplinary research collaborations that are indicative of the national and international technology Grid. SinRG allows students, faculty, and other researchers at UTK, including ICL, to address important challenges of grid-based computing using the advantages of local communication and central administration.

SinRG Deployment on UTK Campus



In addition, we possess an Access Grid (AG) node, which consists of various interfaces and environments on the Grid that support distributed meetings, lectures, tutorials, and other collaborative efforts. The AG comprises multiple video cameras, speakers, projectors, and PCs to form a seamless resource for conducting timely, online collaborative activities. The AG has become an invaluable tool and resource for collaborating with the many organizations and institutions with which we conduct joint research.

PARTNERSHIPS



ICL's success is measured in more than research grants and contracts.

Critical to our achievements have been the incredible, lasting relationships we have forged over the years with institutions and organizations within the high performance computing (HPC) community. The HPC community consists of academic institutions, research centers, branches of the federal government, and various other public and private organizations, both domestic and international. We also routinely develop relationships with researchers whose primary focus is other scientific disciplines, such as biology, chemistry, and physics, which makes our collaborations truly multidisciplinary.

The importance to us of these solid partnerships can not be understated as we continually strive to foster new partnerships to not only enhance our explorations but also maintain our growth. Such mutually beneficial collaborative initiatives over the years have strengthened our research efforts by allowing us to share resources, both material and intellectual. The following lists highlight many of our domestic partners and collaborators. As our list of government and academic partners continues to grow, we hope to also develop additional partnerships with commercial software vendors. Some of the vendors who have incorporated our work in their applications include Intel, Inc. who now develops the KAP/Pro toolset and the Vampir performance visualization and analysis tool, The Mathworks, Inc. who develops Matlab, and Etnus, Inc., developer of the TotalView debugger.

The world map on page 23 shows the location of many of the domestic and international partners and collaborators in research with whom we continue to work.

Domestic Collaborators

Argonne National Laboratory (ANL)	Microsoft Research
California Institute of Technology Center for Advanced Computing Research (CACR)	Morehouse College
Computer Science and Mathematics Division of Oak Ridge National Laboratory (ORNL CSMD)	Myricom
Cray	National Aeronautics and Space Administration (NASA)
Defense Advanced Research Projects Agency (DARPA)	National Computational Science Alliance (NCSA)
DoD High Performance Computing Modernization Program DOE2000	National Institute of Standards and Technology (NIST)
Emory University	National Science Foundation (NSF)
Information Sciences Institute (ISI)	ORNL/UT Joint Institute for Computational Science (JICS)
Intel Corporation	Rice University
International Business Machines (IBM)	San Diego Supercomputing Center (SDSC)
Internet2	Silicon Graphics Incorporated (SGI)
Internet2 Distributed Storage Infrastructure (I2-DSI)	Sun Microsystems
Lawrence Livermore National Laboratory (LLNL)	United States Department of Defense (DoD)
Los Alamos National Laboratory (LANL)	United States Department of Energy (DOE)
Metacenter Regional Alliance (MRA)	University of California, Berkeley
	University of California, San Diego
	University of Kentucky
	University of Tennessee Computer Science Department



International Collaborators

Danish Computing Center for Research and Education Lyngby,
Denmark

Department of Mathematical and Computing Sciences, Tokyo
Institute of Technology – Tokyo, Japan

Department of Mathematics, University of Manchester
– Manchester, England

CERFACS European Centre for Research and Advanced Training in
Scientific Computing – Toulouse, France

Fakultät für Mathematik und Informatik Universität Mannheim
– Mannheim, Germany

Forschungszentrum Jülich Central Institute for Applied
Mathematics – Jülich, Germany

Institut für Wissenschaftliches Rechnen ETH Zentrum – Zurich,
Switzerland

Istituto per le Applicazioni del Calcolo “Mauro icone” del C.N.R.
– Rome, Italy

Intelligent Systems Design Laboratory

Doshisha University – Kyoto, Japan

Kasetsart University – Bangkok, Thailand

Laboratoire de L’Informatique du Parallelisme École Normal
Supérieure de Lyon – Lyon, France

Mathematical Institute Utrecht University – Netherlands

Monash University – Melbourne, Australia

Numerical Algorithms Group Ltd – Oxford, England

Parallel and HPC Application Software Exchange (PHASE)
– Tsukuba, Japan

Queensland University of Technology – Brisbane, Australia

Laboratoire Réseaux Haut Débits et Support d’Applications

Multimedia Jeune Equipe de l’Université Claude Bernard de Lyon
(RESAM) – Lyon, France

Rutherford Appleton Laboratory – Oxford, England

Scole Polytechnique Federale de Lausanne – Lausanne,
Switzerland

Soongsil University – Seoul, South Korea

Technische Universität Wien – Vienna, Austria

Università di Roma “Tor Vergata” – Rome, Italy

University College Dublin – Dublin, Ireland

University of Umeå – Umeå, Sweden



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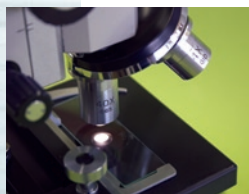
From its inception in the spring of 2001, the Center for Information Technology Research (CITR), directed by Dr. Jack Dongarra and co-located with ICL, has fulfilled all the expectations that the University of Tennessee (UT) had when it established the Research Center program. CITR's mission has been to develop and enhance opportunities for multi-disciplinary and innovative Information Technology Research (ITR) at the University of Tennessee. In order to build up a thriving, well-funded community in basic and applied ITR, CITR's primary strategy has been to invest in a diverse group of ITR laboratories, each one led by an established researcher or an emerging leader in some significant area of ITR. Since first rate students and staff are indispensable to the success of such a strategy, CITR is also working to help develop the kind of educational environment that can recruit and train the people that a top flight IT research University requires.

This year CITR will work with faculty and administrators from several departments and colleges to help establish a new, University wide program in Computational Science that supports advanced degree concentrations in this critical new area across the curriculum. Under this program, students pursuing advanced degrees in a variety of fields of science and engineering will be able to extend their education with special courses of study that teach them both the fundamentals and the latest ideas and techniques from this new era of information intensive research.

Although CITR has also made small investments in collateral activities — challenge grants for new IT researchers, contributions to start up packages for stellar new faculty, enhanced graduate stipends in ITR-related fields — it has concentrated on the ITR laboratories, and this concentration has produced the majority of its successes. Of the nine research centers of excellence — five in Knoxville and four at the Health Science Center in Memphis — CITR ranked second, bringing in \$36.1 million in new research funding, just behind the Center of Genomics and Bioinformatics. Since UT's investment over that period was \$2.7 million, CITR's rate of return on investment has been 13 to 1.

UT's Research Centers of Excellence

The full list of UT's Research Centers of Excellence (and their respective directors), includes the following:



Centers Based in Knoxville

- Center for Information Technology Research**
- Tennessee Advanced Materials Laboratory**
- Center for Environmental Biotechnology**
- Food Safety Center**
- Center for Structural Biology**

- Dr. Jack Dongarra
- Dr. Ward Plummer
- Dr. Gary Saylor
- Dr. Stephen P. Oliver & Dr. Ann Draughon
- Dr. Engin Serpesu



Centers Based in Memphis

- Connective Tissues Diseases Center**
- Center of Genomics and Bioinformatics**
- Center for Neurobiology of Brain Diseases**
- Vascular Biology Center**

- Dr. Andrew H. Kang
- Dr. Dan Goldowitz
- Dr. William A. Pulsinelli
- Dr. Lisa Jennings

Cyberinfrastructure Technology Watch

<http://www.ctwatch.org/>



In collaboration with the NSF funded Cyberinfrastructure Partnership (CIP), which includes the San Diego Supercomputing Center (SDSC) and the National Center for Supercomputing Applications (NCSA), ICL is leading a new and broad ranging publication effort called Cyberinfrastructure Technology Watch (CTWatch). CTWatch is an initiative of the CIP that is intended to serve as a forum for ideas and opinion on issues of importance to the cyberinfrastructure community, and as an ongoing source of information and analysis concerning the latest innovations in cyberinfrastructure technology.

To create the kind of productive mix of news, information, and dialogue that rapid progress in shared cyberinfrastructure today requires, CTWatch has been developed along two complementary paths, one based on a more traditional publishing paradigm and the other including new types of non-traditional, Internet-based communication and publishing. On the conventional front, we have created *CTWatch Quarterly*, an on-line serial publication modeled on a more traditional academic journal. Along a more experimental line, we have created CTWatch Blog, an on-line Weblog that provides frequent updates, commentary, and informative links on the most recent developments and ideas occurring in the national and international cyberinfrastructure community.

Activities during the first year (2005) include the following:

- Designed and developed a Web site (<http://www.ctwatch.org>) to support the promulgation of the *Quarterly* and the Blog.
- Published and publicized the first four issues of *CTWatch Quarterly* on-line (<http://www.ctwatch.org/quarterly/>). A total of more than 1,700 copies of the first three issues of the *Quarterly* have been downloaded.
- Established the format for the *Quarterly* as an on-line publication, implemented as a PDF document designed to support printing on demand with high production values. Each issue focuses on some aspect or subdomain of cyberinfrastructure, rounded out with additional summaries of the reports of national committees and workshops on relevant issues.
- Recruited a Guest Editor for each of the 1st year's issues. The Topic/Guest Editor pairs for the first year's issues included the following: Trends in High Performance Computing (Jack Dongarra); Optical Computing and Networking (Larry Smarr and Phil Papadopoulos); Low Power Computing (Satoshi Matsuoka); and European e-Science and Cyberinfrastructure (Tony Hey and Anne Trefethan).

In the near future we are planning new issues of the *Quarterly* on the state of the art in Computational Biology, collaborative cyberinfrastructure, and international cyberinfrastructure efforts on four continents – Asia, Africa, South America, and Australia. We also plan to expand new media aspects of the web site to include broader participation of the community in CTWatch Blog and new publication modes, such as Wikis and podcasting.



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A complete bibliography of our publications and technical reports from 1999 to present can be found on our web site at <http://icl.cs.utk.edu/>. Most of these are also downloadable.

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INNOVATIVE COMPUTING LABORATORY 2005-2006 REPORT

Edited by Scott Wells

Designed by David Rogers

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The university does not discriminate on the basis of race, sex, or disability in the education programs and activities pursuant to the requirements of Title VI of the Civil Rights Act of 1964, Title IX of the Education Amendments of 1972, Section 504 of the Rehabilitation Act of 1973, and the Americans with Disabilities Act (ADA) of 1990.

Inquiries and charges of violation concerning Title VI, Title IX, Section 504, ADA, the Age Discrimination in Employment Act (ADEA), or any of the other above referenced policies should be directed to the Office of Equity and Diversity (OED), 1840 Melrose Avenue, Knoxville, Tennessee 37996-3560, telephone (865) 974-2498 (V/TTY available) or 974-2440. Requests for accommodation of a disability should be directed to the ADA Coordinator at the UT Knoxville Office of Human Resources, 600 Henley Street, Knoxville, Tennessee 37996-4125.

In accordance with the Tennessee College and University Security Information Act of 1989 and the Student Right-to-Know and Campus Security Act, the University of Tennessee has prepared a report containing campus security policies and procedures, data on campus crimes, and other related information. A free copy of this report may be obtained by any student, employee, or applicant for admission or employment from the Office of the Dean of Students; The University of Tennessee; 413 Student Services Building; Knoxville, Tennessee 37996-0248. Management, 600 Henley Street, Knoxville, Tennessee 37996-4125.



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