

ICL  **UT** 2003-2004 REPORT

INNOVATIVE COMPUTING LABORATORY

COMPUTER SCIENCE DEPARTMENT
UNIVERSITY *of* TENNESSEE

FROM THE DIRECTOR



This has been another productive year for the Innovative Computing Laboratory (ICL) as we continue to improve and expand our activities in the area of high performance computing. I am pleased to report that we have made substantial progress in our programs, increased the size of our organization, and ended the year with a number of new research grants. ICL has the goal of being a leader in defining enabling technologies for high performance computing. As we complete our 14th year of operation, I believe we are well on our way to achieving this goal. It is quite remarkable that ICL, in a relatively short time, has succeeded in establishing a truly multidisciplinary effort with many efforts directed to help computational scientists reach the forefront of scientific investigation. We thrive on collaborating on multidisciplinary projects, as we are well aware of the importance of pooling our research expertise from different traditional disciplinary fields when trying to study and solve complex problems in science and technology.

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 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.

We are building from a firm foundation. Over the past 14 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 ICL's leadership role. Standards and efforts such as PVM, MPI, LAPACK, ScaLAPACK, BLAS, ATLAS, Netlib, NHSE, Top500, and the Linpack Benchmark have all left their mark on the scientific community. We can be proud of the recognition and use our tools receive. We are continuing these efforts with PAPI, NetSolve/GridSolve/GridRPC, HARNESS, HPC Challenge Benchmark, and the Self-Adapting Numerical Software Effort (SANS Effort), as well as other innovative computing projects.

We continue to grow in terms of the resources we have at our disposal. We continue our efforts to strengthen our organization and to ensure the proper balance and integration of research and projects. As we expect the pace of change to continue to accelerate in the coming years, we have positioned ourselves well to discover and exploit new research opportunities.

During these exciting times, I am grateful to our sponsors for their continued endorsement of our efforts. 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

CONTENTS

ICL Overview	2
Research Introduction	4
Numerical Linear Algebra	6
Distributed Computing	8
Performance Evaluation	10
Software Repositories	12
People	14
ICL Staff & Students	15
Recent ICL Visitors & ICL Alumni	18
Hardware	20
Partners	22
Centers of Excellence	24
CITR	25
Publications	26



MISSION STATEMENT

The Innovative Computing Laboratory aspires 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

ICL was established in the fall of 1989 when Dr. Jack Dongarra came to the University of Tennessee (UT) from Argonne National Laboratory (ANL). Dr. Dongarra was given a dual appointment as Distinguished Professor in the Computer Science Department at the university 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. Subsequently, many post-doctoral researchers and professors from various research backgrounds such as mathematics, geology, chemistry, etc. visited the university. Many of these scientists have passed through UT as post-doctoral researchers and worked with Dr. Dongarra to attract other researchers and top graduate students. Below is a list of some of the researchers who were instrumental in helping Dr. Dongarra with the establishment and growth of ICL:

Zhaojun Bai of the University of California, Davis	Robert van de Geijn of University of Texas Austin
Richard Barrett of Los Alamos National Laboratory	Antoine Petitet of Sun Microsystems France
Adam Beguelin of Oracle	Roldan Pozo of NIST
Susan Blackford of Myricom	Erich Strohmaier of Lawrence Berkeley National Laboratory
Henri Casanova of the University of California, San Diego	Françoise Tisseur of Manchester University
Jaeyoung Choi of Soongsil University (Korea)	Bernard Tourancheau of Sun Microsystems Lab
Andy Cleary of Lawrence Livermore National Laboratory	Clint Whaley of Florida State University
Frederic Desprez of ENS Lyon	

Through interactions with colleagues at Rice University, 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 led 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, ICL 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 the ATLAS, BLAS, LAPACK, ScaLAPACK, PVM, MPI, Netlib, and the NHSE. These successes are continuing along with current ICL efforts such as Active Netlib, PAPI, HARNESS, NetSolve, SANS Effort, and the TOP500. In the past decade, four of our projects have earned R&D 100 awards; PVM in 1994, ATLAS and NetSolve in 1999, and PAPI in 2001.



ICL GROUP, 2003

PROFILE

Located in the Claxton building at the heart of the University of Tennessee campus in Knoxville, ICL is part of the Computer Science department. Now in its 14th year of existence, ICL has established itself as one of the foremost academic, enabling technology research laboratories in the world. Our sustained growth during that time has allowed us new accommodations on the Knoxville campus. The Claxton building was expanded in 2000 to house the entire CS department and the ICL. This 70,000 square foot expansion includes a 2500 square machine room, which serves as home to more than 200 machines belonging to both ICL and CS.

Our contributions to both UT and to the HPC community have been well known for more than a decade and our research in information and enabling technology is recognized throughout the world. Perhaps the significance of our laboratory to the research climate here at the university is best expressed by the Chancellor of the Knoxville campus, Dr. Loren Crabtree;

“As the University of Tennessee continues its efforts to be recognized as one of the premier research universities, our ability to attract and retain top researchers is critical. The Innovative Computing Laboratory here at UT, led by Dr. Jack Dongarra, has set the standard for academic research in the 21st century and has helped us establish a strong foundation for our recruiting efforts. With the help of ICL, our university is stretching the boundaries of national and international collaboration that serves to broaden our research initiatives. After more than a decade, the staff and students of ICL continue to be among the leaders both at UT and in the nation in high performance computing and information technology research. As we strive to expand and enrich our successful research environment within the UT system, we must continue to showcase not only the contribution that labs such ICL make to higher education but also the effect that their discoveries have on our state and nation.”

ICL OVERVIEW CONTINUED

ICL PROFILE

Established	1989	Active projects	16
Annual Budget	~\$5 million	International Collaborators	23
Full-time staff	31	Domestic Research Partners	39
Part-time staff	7	Average Annual Publications	30
Students	16	R&D 100 Awards	4

RESEARCH INTRODUCTION

As computational demands continue to increase, so will the opportunities for innovative, engaging research in enabling technology. These demands over the past decade 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 projects has evolved over the course of more than a decade, beginning from a narrow but solid foundation. In 2003-2004, we will support or participate in more than 16 significant projects.

Our work, originating with numerical linear algebra and the numerical libraries that encode its operations in software, has evolved with the increasing computing demands of the 21st century. Driven by the relentless demand for enabling technology in the computational science community, ICL has built upon its successes in the area of numerical libraries and the growing strength of its personnel to break new ground in the areas of high performance and distributed computing. Similarly, our work with numerical libraries has created a strong area of expertise in performance evaluation 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 software repositories.

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 efforts. The areas of distributed and network computing are no exception as we have learned to harness enormous computing power to quickly and efficiently solve mathematical problems that would take humans years or decades to solve by hand.



CLAXTON BUILDING, HOME OF ICL

ACKNOWLEDGEMENT

Research in our four main focus areas – numerical libraries, high performance distributed computing, performance evaluation and benchmarking, and software repositories – is described in more detail in the pages that follow. Our achievements in each of these areas over the past year are also highlighted. Evidence of the perceived value of our work and the importance of our research is apparent in the range of agencies and organizations that have funded, and continue to fund, our efforts. The main source of support has been federal agencies that are charged with investing the nation's research funding: the National Science Foundation (NSF), Department of Energy (DOE), Department of Defense (DoD), the Defense Advanced Research Projects Agency (DARPA), and the National Aeronautics and Space Administration (NASA). However, strong support from private industry has also played a significant role. Some organizations have targeted specific ICL projects while 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:



OVERVIEW

Linear algebra operations occur throughout scientific computing. 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. We have long been a leader in producing standards, algorithms, and software for numerical linear algebra. In collaboration with other researchers and with industry, we have led efforts to standardize and adopt the Basic Linear Algebra Subprograms (BLAS) through the BLAS Technical Forum and the development of libraries such as Linpack, LAPACK, and ScaLAPACK. These efforts have been widely adopted by the scientific community, as well as by the computer industry through inclusion in commercial, standard numerical libraries. In addition to our activities in dense algebra libraries, we have been involved in sparse linear algebra efforts, releasing a performance benchmark for iterative methods.

The above-mentioned libraries focus primarily on algorithmic innovations, moving performance considerations to the kernel level. However, we have made our mark at that level too by releasing the Automatically Tuned Linear Algebra Software (ATLAS) package, which delivers an optimized library in a fraction of the time of hand coding, and which is competitive with vendor-supplied libraries. ATLAS has been widely accepted, having been included in both the MATLAB and OCTAVE linear algebra packages, as well as SciPy – an extension of the Python language for scientific computing.

Reflecting the shift in scientific computing practice from Fortran to Java, our research has begun targeting mathematical software towards this language. Java source

code is compiled into machine independent byte code, which is then interpreted by a Java Virtual Machine (JVM). It is a common and somewhat erroneous belief that Java will always be too slow for scientific computing. Our Fortran to Java (F2J) project is addressing the question of the feasibility of scientific computing via Java through development of a translator that converts programs written in a subset of Fortran 77 into a form that can be executed on JVMs. This translator makes it possible for a Java application or applet to use established legacy numerical code that was originally written in Fortran; as a specific example, a translated version of LAPACK called JLAPACK, has been released.

More recently, considerable research effort here at ICL has been applied to Self-Adapting Numerical Software (SANS) systems, which aim to relieve the user of several levels of decision making in the process of realizing optimally performing numerical software. Such systems adapt the realization process to the computational environment on several levels, including the kernel, network, and algorithmic levels. SANS, a collaborative effort, comprises our projects in kernel level optimization (ATLAS), network level adaptation (LAPACK for Clusters - LFC), and an algorithmic decision-making component (Self-Adapting Large-scale Solver Architecture - SALSA). Combined, these levels constitute a dynamic environment where a user's problem gets solved by an algorithm that is chosen based on characteristics of the input data, scheduled over the current state of the computational grid, and executed with kernels optimally suited to the processors used.

Our LFC project merges the ease of use of LAPACK with the parallel processing capabilities of ScaLAPACK. LFC is a self-contained package with built-in knowledge of how to run

linear algebra software on a cluster. Users are responsible for stating their numerical problems but can assume they are working in a serial environment. The LFC middleware assesses the possibility of solving the problem faster in parallel on some subset of the available resources, based on information describing the state of the system. The user's problem is distributed over the selected processors with a load distribution dependent on the machine loads and relative capabilities, the problem is executed in parallel, and the solution is returned to the user. Experimental results compare favorably with the performance obtained by an expert user in the same environment.

RECENT RESEARCH

We have fully developed an autotools framework for automatic installation of LFC on most of high-end workstations (the sites that participate in the NSF NPACI effort). The functionality that is currently fully supported is double precision decompositional solvers: LU, Cholesky and QR. The solvers work out of the box without user intervention in a sequential or parallel environment - depending on the problem size and available resources. LFC is now installed on NPACI sites (San Diego, CalTech, Univ. of Michigan and others) and other outside locations. Furthermore, we are developing software to make LFC accessible from scripting languages like Matlab and Python. This approach combines the performance of ScaLAPACK, the automatic scheduling of LFC, and the ease of expression of the scripting language. Extending LFC to handle sparse data structures and to operate in grid environments is another direction of our current research.

Our ongoing performance optimization research concerns certain sparse operations: the Automatically Tuned

Multigrid Smoothers package contains smoothers for two-dimensional multigrids that use the ATLAS repertoire of optimizations to good effect.

As an example of an algorithmic component of a SANS system, we continue developing SALSA, software for heuristic decision making for linear and nonlinear system solving. The software currently functions as a testbed for iterative linear system solvers; it contains a number of analysis modules for generating characteristics of user input data, and we have done proof-of-concept tests on using statistical tools for building heuristics. As part of a project for Component-based Programming Frameworks, we have proposed a metadata standard for matrix data that formalizes the matrix characteristics we analyze. We are releasing software that realizes this standard both as an XML file format and as an API for use in numerical codes.

OVERVIEW

Distributed computing provides a fundamental platform for building modern High Performance Applications. Due to its importance, ICL has been involved in distributed computing for over a decade, producing such successful systems as the Parallel Virtual Machine (PVM) jointly with Oak Ridge National Laboratory and Emory University. Currently, we are involved in all three tiers of distributed computing from High Level Problem Solving environments such as NetSolve and GrADS (Grid Application Development System), through middleware technologies such as GridRPC and FT-MPI (Fault Tolerant Message Passing Interface) to low level systems such as HARNESS (Heterogeneous Adaptable Reconfigurable Networked SystemS). Involvement with all levels of distributed computing has allowed for better integration with numeric libraries and applications allowing for very efficient overall system utilization. This is especially important when much of our software supports efficient execution across such a diverse range of systems from SuperComputers to Clusters to the Grid and beyond.

NetSolve is one of our more prominent research projects and has been the basis for a number of complementary projects such as GridSolve and GridRPC. NetSolve 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. Due to the benefits offered to scientists by utilizing specialized numeric libraries together with the power of distributed computing, the NetSolve user community is growing rapidly. A Grid based version of NetSolve, which utilizes Grid services such as

Condor, Network Weather Service (NWS), and the Internet Backplane Protocol (IBP), has also been developed known as GridSolve. A logical extension to this work is the building of a standardized Grid RPC mechanism for general Grid usage. ICL, together with the Global Grid Forum, is well positioned for developing such a standard known as GridRPC. Furthering inter-institutional collaboration on developing Grid applications is managed under the GrADS lead by Rice University. GrADS is a leading edge research project that includes more than a dozen top computer scientists from nine different universities. The GrADS project aims to address the key scientific and technical problems that must be solved in order to make it relatively easy to develop Grid applications for real problems and to tune those applications for high performance.

HARNESS is an experimental Grid computing framework that leverages the success of PVM. Similar to PVM, Harness is built around the concept of multiple collaborative "virtual machines" (VMs) that allows a set of diverse computing resources to be viewed as a single, large, distributed memory computing resource. Building on our collaboration with researchers at ORNL and Emory University, HARNESS extends the framework of modular user definable plug-in services that can provide application, domain specific interfaces. One such interface developed by our research staff is FT-MPI. FT-MPI provides support for fault-tolerant applications that is crucial for large, long running simulations. Currently, fault tolerant applications cannot be built with standard MPI libraries because MPI is unable to handle failures gracefully. Under FT-MPI, applications have flexible control over how failures are handled, allowing message passing applications to be built that can survive

node failures without the need to continuously make expensive state and checkpoint dumps to disk. With FT-MPI, we are also supporting the development of algorithms that can adapt to failures, which is currently not possible with other implementations of MPI.

Our Grid computing research is supported by the Scalable Intracampus Research Grid (SInRG), an NSF funded research infrastructure established by the UT Computer Science department under our leadership. It mirrors within the boundaries of the Knoxville campus both the underlying technologies and the interdisciplinary research collaborations that are characteristic of the national and international technology Grid allowing ICL and UT researchers to address the key research challenges of grid-based computing using the advantages of local communication and central administration.

RECENT RESEARCH

Over the past year, our GrADS work has produced an integrated system architecture and prototype software called GrADSoft that prepares, schedules, and executes programs on the Grid. Parallel linear algebra applications not meeting an expected performance level are automatically detected and can migrate to alternative Grid resources, even migrating from N resources to M resources. This enables reliable and efficient performance on volatile resources.

In addition, NetSolve has been integrated with GrADS, providing a simple RPC style front end to GrADS's powerful scheduling and execution environment. This enables parallel libraries and distributed Grid resources to be easily accessed using front ends such as Matlab and serial C or Fortran programs. Furthermore, NetSolve 2.0 includes an implementation of the GridRPC API. NetSolve/GridSolve-

2.0 will be an integral part of the NSF Middleware Initiative Release 4 suite, being released later this year. NetSolve and the Internet Backplane Protocol (IBP), two SInRG middlewares, have been combined into partner applications now supporting researchers in Computational Ecology, Medical Imaging, Computational Combinatorics, as well as Statistical Parametric Mapping (SPM) and remote users of ATLSS (Across Trophic Level System Simulation). These applications represent initial realizations of one of the key goals of the SInRG project, viz. to make grid computing a routine part of the working environment for computational scientists.

The maturity of the HARNESS system has prompted its utilization by scientists at the General Hospital in Vienna to handle simulations using the PEBBLES solver to calculate electric fields within muscles, which allows for external electrical simulation benefiting some paralyzed patients with a limited ability to walk.

FT-MPI has reached beta release status and now supports the full MPI 1.2 specification as well as multiple chapters of the MPI-2 standard including the C++ API binding. A full release is expected in the 4th quarter of 2003.

OVERVIEW

ICL has long been a leader in benchmarking and performance evaluation efforts that measure and report performance on high performance computing machines. Our researchers have developed a number of benchmark codes. The Linpack Benchmark is a numerically intensive test that has been used for years to measure the floating-point performance of computers. Performance on this benchmark is also the basis of the semi-annual TOP500 list that ranks the fastest 500 computers in the world. For the TOP500, the version is used that allows the user to scale the size of the problem and to optimize the software to achieve the best performance for a given machine. Linpack performance does not reflect the overall performance of a given system, as no single number ever can. However, it does reflect the performance of a dedicated system for solving a dense system of linear equations. In addition to the semi-annual TOP500 list published by ICL and University of Mannheim, ICL Director Jack Dongarra and colleague Aad J. van der Steen publish a yearly Overview of Recent Supercomputers which reflects the technical state of the supercomputer arena as accurately as possible.

Our researchers have 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, so as to leave the user with the opportunity of experimentally determining an optimal set of parameters for a given machine configuration. State-of-the-art algorithms are used, including recursive panel factorization with pivot search and column broadcast combined and a bandwidth-reducing

swap broadcast algorithm. The algorithms are scalable in the sense that their parallel efficiency is maintained constant with respect to the per processor memory usage. In addition to providing a means for obtaining Linpack results, HPL exemplifies the coding practices needed to obtain near peak performance on modern parallel architectures. Our researchers have also helped develop the SparseBench Benchmark suite for iterative methods on sparse matrices. Solution of sparse linear systems, such as those derived from Partial Differential Equations (PDEs), form an important problem area in numerical analysis as well as being the basis of computational problems in a number of application areas, including computational fluid dynamics and structural mechanics. Unlike in the case of dense linear systems, solution of sparse systems does not entail much reuse of data. Thus, algorithms for sparse matrices will be more bound by memory speed than by processor speed. SparseBench uses common iterative methods, preconditioners, and storage schemes to evaluate machine performance on typical sparse operations.

In addition to developing benchmarks, our research staff is actively involved in the development of performance evaluation tools and methodologies. As a basis for collecting accurate and relevant performance data, we have developed a portable library interface for access to hardware performance counters on most modern microprocessors. These counters exist as a small set of registers that count events, which are occurrences of specific signals related to the processor's function. Monitoring these events facilitates correlation between the structure of source/object code and the efficiency of the mapping of that code to the underlying architecture. This correlation has a variety of uses in

performance analysis including hand tuning, compiler optimization, debugging, benchmarking, monitoring and performance modeling. 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.

RECENT RESEARCH

Reflecting the strong emerging trend of cluster computing in high performance computing, the TOP500 team, in collaboration with the IEEE Task Force on Cluster Computing (IEEE TFCC), is developing a list similar to the TOP500 to rank the world's top 100 cluster computing systems.

In addition, our research staff has been instrumental in assisting with recent major benchmarking efforts such as those carried out by the Department of Energy Advanced Simulation and Computing program (DOE ASC, formerly DOE ASCI), the Department of Defense High Performance Computing Modernization Program (DoD HPCMP) and DARPA High Productivity Computing Systems (HPCS). Our activities in these efforts have included assisting with tuning the benchmark codes, defining the performance metrics to be collected, providing tools for collecting the data, and interpreting the benchmark data. We have also recently started an effort to expand the scope of benchmarking beyond the Linpack Benchmark. For DARPA, we are aiding

in the development of a new benchmark suite, called the HPC Challenge Benchmark, which currently consists of four benchmarks; HPL, Streams, RandomAccess, and PTRANS. HPL is the Linpack TPP benchmark, which tests the floating point performance of a system. Streams is a benchmark that measures sustainable memory bandwidth (in GB/s), RandomAccess measures the rate of random updates of memory. PTRANS (parallel matrix transpose) measures the rate of transfer for large arrays of data from multiprocessor memory.

The PAPI library interface and reference implementations have become widely adopted by performance tool developers, including the HPCView project at Rice University, the SvPablo project at the University of Illinois, the TAU project at the University of Oregon, and the VProf project at Sandia National Laboratories. The PAPI library and tools that rely on it are also in use at major HPC sites in the US and worldwide for performance evaluation and tuning of applications in areas such as climate and weather modeling, environmental quality modeling, computational fluid dynamics, and signal image processing.

Our recent efforts on the PAPI project have focused on streamlining the implementation to reduce data collection overheads and on implementing new features such as multiple counter overflow support and counter sampling. The overhead for starting, reading, and stopping the counters has been lowered to a few hundred cycles on several platforms. In addition, we have developed a web-based performance optimization tutorial that gives instruction on how to analyze and tune application performance using PAPI and other tools.

OVERVIEW

The foundation for our work in software repositories can be traced back to the tremendous success of Netlib in the 1980s and the benefits its mathematical software and resources provided (and still provides) to the HPC community. The open source Netlib effort has recorded more than 230 million requests to date with primary servers maintained both here at ICL and at Bell Laboratories in New Jersey. As a result of the tremendous success of Netlib and the ever increasing demands for software reuse generated by the proliferation of scientific computing and simulation here in the US, the National HPC 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 of the products of the NHSE effort was the Repository in a Box (RIB) toolkit, which was developed to enable the creation and interoperability of discipline-oriented, web-based software repositories, specifically 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. Our staff currently maintains several domain specific software repositories built with RIB including the Parallel Tools Library (PTLib) and the High Performance Netlib (HPC-Netlib) Library. The Department of Defense (DoD) and the Department of Energy (DOE) also maintain RIB-based repositories. Leveraging the many advantages of RIB and drawing upon

the vast Netlib resources, we continue our work of providing tools for sharing metadata and libraries through the creation of the Active Netlib project, which has the goal of providing an interactive, inquiry-based learning environment about mathematical software for undergraduate engineering students, teachers, and practicing engineers. Active Netlib utilizes NetSolve (also produced here at ICL), RIB, and Netlib and is part of the NSF National Scientific Digital Library (NSDL) program. Active Netlib was developed as a joint project with Morehouse College, the Joint Institute for Computational Science (JICS), and the Computational Fluid Dynamics Laboratory here at UT.

The progression of our repository efforts also continues with our work on NetBuild, which is a project to make it easier for authors and users of scientific computation software to utilize standardized mathematical software libraries, many of which may be located in the Netlib repository or similar collections. Specifically, the NetBuild tool suite attempts to eliminate the need for authors and users to locate, download, configure, compile, and install each of the mathematical software libraries that are required by a program. In contrast to Active Netlib, which provides facilities for remote execution of computations on the user's data using NetSolve servers, the netbuild program securely downloads the code necessary to perform those computations on the user's computer.

RECENT RESEARCH

The past year has seen many changes, not only in the processing demands of computationally intensive applications, but also in the demands of these applications to move, share and store data, metadata, and other software resources. In order to keep pace with changes in data and

resource demands, the current RIB toolkit is undergoing a complete overhaul. In the summer of 2003, work began on the next generation repository building application, with an as yet to be determined name. Completely rewritten in Java and no longer packaged with a web server, a database, or the necessary scripts to run it all, the new incarnation of RIB will be streamlined and improved to decrease install time and accommodate any type of data model while still providing flexibility for catalog building and robust metadata interoperation.

Our Active Netlib project has reached its goal for providing an inquiry-based learning environment for engineering students and faculty. With NetSolve servers running at both UT and Morehouse College, Active Netlib now provides resources such as Mathworld articles and engineering applications to both students and faculty. Using multiple interfaces including Open Archives Initiatives (OAI) and Iterative solvers, JICS located in Oak Ridge, Tennessee has successfully utilized Active Netlib to archive simulation data for teaching. Active Netlib essentially takes advantage of the existing Netlib resources and extends them through the use of RIB, which allows the Netlib collection to be selectively mirrored and contributed to by multiple participants. In the near future, all of the components of Active Netlib will be bundled together and combined with the NSF NSDL program.

NetBuild has been extended over the past several months to support a wider variety of platforms. The tools for building libraries can now compile a set of libraries for each of several variants of a platform (depending on cpu features, cache size, etc.) and generate appropriate metadata for each one. The netbuild program can then select the best one of these

for the target platform. The NetBuild tool suite also now has the ability to impose constraints on the use of libraries based on various features of the target platform, such as whether the platform has other libraries installed. A precedence expression is used to determine which library to use among those for which the constraints are met. For example, on a platform that has a vendor BLAS installed, netbuild can be told whether or not it is better to use that BLAS, an ATLAS BLAS, or some other library. In addition, the tools are now more robust and more portable, and there are now better tools for managing collections of libraries on the netbuild server.

Just like with most organizations, our employees are the key to our success. It is also the working relationships we have established with individuals and organizations within the high performance computing (HPC) community that are instrumental in our achievements. Our staff, our partners and collaborators, and the many commercial vendors with which we work have helped us create a strong foundation for fostering creative, original research.

Both our reputation and achievements have allowed us to build a research staff comprising some of the finest research minds in the world. With a large number of staff, we are able to apply adequate people resources to the projects on which we work. Currently, we employ 38 full or part-time staff, most of whom have advanced degrees and many of whom worked for us as student assistants. Proudly, our staff includes representatives from nearly a dozen countries. Our ability to attract such experts from around the world is only one reason ICL remains an HPC research leader.

Also integral to our success are our many student employees. As an academic research group, we have an inherent responsibility to teach. Because we are part of the computer science (CS) department of a large university, we have access to both graduate and undergraduate students. With a CS program consisting of nearly 200 students, additional help with our projects is just a job posting away. These students represent a resource that is not readily available to many research groups, and we have been very proactive in securing internships and assistantships for those students who are motivated, hard working, and willing to learn. In addition to our large staff, we are proud to currently support 16 students, both graduate and undergraduate.

In addition to our staff and students, we 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 from many research institutions. Furthermore, 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. In fact, many Ph.D. students from universities as far away as Japan have passed through our doors in an effort to broaden their understanding of linear algebra techniques and how we apply them to our research. 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. See page 18 for the many guests who have stopped by in the last year to exchange ideas and share their expertise with us. We have worked hard to create and maintain collaborative relationships and are always eager to open doors to new opportunities for sharing research endeavors.

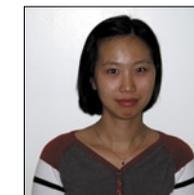
We also proudly boast that many of our former students and staff have moved on to do further interesting and useful research at places around the world. Many of our alumni have gone on to apply the knowledge gained from their time at ICL with companies such as Hewlett-Packard, Hitachi, IBM, Inktomi, Intel, Microsoft, Myricom, NEC, SGI, Sun Microsystems, and many others.



Sudesh Agrawal
Research Associate



Cynthia Browne
Undergraduate Student Assistant



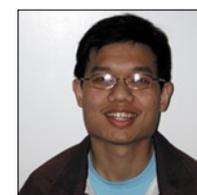
Jun Ding
Graduate Research Assistant



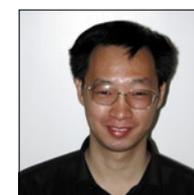
Brett Ellis
Senior Computer Systems Specialist



Teresa Finchum
Administrative Services Assistant



Thara Angskun
Graduate Research Assistant



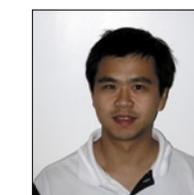
Zizhong Chen
Graduate Research Assistant



Jack Dongarra
Univ. Distinguished Professor



Lisa Ezzell
Administrative Support Assistant



Xiaoquan Fu
Graduate Research Assistant



Nikhil Bhatia
Graduate Research Assistant



Tom Cortese
Research Scientist
CE Onsite Lead



Brian Drum
Consultant



Graham Fagg
Research Associate Professor



Erika Fuentes
Graduate Research Assistant



George Bosilca
Senior Research Associate



David Cronk
Research Leader



Victor Eijkhout
Research Assistant Professor



Don Fike
Research Assistant



Edgar Gabriel
Senior Research Associate

ICL STAFF AND STUDENTS CONTINUED



Nathan Garner
Research Consultant



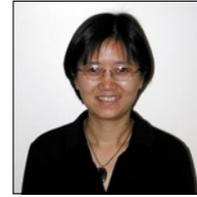
Jeff Larkin
Graduate Research Assistant



Eric Meek
consultant



Phil Mucci
Research Consultant



Mei Ran
Graduate Research Assistant



Keith Seymour
Senior Research Associate



Joe Thomas
Research Associate



Asim YarKhan
Senior Research Associate



Jan Jones
Publications Coordinator



Tracy Lee
Senior Budget Assistant



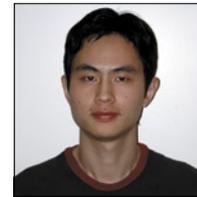
Shirley Moore
Associate Director



Paul Peltz
IT Administrator



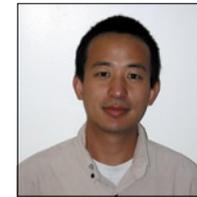
Ken Roche
Senior Research Associate



Zhiao Shi
Graduate Research Assistant



Michael Walters
Undergraduate Student
Assistant



Haihang You
Research Associate



Amanda Laake
Graduate Research Assistant



Kevin London
Research Assistant



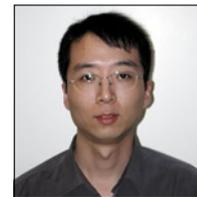
Keith Moore
Senior Research Associate



Jelena Pjesivac-Grbovic
Graduate Research Assistant



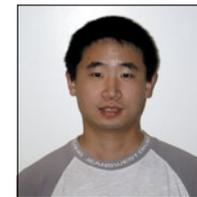
David Rogers
Graphic Designer



Fengguang Song
Graduate Research Assistant



Scott Wells
Assistant Director



Yuanlei Zhang
Graduate Research Assistant



Julien Langou
Senior Research Associate



Piotr Luszczek
Senior Research Associate



Terry Moore
Associate Director



Tracy Rafferty
Business Manager



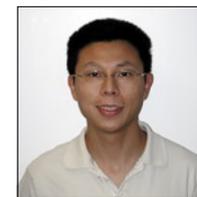
Kiran Sagi
Research Associate



Dan Terpstra
Research Leader



Felix Wolf
Senior Research Associate



Min Zhou
Graduate Research Assistant

RECENT VISITORS TO ICL

Javier Cuenca Universidad de Murcia – Spain	John Levesque Cray, Inc. – US
Thom Dunning Joint Institute for Computational Science – US	Mitsunori Miki Doshisha University – Japan
Shawn Ericson Joint Institute for Computational Science – US	Bernd Mohr John von Neumann Institut für Computing – Germany
Christoph Fabianek Vienna University of Technology – Austria	Jeff Nichols Oak Ridge National Laboratory – US
Patrick Geoffray Myricom, Inc. – US	Tom Rittenberry Silicon Graphics, Inc. – US
Tomo Hiroyasu Doshisha University – Japan	Carlos Rojas Silicon Graphics, Inc. – US
John Hurley Clark Atlanta University – US	Yusuke Tanimura Doshisha University – Japan
Ricky Kendall Ames Laboratory – US	Brian Worley Oak Ridge National Laboratory – US

ICL ALUMNI

Carolyn Aebischer 1990-1993	Adam Beguelin 1991	Greg Bunch 1995	Jin Ding 2003
Ed Anderson 1989-1991	Annamaria Benzoni 1991	Henri Casanova 1995-1998	Martin Do 1993-1994
Papa Arkhurst 2003	Scott Betts 1997-1998	Sharon Chambers 1998-2000	Leon Dong 2000-2001
Dorian Arnold 1999-2001	Noel Black 2003	Jaeyoung Choi 1994-1995	David Doolin 1997
Zhaojun Bai 1990-1992	Susan Blackford 1989-2001	Eric Clarkson 1998	Andrew Downey 1998 - 2003
Ashwin Balakrishnan 2001-2002	Fernando Bond 1999-2000	Andy Cleary 1995-1997	Mary Drake 1989-1992
Richard Barrett 1992-1994	Randy Brown 1997-1999	Jason Cox 1993-1997	Julio Driggs 2002 - 2003
Alex Bassi 2000-2001	Murray Browne 1998-1999	Cricket Deane 1998-1999	Zachary Eycler-Walker 1997-1998
Micah Beck 2000-2001	Antonin Bukovsky 1998 - 2003	Frederic Desprez 1994-1995	Markus Fischer 1997-1998

ICL ALUMNI CONTINUED

Lynn Gangwer 2000-2001	Weizhong Ji 1999-2000	Cindy Mitchell 2001 - 2002	Daisuke Takahashi 2002
Tracy Gangwer 1992-1993	Weicheng Jiang 1992-1995	Steven Moulton 1991-1993	Judi Talley 1993-1999
Kelley Garner 1998	Song Jin 1997-1998	Peter Newton 1994-1995	Keita Teranishi 1998
Jonathan Gettler 1996	Balajee Kannan 2001	Caroline Papadopoulos 1997-1998	John Thurman 1998-1999
Eric Greaser 1993	David Katz 2002	Leelinda Parker 2002	Francoise Tisseur 1997
Stan Green 1992-1996	Youngbae Kim 1992-1996	Antoine Petitot 1993-2001	Bernard Tourancheau 1993-1994
Hunter Hagewood 2000-2001	MyungHo Kim 1998	Roldan Pozo 1992-1994	Sathish Vadhiyar 1999 - 2003
Christian Halloy 1996-1997	Michael Kolatis 1993-1996	Tammy Race 1999-2001	Robert van de Geijn 1990-1991
Sven Hammarling 1996-1997	DongWoo Lee 2000 - 2002	Ganapathy Raman 1998-2000	Scott Venckus 1993-1995
Hidehiko Hasegawa 1995-1996	Todd Letsche 1993-1994	Kamesh Ramani 2003	Reed Wade 1990-1996
Satomi Hasegawa 1995-1996	Sharon Lewis 1992-1995	Yves Robert 1996-1997	R. Clint Whaley 1991-2001
Chris Hastings 1996	Xiang Li 2001	Tom Rothrock 1997-1998	Susan Wo 2000-2001
David Henderson 1999-2001	Weiran Li 2002	Tom Rowan 1993-1997	Tinghua Xu 1998-2000
Greg Henry 1996	Chaoyang Liu 2000	Evelyn Sams 1998-1999	Tao Yang 1999
Sid Hill 1996-1998	Matt Longley 1999	Farial Shahnaz 2001	Yong Zheng 2001
George Ho 1998-2000	Richard Luczak 2000-2001	Majed Sidani 1991-1992	Luke Zhou 2000-2001
Jeff Horner 1995-1999	Robert Manchek 1990-1996	Shilpa Singhal 1996-1998	
Yan Huang 2000-2001	Paul McMahan 1994-2000	Thomas Spencer 1999-2001	
Chris Hurt 2002	Jeremy Millar 1998-2002	Erich Strohmaier 1995-2001	
Paul Jacobs 1992-1995	Michelle Miller 1999 - 2003	Martin Swany 1996-1999	

HARDWARE



Keeping pace with scientific discovery in high performance computing (HPC) demands that we have access to a variety of hardware resources. Our ability to develop and test our efforts on the best equipment is one reason we are able to remain at the forefront of research in enabling technology. Here at ICL, we maintain systems ranging from individual desktops to large, networked clusters. In addition, we have the heterogeneous resources necessary to parallelize many applications that previously ran only sequentially.

The in-house computing systems on which we develop and test our ideas and applications include the following:

- Commodity-based Itanium clusters
- Compaq Alphas
- IBM Power 3s
- SGI Altix (32 processor)
- SGI Octane

As part of the CS department, we also retain access to additional resources including several server class machines and several HPC clusters. These clusters consist of multiple architectures including Itaniums, Itanium2s, Pentium IIIs, Pentium 4s, and AMD processors and comprise over 100 machines with various architectures ranging from Sun Enterprises and Quad PIIIs to dual P4s. Recently, we began working with the CS department to build a 64 node cluster consisting of 128 AMD Opteron 240s with two Gigabytes of memory



per node and a donated switch by Myricom. All of our clusters are arranged in the classic Beowulf configuration in which machines are connected by low latency, high-speed network switches.

Because of the many wonderful collaborations we have established around the country, we are granted remote access to many other HPC machines and architectures. Below are some of the systems that we currently have access to and use:

- Compaq SC40 and 45
- Cray T3E, SV1, SV1ex, and X1
- IBM SP, Power 3 and 4, and Cluster 1600
- Several large Linux Clusters
- SGI Origin 2000, 3000, 3800, 3900
- Sun E10000

Over the past year, we have also installed 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.

PARTNERS

ICL has enjoyed many working relationships with institutions all over the globe. The high performance computing (HPC) community consists of academic institutions, research centers, branches of the federal government, and various other public and private organizations, both domestic and international. The map on the next page shows the locations of our partners and collaborators. These solid partnership foundations have been instrumental in our growth and success and we are always eager to establish new relationships. Our mutually beneficial collaborative initiatives have strengthened our research efforts by allowing us to share both material and intellectual resources. 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 (formerly developed by Kuck and Associates) and the Vampir performance visualization and analysis tool (formerly developed by Pallas GmbH), The Mathworks, Inc. who develops Matlab, and Etnus, Inc., developer of the TotalView debugger.

DOMESTIC PARTNERS AND COLLABORATORS

Argonne National Laboratory	Microsoft Research
The Basic Linear Algebra Subprograms Technical Forum	MetaCenter Regional Alliance (MRA)
California Institute of Technology Center for Advanced Computing Research (CACR)	Morehouse College
The Computational Fluid Dynamics (CFD) Lab, UT College of Engineering	National Aeronautics and Space Administration (NASA)
Defense Advanced Research Projects Agency (DARPA)	National Computational Science Alliance (NCSA)
The United States Department of Defense (DoD)	National HPCC Software Exchange (NHSE)
The DoD High Performance Computing Modernization Program (DoD HPCMP)	National Institute of Standards and Technology (NIST)
The United States Department of Energy (DOE)	National Partnership for Advanced Computational Infrastructure (NPACI)
DOE2000	National Science Foundation (NSF)
Emory University	The Computer Science and Mathematics Division of Oak Ridge National Laboratory (ORNL CSMD)
Information Sciences Institute (ISI)	Rice University
International Business Machines (IBM)	San Diego Supercomputing Center (SDSC)
Intel Corporation	Silicon Graphics Incorporated (SGI)
Internet2	Sun Microsystems
The Internet2 Distributed Storage Infrastructure (I2-DSI)	University of California, Berkeley
Joint Institute for Computational Science (JICS)	University of California, San Diego
Lawrence Livermore National Laboratory (LLNL)	University of California, Santa Barbara
The Logistical Computing and Internetworking Laboratory (LoCI)	University of Kentucky
Los Alamos National Laboratory (LANL)	University of Tennessee Computer Science Department (UTK-CS)



ICL PARTNERS AND COLLABORATORS

INTERNATIONAL PARTNERS AND COLLABORATORS

Central Institute for Applied Mathematics (ZAM) - Research Centre Jülich Jülich, Germany	Laboratoire Réseaux Haut Débits et Support d'Applications Multimedia (RESAM) Lyon, France
Danish Computing Centre for Research and Education Lyngby, Denmark	Mathematical Institute, Utrecht University Netherlands
Dept. of Mathematical and Computing Sciences Tokyo Institute of Technology Tokyo, Japan	Monash University Melbourne, Australia
Department of Mathematics, University of Manchester Manchester, England	The Numerical Algorithms Group Ltd. Oxford, England
Doshisha University Kyoto, Japan	Parallel and HPC Application Software Exchange (PHASE) Tsukuba, Japan
Electrotechnical Laboratory, Computer Systems Division Tsukuba, Japan	Queensland Institute of Technology Brisbane, Australia
European Centre for Research and Advanced Training in Scientific Computing (CERFACS) Toulouse, France	Rutherford Appleton Laboratory Oxford, England
Fakultät für Mathematik und Informatik, Universität Mannheim Mannheim, Germany	École Polytechnique Fédérale de Lausanne Lausanne, Switzerland
Institut für Wissenschaftliches Rechnen, ETH Zentrum Zürich, Switzerland	Soongsil University Seoul, South Korea
Istituto per le Applicazioni del Calcolo "Mauro Picone" del C.N.R. Rome, Italy	Technische Universitaet Wien Vienna, Austria
Kasetsart University Bangkok, Thailand	University of Umeå Umeå, Sweden
Laboratoire de l'Informatique du Parallelisme, École Normale Supérieure de Lyon Lyon, France	

CENTERS OF EXCELLENCE



In 2003 the University of Tennessee's nine new Research Centers of Excellence (RCEs) completed their second year of operation. As part of a strategic effort to become one of America's top 25 public research universities, in 2000 the University began a five-year, \$335 million Tennessee Plan for Academic Excellence, including the establishment of nine new RCEs. These research centers of excellence — five in Knoxville and four at the Health Science Center in Memphis — promise to dramatically enhance the flow of research funding into the university, as well as impact the state's economy by creating new jobs and spawning new companies. The centers represent a \$280 million investment, including \$56 million from the university and the state with the balance primarily from grants. Below is a list of each of these centers (and their respective directors), including the Center for Information Technology Research (CITR), which is directed by Dr. Jack Dongarra and is co-located with ICL:

CENTERS BASED IN KNOXVILLE

Advanced Materials Center	Director: Dr. Ward Plummer
Center for Information Technology Research	Director: Dr. Jack Dongarra
Environmental Biotechnology Center	Director: Dr. Gary Saylor
Food Safety Center	Directors: Dr. Stephen P. Oliver & Dr. Ann Draughon
Structural Biology Center	Director: Dr. Engin Serpersu

CENTERS BASED IN MEMPHIS

Connective Tissues Diseases Center	Director: Dr. Andrew H. Kang
Genomics and Bioinformatics Center	Director: Dr. Dan Goldowitz
Neurobiology & Imaging of Brain Disease Center	Director: Dr. S. T. Kitai
Vascular Biology Center	Director: Dr. Lisa Jennings

BACKGROUND

CITR was established in the spring of 2001 with the goal to drive the growth and development of leading edge Information Technology Research (ITR) at the University of Tennessee. Information Technology Research (ITR) is a broad, multi-disciplinary area that investigates ways in which fundamental innovations in Information Technology affect, and are affected, by the research process.

The mission of CITR is to build up a thriving, well-funded community in basic and applied ITR at the University of Tennessee in order to help the University capitalize on the rich supply of research opportunities that now exist in this area. To carry out this mission, CITR has implemented a two pronged strategy: First, CITR is investing in a diverse group of ITR laboratories, each one led by an established researcher or an emerging leader in some significant area of ITR. Second, CITR is developing a complimentary set of university-wide programs that can serve to foster innovative research ideas in the University community, seed the creation of new CITR laboratories, and help the University exploit the broadest possible spectrum of ITR opportunities. In its second year of operation, CITR made major progress on both of these fronts.

CITR LABORATORIES

CITR is making strategic investments in several ITR Laboratories, targeting researchers with the potential for generating well-funded research and also with an eye toward diversifying the range of research opportunities and funding sources that UT can address. The first CITR laboratory, and the model for others, is the ICL. In addition to ICL, two more CITR Laboratories have been formed: The



CITR

Logistical Computing and Internetworking (LoCI) Lab, co-directed by Professors Micah Beck and Jim Plank from the Computer Science Department; and The Institute for Environmental Modeling (TIEM) run by Professor Lou Gross from the Departments of

Ecology and Evolutionary Biology and Mathematics. During the first two years of operation, CITR has generated more than \$17 million in new research funding, the vast majority of it deriving from its investments in its laboratories.

UNIVERSITY WIDE PROGRAMS

CITR has created several university wide programs to complement its ITR laboratory thrust. The most significant program offers Challenge Grants to IT researchers who will be applying for agency funding in the near future. The goal of the Challenge Grant program is to provide UT faculty with seed money to support the pursuit of new funding opportunities in diverse areas of ITR. Challenge Grants represent an investment in the overall work of particular IT investigators or groups for a given year, an investment that can be used to hire a promising graduate student, support relevant travel, purchase special equipment, develop early prototypes, help in the proposal process, and so on. The Challenge Grants that have been awarded during the first two years have not only lead to successful research proposals of more than a million dollars, they have elicited successful new proposals from researchers who had previously been unfunded.

In addition, CITR provides start-up funding to support the recruitment of outstanding new faculty in different areas of ITR, scholarships to attract Ph.D. students of exceptional promise to UT, and supplemental funding for ITR related conferences at UT.

PUBLICATIONS

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/publications/>. Most of these are also downloadable.

2004
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Eidson, T., Dongarra, J., Eijkhout, V. "Applying Aspect-Oriented Programming Concepts to a Component-based Programming Model," *IPDPS 2003, Workshop on NSF-Next Generation Software*, Nice, France, April 22, 2003.

Fagg, G., Gabriel, E., Chen, Z., Angskun, T., Bosilca, G., Bukovsky, A., Dongarra, J. "Fault Tolerant Communication Library and Applications for High Performance Computing," *Los Alamos Computer Science Institute Symposium* (to appear), Santa Fe, NM, October 27-29, 2003.

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ICL CONTACT INFO

ADDRESS

Innovative Computing Laboratory
Suite 413
Computer Science Department
1122 Volunteer Blvd
University of Tennessee
Knoxville, TN 37996-3450

WEB SITE

<http://icl.cs.utk.edu/>

E - MAIL

icl@cs.utk.edu

PHONE

865-974-8295

FAX

865-974-8296

Innovative Computing Laboratory 2003-2004 Report

Edited by Scott Wells
Designed by David Rogers

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The University of Tennessee - Knoxville
EEO/Title IX/Section 504/ADA Statement

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UT does not discriminate on the basis of race, sex, or disability in the education programs and activities which it operates, pursuant to requirements of Title VI of the Civil Rights Act of 1964, Title IX of the Educational 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 or the Age Discrimination in Employment Act (ADEA), or any of the other above referenced policies should be directed to the Office of Diversity Resources and Educational Services (DRES), 1818 Lake Avenue, Knoxville, TN 37996-3560, telephone (865) 974-2498 (TTY available). Requests for accommodation of a disability should be directed to the ADA Coordinator at the Office of Human Resources Management, 600 Henley Street, Knoxville, TN 37996-4125.



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