INNOVATIVE COMPUTING LABORATORY

THE UNIVERSITY of TENNESSEE

2013/2014 REPORT

INNOVATIVE COMPUTING LABORATORY 2013/2014 REPORT

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FROM THE DIRECTOR

Jack Dongarra
DIRECTOR, ICL

A variety of factors, ranging from the ongoing struggles over the federal budget in Washington to the disruptive emergence of "Big Data" as a dominating issue for computational science, made 2013 both exceptionally challenging and exceptionally exciting for ICL. As we enter 2014, and ICL begins its twenty-fifth year at the University of Tennessee, this report gives us a chance to review the achievements of the year just past, highlighting the results of all the incredibly hard work that the talented people of ICL put in. It is one of the best ways I know of to prepare for what promises to be an equally remarkable year to come.

The chart of ICL alumni and the timeline of major ICL projects with which we traditionally begin our report is intended to serve as a reminder of the fact that we are building on the rich legacy left to us by the hundreds of remarkably creative and energetic people who have come through ICL over the years. The names of the projects that they have helped lead—PVM, MPI, LAPACK, ScaLAPACK, BLAS, ATLAS, Netlib, NHSE, TOP500, PAPI, NetSolve, Open-MPI, FT-MPI, the HPC Challenge, LINPACK, and the HPCG benchmark—are familiar to HPC users around the world. And the software that they have produced now provides critical research infrastructure for hundreds of thousands, if not millions, of users.

In recent years, our efforts to build on this legacy have focused on finding new solutions to the daunting problems posed by the ongoing revolution in processor design and extreme-scale system architecture. In 2013, we developed successful proposals and funded new projects along this line in all of ICL's core research areas: the NSF is supporting innovative research in the area of software autotuning (BEAST); the DOE awarded research projects (PaRSEC and

ARGO) in distributed computing and exascale operating systems; and the Department of Defense is now funding ICL research (CoDAASH) in advanced performance monitoring. But beyond the more purely research efforts, it was also very gratifying to receive support, via the NSF's highly competitive Software Infrastructure for Sustained Innovation (SI2) program, for the SILAS and ADAPT projects, which focus on translating the results of our leading edge research into deployment-ready software infrastructure for computational science. I am confident that all these efforts will add substantially to the reputation we have been building since ICL's earliest days—doing original and first-rate Computer Science research that becomes software, which benefits scientific computing generally.

This past year also saw the advent of what one has to regard as a new era of "Big Data." This fact was reflected in three very different facets of ICL's work in 2013. First, on the research front, ICL joined the SciDB project of the Intel Science and Technology Center (ISTC) for Big Data, which is a collaboration between MIT and the Intel Parallel Computing Laboratory. For SciDB, we are providing expertise in both linear algebra for HPC and fault-tolerant distributed computing to solve the problems of doing high-performance data analytics in parallel databases. Second, as our contribution to the HPC community's exascale computing initiative, we helped to stage and lead the first international Big Data and Extreme-scale Computing (BDEC) workshop in Charleston, SC. The initial meeting in a series of at least three workshops, the BDEC represents a further, big-data-driven evolution of the International Exascale Software Project (IESP), in which we also played a major role over the past four years. Finally, as the educational side of ICL's mission, we began discussions with UT colleagues and administrators to transform our IGMCS graduate program into a true interdisciplinary PhD program. Surprisingly however, it appears that the IGMCS is on track to spawn not one, but two interdisciplinary PhDs: one in computational science and engineering, and one in data analytics. Prior to the Big Data tsunami of 2012 and 2013, it is far more likely that we would have seen just the former, but not the latter.

So the stage is set for what promises to be a very exciting and rewarding year for ICL, both in its main areas of research and in its work to grow and strengthen UTK and its broader community. During these exciting times, I am grateful to our sponsors for their continued support for our efforts. My special thanks and congratulations go to the ICL staff and students for their skill, dedication, and tireless efforts to make ICL one of the best centers in the world for scientific computing technologies.

– Jack Dongarra

INTRODUCTION

The Innovative Computing Laboratory (ICL) is a large Computer Science research and development group situated in the heart of the University of Tennessee's Knoxville campus. ICL's mission is to establish and maintain the University of Tennessee as a world leader in advanced scientific and high performance computing through research, education, and collaboration.

ICL's founder, Dr. Jack Dongarra, established the lab in 1989 when he received a dual appointment as a Distinguished Professor at UTK and as a Distinguished Scientist at Oak Ridge National Laboratory. Since then, ICL has grown into an internationally recognized research laboratory, specializing in Numerical Linear Algebra, Distributed Computing, and Performance Evaluation and Benchmarking. The lab now employs nearly forty researchers, students, and staff, and has earned many accolades, including four R&D100 awards.

Claxton Building
HOME OF ICL

HISTORY

KEY ICL RESEARCH PROJECTS

1989 PVM, Level 3 BLAS
1992 LAPACK, BLACS
1993 TOP500
1994 MPI
1995 ScaLAPACK
1997 NetSolve, ATLAS, RIB
1999 PAPI, HARNESS
2000 HPL
2002 FT-MPI, GCO
2003 LAPACK for Clusters, HPC Challenge
2006 Open MPI, FT-LA
2008 PLASMA, MAGMA
2009 Blackjack, MuMMI
2010 DPLASMA
2011 PULSAR
2012 PaRSEC
2013 BEAST, HPCG

SELECTED ICL ALUMNI

1991-1992 Adam Beguelin — SENSR.NET
1995-1996 Sven Hammarling — NUMERICAL ALGORITHMS GROUP
2004-2007 Alfredo Buttari — CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE
1991-2001 Clint Whaley — LOUISIANA STATE UNIVERSITY
1995-1998 Henri Casanova — UNIVERSITY OF HAWAII, MANOA
2003-2004 Edgar Gabriel — UNIVERSITY OF HOUSTON
2006-2008 Karl Fuerlinger — LUDWIG-MAXIMILIANS-UNIVERSITY MUNICH
1989-2001 Susan Blackford — CSP, INC.
1994-2009 Keith Seymour
1992-2005 Victor Eijkhout — UNIVERSITY OF TEXAS, AUSTIN
1992-1995 Jaeyoung Choi — SOONGSIL UNIVERSITY, KOREA
1996-2001 Dorian Arnold — UNIVERSITY OF NEW MEXICO
2004-2009 Haihang You — NATIONAL INSTITUTE FOR COMPUTATIONAL SCIENCES
1993-2001 Antoine Petitet — ESI GROUP, FRANCE
2003-2006 Julien Langou — UNIVERSITY OF COLORADO, DENVER
1989-1991 Ed Anderson — EPA
1996-2006 Graham Fagg — MICROSOFT
1991-1994 Roldan Pozo — NIST
1995-2001 Erich Strohmaier — LAWRENCE BERKELEY NATIONAL LABORATORY
2003-2006 Felix Wolf — JÜLICH SUPERCOMPUTING CENTRE
1992-1994 Richard Barrett — SANDIA NATIONAL LABORATORIES
1996-1997 Yves Robert — ENS-LYON, FRANCE
2009 Emmanuel Agullo — INRIA, FRANCE
1989-1990 Zhaojun Bai — UNIVERSITY OF CALIFORNIA, DAVIS
1995-1996 Greg Henry — INTEL
1999-2003 Sathish Vadhiyar — INDIAN INSTITUTE OF SCIENCE, INDIA
1990-1996 Bob Manchek — STRATUS TECHNOLOGIES
1999-2010 David Cronk — LOCKHEED-MARTIN
1990-1991 Robert van de Geijn — UNIVERSITY OF TEXAS, AUSTIN
1995-1996 Andy Cleary — AMAZON
2001-2006 Zizhong (Jeffrey) Chen — UNIVERSITY OF CALIFORNIA, RIVERSIDE
2008-2011 Hatem Ltaief — KAUST, SAUDI ARABIA
1993-1994 Bernard Tourancheau — UNIVERSITÉ JOSEPH FOURIER DE GRENOBLE, FRANCE
1994 Frederic Desprez — ENS-LYON, FRANCE
1999-2004 Ken Roche — UNIVERSITY OF WASHINGTON
1993-2012 Shirley Moore — UNIVERSITY OF TEXAS AT EL-PASO
1994-2004 Phil Mucci
1990-1996 Reed Wade — WETA DIGITAL
1997 Françoise Tisseur — MANCHESTER UNIVERSITY, ENGLAND

2013

2013 BY THE NUMBERS

61 PUBLICATIONS > PAGE 20

JOURNALS	17
CONFERENCE PROCEEDINGS	22
TECH REPORTS	16
BOOK CHAPTERS	6

CONFERENCES PARTICPATED IN > PAGE 22 **39**

SOFTWARE RELEASES **14**

STUDENTS ICL AND IGMCS
AS OF DECEMBER 2013

CURRENT ICL GRADUATE RESEARCH ASSISTANTS **9**

31 STUDENTS ENROLLED IN IGMCS

TOTAL IGMCS GRADUATES **40**

HIGHLIGHTS

For ICL, 2013 marks the 24th year of conducting innovative research in high performance computing and cyberinfrastructure, and the lab made significant contributions to the HPC community during the past year. The sections below illustrate ICL's commitment to excellence as well as set the bar for continued progress in our areas of research.

INDUSTRY EXCELLENCE

For years, ICL has been recognized by industry as a leader in information technology research. Vendors like NVIDIA and Intel regularly collaborate with the lab's research scientists, exchanging hardware and expertise, in an effort to improve both the hardware and software used in their products. These collaborations have led to very close working relationships and recognition of ICL's efforts among vendors.

NVIDIA CUDA Center of Excellence

ICL is part of a very small and select group of labs given a CUDA Center of Excellence (CCOE) designation. First awarded in 2009 and extended in 2013, UTK's CCOE focuses on the development of numerical linear algebra libraries for CUDA-based hybrid architectures. ICL's work on the Matrix Algebra on GPU and Multicore Architectures (MAGMA) project further enables and expands our CUDA-based software library efforts, especially in the area of high-performance scientific computing.

The CCOE designation also led to the establishment of a productive long-term collaboration between ICL and NVIDIA. As part of the collaboration and CCOE designation, ICL has continuously received hardware, financial support, and other resources from NVIDIA.

Intel Science and Technology Center for Big Data

ICL joined the SciDB project of the Intel Science and Technology Center (ISTC) for Big Data, one of a series of research collaborations that Intel is establishing with universities in the U.S. to identify and prototype revolutionary technology opportunities, and exchange expertise in various fields of high performance computing.

In the case of ICL, the lab will help improve the efficiency of large scale data analytics by providing efficient codes for linear algebra on the Intel Xeon Phi. The lab will also provide expertise on fault tolerance to help make the compute intensive portion of data management more resilient, which is essential given the large databases used in Big Data applications. Finally, the distributed nature of large data processing calls for optimal data distribution and redistribution operations, which has long been one of ICL's core strengths.

PHOTO Courtesy of Dirk Van den Poel

Jack Dongarra receiving the 2013 ACM-IEEE Ken Kennedy Award
NOVEMBER 2013

ACCOLADES

Hard work seldom goes unnoticed, and in 2013 members of the ICL team earned several awards in recognition of the lab's research efforts and history of excellence.

ACM-IEEE Ken Kennedy Award

On November 19th, Jack Dongarra received the ACM-IEEE Ken Kennedy Award at an SC13 ceremony in Denver, Colorado. The award recognizes Jack for his leadership in designing and promoting standards for mathematical software used to solve numerical problems common in HPC, and for his work in the development of major software libraries that boost performance and portability in HPC environments.

Best Paper at IPDPS

On May 23rd, ICL's Ichitaro Yamazaki and his co-authors were presented with a best paper award for their entry in the 27th IEEE International Parallel & Distributed Processing Symposium (IPDPS) in Boston, Massachusetts.

The paper, "Implementing a Blocked Aasen's Algorithm with a Dynamic Scheduler on Multicore Architectures," describes the authors' experiments, which show that the Blocked Aasen's algorithm has the potential to be the first scalable and provably stable algorithm for solving dense symmetric indefinite problems.

Illinois Institute of Technology's Professional Achievement Award

On April 19th, Jack Dongarra received a Professional Achievement Award from the Illinois Institute of Technology (IIT). Dr. Dongarra graduated from IIT with an MS in Computer Science in 1973, and was among four winners of this year's IIT Professional Achievement Award, which honors IIT alumni whose achievements in their fields have brought great distinction to themselves as well as credit to IIT.

"For influential contributions to mathematical software, performance measurement, and parallel programming, and significant leadership and service within the HPC community."

RESEARCH

Increased efforts to keep pace with the evolution in HPC hardware and software represent unique challenges that only a handful of enabling technology researchers are capable of addressing successfully. Our cutting-edge research efforts of the past have provided the foundation for addressing these challenges and serve as catalysts for success in our ever growing research portfolio. Our vision, our expertise, our determination, and our track record continue to position ICL as a leader in academic research.

What originally began more than 20 years ago as in-depth investigations of the numerical libraries that encode the use of linear algebra in software, has grown into an extensive research portfolio. We have evolved and expanded our research agenda to accommodate the aforementioned evolution of the HPC community, which includes a focus on algorithms and libraries for multicore and hybrid computing. As we have gained a solid understanding of the challenges presented in these domains, we have further expanded our research to include work in performance evaluation and benchmarking for high-end computers, as well as work in high performance parallel and distributed computing, with efforts focused on message passing and fault tolerance.

Demonstrating the range and diversity of our research, we will be engaged in more than 25 significant research projects during 2013-2014 across our main areas of focus. On the following pages, we provide brief summaries of some of our efforts in these research areas. For more detailed information about our research, visit our website – http://icl.utk.edu/.

NUMERICAL LINEAR ALGEBRA

Numerical Linear Algebra algorithms and software form the backbone of many scientific applications in use today. With the ever-changing landscape of computer architectures, such as the massive increase in parallelism and the introduction of hybrid platforms utilizing both traditional CPUs as well as accelerators, these libraries must be revolutionized in order to achieve high performance and efficiency on these new hardware platforms. ICL has a long history of developing and standardizing these libraries in order to meet this demand, and we have multiple projects under development in this arena.

ICL TEAM

Hartwig Anzt
Chongxiao Cao
Simplice Donfack
Tingxing Dong
Mark Gates
Azzam Haidar
Blake Haugen
Yulu Jia
Khairul Kabir
Jakub Kurzak
Julie Langou
Piotr Luszczek
Yves Robert
Stanimire Tomov
Ichitaro Yamazaki
Asim YarKhan

DISTRIBUTED COMPUTING

Distributed Computing is an integral part of the high performance computing landscape. As the number of cores, nodes, and other components in an HPC system continue to grow explosively, applications need runtime systems that can exploit all this parallelism. Moreover, the drastically lower meantime to failure of these components must be addressed with fault tolerant software and hardware, and the escalating communication traffic that they generate must be addressed with smarter and more efficient message passing standards and practices. Distributed Computing research at ICL has been a priority for nearly two decades, and the lab has several projects in that arena under active development.

ICL TEAM

George Bosilca
Aurelien Bouteiller
Anthony Danalis
Peter Gaultney
Thomas Herault
Reazul Hoque
Thananon Patinyasakdikul
Wei Wu

PERFORMANCE EVALUATION AND BENCHMARKING

Performance Evaluation and Benchmarking are vital to developing science and engineering applications that run efficiently in an HPC environment. ICL's Performance Evaluation tools allow programmers to see the correlation between the structure of source/object code and the efficiency of the mapping of that code to the underlying architecture. These correlations are important for performance tuning, compiler optimization, debugging, and finding and correcting performance bottlenecks. ICL's benchmark software is widely used to determine the performance profile of modern HPC machines, and has come to play an essential role in the purchasing and management of major computing infrastructure by government and industry around the world.

ICL TEAM

Piotr Luszczek
Gabriel Marin
Heike McCraw
Shirley Moore
James Ralph
Dan Terpstra

ADAPT

Next-Gen Open MPI

The ADAPT project proposes to enhance, harden, and modernize the Open MPI library in the context of the ongoing revolution in processor architecture and system design. On the large systems, expected before the end of this decade, the degree of parallelism (intra and inter node) is expected to increase by several orders of magnitude (based on the IESP predictions). To efficiently handle such systems, MPI implementations will have to adopt more asynchronous and thread-friendly behaviors to perform better than they do on today's systems.

In this project we seek to create a viable foundation for a new generation of Open MPI components, which enables a rapid exploration of new physical capabilities, provides greatly improved performance portability, and works toward full interoperability between classes of components. ADAPT explores process placement, distributed topologies, file accesses, point-to-point and collective communications, and different approaches to fault tolerance.

ARGO

A new architecture for Exascale compting

The ARGO project is developing a new Exascale Operating System and Runtime (OS/R) designed to support extreme-scale scientific computation. Disruptive new computing technologies, such as 3D memory, ultra-low-power cores, and embedded network controllers, are changing the scientific computing landscape. As it becomes clear that incremental approaches to operating systems and runtimes (OS/R) cannot grow into an Exascale solution, we propose a novel radical approach.

ARGO is designed on an agile, new modular architecture that supports both global optimization and local control. It aims to efficiently leverage new chip and interconnect technologies while addressing the new modalities, programming environments, and workflows expected at Exascale. It is designed from the ground up to run future HPC applications at extreme scales.

BEAST

Bench-testing Environment for Automated Software Tuning

> FIND OUT MORE AT http://icl.utk.edu/beast/

The objective of the Bench-testing Environment for Automated Software Tuning (BEAST) project is to embrace the nature of accelerators, such as Graphics Processing Units (GPUs) from NVIDIA and AMD, and Xeon Phi coprocessors from Intel, which offer an order of magnitude more computing power and an order of magnitude more memory bandwidth than standard processors, and create an unprecedented opportunity for breakthroughs in science and engineering.

Accelerators are a different kind of beast when it comes to performance tuning, and their architectural features usually pose unique programming challenges. For example, accelerators have massive numbers of simple cores, with static pipelines, and no branch prediction, and a multitude of constraints that can obliterate performance in numerous situations. BEAST allows a user to write high performance kernels in a tunable manner, sweep through a large search space, collect massive amounts of performance data, and plow through that data with machine learning techniques. These features enable a user to optimize code to the metal, without descending into the dark abyss of assembly programming.

CoDAASH

Co-design Approach for Advances in Software and Hardware

The Co-design Approach for Advances in Software and Hardware (CoDAASH) project focuses on understanding the relationship between algorithms and hardware platforms and how to jointly optimize the software and hardware in order to achieve efficient implementations for materials science applications. CoDAASH is a joint effort between the University of Tennessee, the University of Texas, El Paso, and the University of California, San Diego, and is funded by the United States Air Force Office of Scientific Research (AFOSR).

One of the project milestones focuses on expressing certain computational chemistry algorithms in the form of a data flow graph (DAG) and subsequently mapping the DAG representation of the kernels to the hardware platforms. This representation allows capturing the essential properties of the algorithm and its data dependencies in order to provide a true picture of the relationship between the algorithm and the architecture. For the definition of the dependencies as well as the management and scheduling of the tasks, the PaRSEC runtime is successfully employed, and extended. In CoDAASH's first year, a new machine named "Bolt" was acquired and installed specifically for this work. This resource provides an excellent testbed for the architectural experimentation needed for CoDAASH research.

DOD PETTT CREATE

High-Performance Numerical Libraries with Support for Low-Rank Matrix Computations

The main objective of the High-Performance Numerical Libraries with Support for Low-Rank Matrix Computations project is to reinforce a number of hybrid finite element/boundary integral analysis codes with high-performance numerical libraries that will enable them to efficiently use current and upcoming heterogeneous multi/many-core CPU and GPU-based architectures. The applications of interest use matrix compression techniques to reduce the complexity in both computer memory and computations. The compression techniques use adaptive cross approximation and SVD approaches that lead to low-rank matrix computations. Matrix factorizations and system solvers are similar to non-compressed methods except that the underlying matrix computations are performed in low-rank form.

ICL's work on this project focuses on the development of GPU algorithms, and their CUDA/OpenCL implementations for the required low-rank matrix computations, as well as the high level factorizations and solvers that will support matrix compression through the newly developed low-rank matrix computations. Of interest are factorizations and solvers for dense matrices, and multi-frontal methods for sparse matrices.

DPLASMA

Distributed Parallel Linear Algebra Software for Multicore Architectures

> FIND OUT MORE AT http://icl.utk.edu/dplasma/

The Distributed Parallel Linear Algebra Software for Multicore Architectures (DPLASMA) package is the leading implementation of a dense linear algebra package for distributed heterogeneous systems. It is designed to deliver sustained performance for distributed systems where each node features multiple sockets of multicore processors, and if available, accelerators like GPUs or Intel Xeon Phi. DPLASMA achieves this objective through the state-of-the-art PaRSEC runtime by leveraging the Parallel Linear Algebra Software for Multicore Architectures (PLASMA) algorithms on the distributed memory realm.

In addition to traditional ScaLAPACK data distribution, DPLASMA provides interfaces for users to expose arbitrary tile distributions. The algorithms transparently operate on local data, or introduce implicit communications to resolve dependencies, removing the burden of initial data re-shuffle, and providing to the user a novel approach to address load balance.

EASIR

Extreme-scale Algorithms and Solver Resilience

The mission of the Extreme-scale Algorithms and Solver Resilience (EASIR) project is to close the performance gap between the peak capabilities of HPC hardware and the performance realized by high performance computing applications. To carry out this mission, the EASIR project team develops architecture-aware algorithms and libraries, and the supporting runtime capabilities, to achieve scalable performance and resilience on heterogeneous architectures.

The project team includes personnel from Oak Ridge National Laboratory, Sandia National Laboratories, University of Illinois, University of California Berkeley, and the University of Tennessee (ICL). ICL's efforts focus on providing components and services in a vertically integrated software stack, from low-level runtime process and thread scheduling to multicore aware library interfaces, multicore dense linear algebra, scalable iterative methods, and advanced parallel algorithms that break traditional parallelism bottlenecks.

FT-LA

Fault Tolerant Linear Algebra

> FIND OUT MORE AT http://icl.utk.edu/ft-la/

The Fault Tolerant Linear Algebra (FT-LA) research effort is aimed at understanding and developing Algorithm Based Fault Tolerance (ABFT) into major dense linear algebra kernels. With distributed machines currently reaching up to 300,000 cores, fault-tolerance has never been so paramount. The scientific community has to tackle process failures from two directions: first, efficient middleware needs to be designed to detect failures, and second, the numerical applications have to be flexible enough to permit the recovery of the lost data structures.

At ICL, we have successfully developed Fault Tolerant MPI (FT-MPI) middleware and, more recently, an FT-LA library that will efficiently handle several process failures. The project team has also integrated FT-LA in the CIFTS (Coordinated Infrastructure for Fault Tolerant Systems) environment to provide better communication and fault management between the system's software components and scientific applications. Future work in this area involves the development of scalable fault-tolerant, one-sided (Cholesky, LU, and QR) and two-sided (Hessenberg, tri-diagonalization, and bi-diagonalization) factorizations, following the ABFT principles.

FutureGrid

A distributed testbed for parallel, grid, and cloud computing

> FIND OUT MORE AT http://portal.futuregrid.org/

FutureGrid is a distributed computing infrastructure that uses the nation's high performance research networks to create a wide area testbed for developing and testing novel approaches to parallel, grid, and cloud computing. In order to present a homogeneous resource to users, FutureGrid uses virtualization technology to create a cloud computing environment that applications can access and utilize in a uniform way. FutureGrid partners are deploying different kinds of high performance computing clusters at their sites and connecting them to XSEDE — the Extreme Science and Engineering Discovery Environment, funded by the NSF and based at NCSA. XSEDE, which is a follow-on to the TeraGrid project, is the NSF's newest national cyberinfrastructure for scientific research.

ICL is contributing to the project in the areas of performance measurement and application benchmarking, which pose very difficult problems for virtualized environments like FutureGrid. Recent releases of PAPI, since version 5.0, also known as PAPI-V, provide support for virtual and cloud environments, and have been deployed both on physical hardware for FutureGrid and in virtual space. For application benchmarking, ICL's Grid Benchmark Challenge effort applies the principles behind the HPC Challenge to assess virtualization overheads in controlled benchmarking scenarios.

G8 ECS

Enabling Climate Simulation at Extreme Scale

The objective of the G8 Enabling Climate Simulation at Extreme Scale (G8 ECS) project is to investigate how climate scientists can efficiently run climate simulations on future Exascale systems. Exascale supercomputers will appear in 2018–2020 featuring a hierarchical design, and will utilize hundreds of millions of computing cores. The numerical models of the physics, chemistry, and biology affecting the climate system need to be improved to run efficiently on these massive systems.

This project gathers top minds in climate research and computer science to focus on the challenges in resilience, performance, and scalability when running these simulations at extreme scale. The project team includes personnel from the University of Illinois at Urbana-Champaign, University of Tennessee (ICL), University of Victoria, the German Research School for Simulation Sciences, INRIA, Barcelona Supercomputing Center, Tokyo Institute of Technology, and the University of Tsukuba. ICL's main role in the ECS project is moving widely used climate model code toward Exascale, starting with node level performance and scalability, and then application resilience.

GridPAC

The Grid with Power-Aware Computing

> FIND OUT MORE AT http://icl.utk.edu/gridpac/

The Grid with Power-Aware Computing (GridPAC) project is a collaborative effort between the University of Texas Arlington, University of Florida, Virginia Tech, and the University of Tennessee, Knoxville, that develops resource management systems for energy and performance optimization on computational grids.

UTK/ICL's contribution to this project is in designing and implementing scalable, high performance tiled linear algebra applications for heterogeneous and dynamic architectures. These linear algebra applications generate large-scale workflows instantiated as task-DAGs with data dependencies linking the tasks. UTK/ICL designed and experimented with several execution environments for scheduling and executing the generated workflows. The end architectures included GPUs, shared-memory multicore machines, and distributed-memory environments. The energy footprint of these tiled linear algorithms was compared to standard approaches on multicore architectures using PowerPack instrumentation.

HPCC

HPC Challenge

> FIND OUT MORE AT http://icl.utk.edu/hpcc/

The HPC Challenge (HPCC) benchmark suite is designed to establish, through rigorous testing and measurement, the bounds of performance on many real-world applications for computational science at extreme scale. To this end, the benchmark includes a suite of tests for sustained floating point operations, memory bandwidth, rate of random memory updates, interconnect latency, and interconnect bandwidth. The main factors that differentiate the various components of the suite are the memory access patterns that, in a meaningful way, span the memory utilization space of temporal and spatial locality. The components of the suite are brought together inside HPCC, which allows information to pass between the components and provide a comprehensive testing and measurement framework that goes beyond the sum of its parts.

Each year, the HPCC Awards competition features contestants who submit performance numbers from the world's largest supercomputer installations, as well as alternative implementations that use a vast array of parallel programming environments. Results from the competition are announced at the annual Supercomputing Conference, and are available to the public to help track the progress of both the high-end computing arena and the commodity hardware segment.

HPCG

The HPC Preconditioned Conjugate Gradient Benchmark

The HPC Preconditioned Conjugate Gradient (HPCG) benchmark is designed to measure performance that is representative of modern HPC capability by simulating patterns commonly found in real science and engineering applications based on sparse iterative solvers. HPCG exhibits the same irregular accesses to memory and fine-grain recursive computations that dominate large-scale scientific workloads used to simulate complex physical phenomena. Intended as a candidate for a new HPC metric, HPCG implements the preconditioned conjugate gradient method with a local symmetric Gauss-Seidel preconditioner.

HPCG 1.0 was released on November 19, 2013, and coincided with the SC13 conference in Denver, Colorado. This initial release code includes both testing and verification of the run, and allows users to supply optimized kernels for computationally intensive portions of the code. The community's reception of the benchmark has been overwhelmingly positive, and the constant feedback feeds the continuous improvement of the code and its scope. Future releases will include additional refinements that allow HPCG to reflect the behavior of multigrid solvers.

HPL

High Performance LINPACK Benchmark

> FIND OUT MORE AT http://icl.utk.edu/hpl/

The High Performance LINPACK (HPL) benchmark is a software package that solves a (randomly generated) dense linear system in double precision (64-bit) arithmetic on distributed-memory computers. Written in a portable ANSI C and requiring an MPI implementation as well as either the BLAS or VSIPL library, HPL is often one of the first programs to run on large computer installations, producing a result that can be submitted to the biannual TOP500 list of the world's fastest supercomputers.

HPL 2.1, released in 2012, includes several major bug fixes and accuracy enhancements based on user feedback. The major focus of HPL 2.1 is to improve the accuracy of reported benchmark results, and ensure scalability of the code on large supercomputer installations with hundreds of thousands of computational cores. The new version also features detailed time-of-run accounting to help with assessing power requirements at the time of execution, a metric which has been reported with TOP500 results since 2007 and is also highlighted on the Green500 list. In 2011, the LINPACK benchmark app for iOS achieved performance of over 1 gigaflop/s on an Apple iPad 2, with per-Watt performance easily beating supercomputing solutions, including the most power-efficient systems based on hardware accelerators.

Keeneland

Bringing emerging hardware architectures to the open science community

> FIND OUT MORE AT http://keeneland.gatech.edu/

Keeneland is a five-year, $12 million cyberinfrastructure project, awarded in 2009 under the NSF's Track 2D program, designed to bring emerging hardware architectures to the open science community. ICL partnered with project leader Georgia Tech, as well as Oak Ridge National Laboratory, UT's National Institute for Computational Sciences, Hewlett-Packard, and NVIDIA, to develop and deploy Keeneland's innovative and experimental system.

As part of our contribution, ICL performed education and outreach activities, developed numerical libraries to leverage the power of NVIDIA's CUDA-based GPUs used in the Keeneland machine, and teamed up with early adopters to map their applications to the Keeneland architecture. In 2012, the Keeneland Full Scale (KFS) system was accepted by the NSF and went into production. KFS is a ~615 Teraflop, 264-node HP SL250 system with 528 Intel Sandy Bridge CPUs and 792 NVIDIA M2090 graphics processors, connected by an InfiniBand FDR network.

LAPACK

Linear Algebra PACKage

> FIND OUT MORE AT http://www.netlib.org/lapack/

ScaLAPACK

Scalable LAPACK

> FIND OUT MORE AT http://www.netlib.org/scalapack/

The Linear Algebra PACKage (LAPACK) and Scalable LAPACK (ScaLAPACK) are widely used libraries for efficiently solving dense linear algebra problems. ICL has been a major contributor to the development and maintenance of these two packages since their inception. LAPACK is sequential, relies on the BLAS library, and benefits from the multicore BLAS library. ScaLAPACK is parallel distributed and relies on BLAS, LAPACK, MPI, and BLACS libraries.

LAPACK 3.5.0 was released in November 2013. LAPACK 3.5.0 includes Symmetric/Hermitian LDLT factorization routines with rook pivoting algorithms, 2-by-1 CSD to be used for tall and skinny matrices with orthonormal columns, and new stopping criteria for balancing. Since 2011, LAPACK has included LAPACKE, a native C interface for LAPACK developed in collaboration with INTEL, which provides NAN check and automatic workspace allocation. There were two new LAPACK releases in 2012 (3.4.1 and 3.4.2) for minor bug fixes. ScaLAPACK 2.0.0, which includes the MRRR algorithm and new Nonsymmetric Eigenvalue Problem routines, was released in November 2011. Two additional ScaLAPACK versions (2.0.1 and 2.0.2) were released in 2012 for minor bug fixes.

MAGMA

Matrix Algebra on GPU and Multicore Architectures

> FIND OUT MORE AT http://icl.utk.edu/magma/

Matrix Algebra on GPU and Multicore Architectures (MAGMA) is a collection of next generation linear algebra (LA) libraries for heterogeneous architectures. The MAGMA package supports interfaces for current LA packages and standards, e.g., LAPACK and BLAS, to allow computational scientists to easily port any LA-reliant software components to heterogeneous architectures. MAGMA allows applications to fully exploit the power of current heterogeneous systems of multi/many-core CPUs and multi-GPUs/coprocessors to deliver the fastest possible time to accurate solution within given energy constraints.

MAGMA 1.4 features top performance and high accuracy LAPACK compliant routines for multicore CPUs enhanced with NVIDIA GPUs. The MAGMA 1.4 release includes more than 320 routines, covering one-sided dense matrix factorizations and solvers, two-sided factorizations and eigen/singular-value problem solvers, as well as a subset of highly optimized BLAS for GPUs. MAGMA provides multiple precision arithmetic support (S/D/C/Z, including mixed-precision). All algorithms are hybrid, using both multicore CPUs and GPUs. Support for AMD GPUs (OpenCL) and Intel Xeon Phi Coprocessors is provided correspondingly in the clMAGMA 1.1 and MAGMA MIC 1.1 releases.

MuMMI

Multiple Metrics Modeling Infrastructure

> FIND OUT MORE AT http://icl.utk.edu/mummi/

The Multiple Metrics Modeling Infrastructure (MuMMI) project is developing a framework to facilitate systematic measurement, modeling, and prediction of performance, power consumption, and performance-power tradeoffs for applications running on multicore systems. MuMMI combines UTK's PAPI hardware performance monitoring capabilities with Texas A&M's Prophesy performance modeling interface and Virginia Tech's Power-Pack power-performance measurement and analysis system.

PAPI has been integrated with Power-Pack and Prophesy, and performance and power consumption data have been collected for a range of benchmarks and applications running on multicore systems. Recent research activities at UTK have focused on extending PAPI power measurement to new architectures such as Intel Xeon Phi, and on integrating MuMMI power measurements with the Score-P measurement infrastructure.

Open MPI

Open source MPI

> FIND OUT MORE AT http://icl.cs.utk.edu/open-mpi/

The Open MPI Project is an open source Message Passing Interface (MPI) implementation that is developed and maintained by a consortium of academic, research, and industry partners. MPI primarily addresses the message-passing parallel programming model, in which data is moved from the address space of one process to that of another process through cooperative operations on each process. Open MPI integrates technologies and resources from several other projects (HARNESS/FT-MPI, LA-MPI, LAM/MPI, and PACX-MPI) in order to build the best MPI library available. A completely new MPI-2.2 compliant implementation, Open MPI offers advantages for system and software vendors, application developers, and computer science researchers.

ICL's efforts in the context of Open MPI have significantly improved its scalability, performance on many-core environments, and architecture-aware capabilities, such as adaptive shared memory behaviors and dynamic collective selection, making it ready for the next generation exascale challenges.

PAPI

The Performance API

> FIND OUT MORE AT http://icl.utk.edu/papi/

The Performance API (PAPI) has become the de facto standard within the HPC community for providing access to the hardware performance counters found on modern high performance computing systems. Provided as a linkable library or shared object, PAPI can be called directly in a user program, or used transparently through a variety of third party tools. Architecturally, PAPI provides simultaneous access to both on-processor and off-processor counters and sensors. PAPI continues to be ported to the architectures of greatest interest to the high performance computing community, including heterogeneous computing systems and virtual computing environments. Industry liaisons with Cray, Intel, IBM, NVIDIA, and others ensure seamless integration of PAPI with new architectures at or near their release. For example, close collaboration with IBM engineers allowed full PAPI support of the IBM Blue Gene/Q architecture when it was released, and collaboration with Intel engineers ensured full support for PAPI on the Intel Xeon Phi architecture.

Now supporting component technology, PAPI can measure performance beyond just the CPU. Components are available for network counters, GPGPUs such as NVIDIA, system health monitoring, and power and energy measurement. Virtual PAPI, or PAPI-V—supported by NSF and VMware—has been supported since PAPI 5.0. This version of PAPI provides performance measurement standards in virtual environments, which are common in cloud computing. As power and energy consumption become an increasingly important aspect of high performance computing, PAPI is developing components to aid in their measurement. Recent versions of PAPI support measuring energy consumption on Intel Sandy Bridge and Ivy Bridge processors through the RAPL (Running Average Power Limit) interface, and power measurements are now possible through both a native and host-based power component for Intel Xeon Phi. Work is underway to support other methods for power and energy measurement as they become available. As the PAPI component ecosystem becomes more populated, performance tools that interface with PAPI automatically inherit the ability to measure these new data sources, usually with no changes at the user level. This provides a richer environment in which performance analysts can work.

PaRSEC

Parallel Runtime Scheduling and Execution Controller

> FIND OUT MORE AT http://icl.utk.edu/parsec/

The Parallel Runtime Scheduling and Execution Controller (PaRSEC) is a generic framework for architecture-aware scheduling and management of micro-tasks on distributed many-core heterogeneous architectures. Applications we consider are expressed as a Direct Acyclic Graph (DAG) of tasks, with edges designating data dependencies. DAGs are represented in a compact problem-size independent format that can be queried to discover data dependencies in a totally distributed fashion, a drastic shift from today's programming models, which are based on sequential flow of execution.

PaRSEC assigns computation threads to the cores, overlaps communications and computations, and uses a dynamic, fully-distributed scheduler based on architectural features such as NUMA nodes and algorithmic features such as data reuse. PaRSEC includes a set of tools to generate the DAGs and integrate them in legacy codes, a runtime library to schedule the micro-tasks on heterogeneous resources, and tools to evaluate and visualize the efficiency of the scheduling. Many dense and sparse linear algebra extensions have been implemented, and computational kernels have been re-implemented using PaRSEC, enabling better performance on distributed many-core systems.

PetaApps

A Petaflop Cyberinfrastructure for Computing Free Energy Landscapes of Macro-and Biomolecular Systems

The objective of the Petaflop Cyberinfrastructure for Computing Free Energy Landscapes of Macro-and Biomolecular Systems project is to develop an exascale cyberinfrastructure for the efficient calculation of free energy landscapes for complex macro-and bio-molecular systems. The project team plans to demonstrate its effectiveness by applying it to two outstanding science problems: conformations of a linker protein in solution and self-assembly of lipids. In the context of this project, we have begun investigating, implementing, and evaluating different approaches to improve the scalability and the resilience of the cyberinfrastructure software computing for free energy landscapes. Our efforts are aimed at two axes of research. On one side, we are analyzing the current scalability of the existing framework and potential ways to drastically improve it. On the other side, we are investigating the software needs in order to achieve a reasonable level of resilience in this cyberinfrastructure.

PLASMA

Parallel Linear Algebra Software for Multicore Architectures

> FIND OUT MORE AT http://icl.utk.edu/plasma/

The Parallel Linear Algebra Software for Multicore Architectures (PLASMA) package is a dense linear algebra package at the forefront of multicore computing, designed to deliver the highest possible performance from a system with multiple sockets of multicore processors. PLASMA achieves this objective by combining state-of-the-art solutions in parallel algorithms, scheduling, and software engineering. Currently, PLASMA offers a collection of routines for solving linear systems of equations, least square problems, eigenvalue problems, and singular value problems.

PLASMA relies on runtime scheduling of parallel tasks, which is based on the idea of assigning work to cores based on the availability of data for processing at any given point in time. The concept, which is sometimes called data-driven scheduling, is closely related to the idea of expressing computation through a task graph, often referred to as the DAG (Directed Acyclic Graph), and the flexibility of exploring the DAG at runtime.

PULSAR

Parallel Unified Linear Algebra with Systolic Arrays

> FIND OUT MORE AT http://icl.utk.edu/pulsar/

The objective of the Parallel Unified Linear Algebra with Systolic Arrays (PULSAR) project is to address the challenges of extreme scale computing by applying the dataflow principles of Systolic Array architectures. PULSAR's solution is a Virtual Systolic Array (VSA) architecture, where multidimensional virtual systolic arrays are designed for various scientific workloads and successively mapped to the hardware architecture by a virtualization layer with a substantial runtime component.

The PULSAR Runtime offers a complete API for building and executing a Virtual Systolic Array, which is a collection of Virtual Data Processors, connected with data channels, and communicating via packets. The runtime supports distributed memory systems with multicore processors, and relies on POSIX Threads (a.k.a., pthreads) for intra-node multithreading, and on the Message Passing Interface (MPI) for inter-node communication. Support for hardware accelerators, such as NVIDIA GPUs, AMD GPUs, and Intel Xeon Phi coprocessors, is planned in the near future.

QUARK

QUeuing And Runtime for Kernels

> FIND OUT MORE AT http://icl.utk.edu/quark/

The QUeuing And Runtime for Kernels (QUARK) provides a library that enables the dynamic execution of tasks with data dependencies in a multi-core, multi-socket, shared-memory environment. QUARK infers data dependencies and precedence constraints between tasks based on the way the data is used, and then executes the tasks in an asynchronous, dynamic fashion in order to achieve a high utilization of the available resources.

QUARK is designed to be easy to use, is intended to scale to large numbers of cores, and should enable the efficient expression and implementation of complex algorithms. The driving application behind the development of QUARK is the PLASMA linear algebra library, and the QUARK runtime contains several optimizations inspired by the algorithms in PLASMA.

SILAS

Sustained Innovation for Linear Algebra Software

The NSF funded project on Sustained Innovation for Linear Algebra Software (SILAS) updates two of the most widely used numerical libraries in the history of Computational Science and Engineering—LAPACK and ScaLAPACK. Working with partners at the University of California, Berkeley and the University of Colorado, Denver, ICL is using SILAS to enhance and harden these essential libraries for the ongoing revolution in processor architecture and system design.

SILAS is organized around three complementary objectives: 1) Wherever possible, SILAS delivers seamless access to the most up-to-date algorithms, numerical implementations, and performance, by way of the familiar Sca/LAPACK programming interface; 2) Wherever necessary, SILAS makes advanced algorithms, numerical implementations and performance capabilities available through new interface extensions; and 3) SILAS provides a well engineered conduit through which new discoveries at the frontiers of research in these areas can be channeled as quickly as possible to all the application communities.

SUPER

The Institute for Sustained Performance, Energy, and Resilience

> FIND OUT MORE AT http://super-scidac.org/

The Institute for Sustained Performance, Energy, and Resilience (SUPER), led by the University of Southern California, has organized a broad-based project involving several universities and DOE laboratories with expertise in compilers, system tools, performance engineering, energy management, and resilience to ensure that DOE's computational scientists can successfully exploit the emerging generation of high performance computing (HPC) systems.

SUPER is extending performance modeling and autotuning technology to heterogeneous and petascale computing systems, investigating application-level energy efficiency techniques, exploring resilience strategies for petascale applications, and developing strategies that collectively optimize performance, energy efficiency, and resilience. UTK work focuses on performance measurement, power and energy measurements, and resilience techniques for hard and soft errors.

TOP500

Ranking the 500 fastest computers in the world

> FIND OUT MORE AT http://top500.org/

Since 1993, a ranking of the top 500 fastest computers in the world has been compiled biannually with published results released in June and November. Each machine on the TOP500 is ranked based on performance results from running the computationally intensive High Performance LINPACK (HPL) benchmark developed by ICL.

While other benchmarks, including HPCC, have been developed to measure performance of HPC systems, the TOP500 still relies on the HPL benchmark and remains the de-facto ranking relied upon by commercial, industrial, government, and academic institutions. ICL continues to partner with NERSC/Lawrence Berkeley National Laboratory and the University of Mannheim, Germany to produce the rankings.

In June 2013, China's Tianhe-2 supercomputer took the #1 spot on the TOP500 at an astounding 33.86 petaflop/s, and maintained that position in November 2013. The surprise appearance of Tianhe-2, two years ahead of the expected deployment, marks China's first return to the #1 position since November 2010, when Tianhe-1A was the top system. Tianhe-2 has 16,000 nodes, each with two Intel Xeon Ivy Bridge processors and three Xeon Phi coprocessors for a combined total of 3,120,000 computing cores.

ULFM

User Level Failure Mitigation

> FIND OUT MORE AT http://fault-tolerance.org/

User Level Failure Mitigation (ULFM) is a set of new interfaces for MPI that enables Message Passing programs to restore MPI functionality affected by process failures. The MPI implementation is spared the expense of internally taking protective and corrective actions against failures. Instead, it reports operations whose completions were rendered impossible by failures.

Using the constructs defined by ULFM, applications and libraries drive the recovery of the MPI state. Consistency issues resulting from failures are addressed according to an application's needs and the recovery actions are limited to the necessary MPI communication objects. Therefore, the recovery scheme is more efficient than a generic, automatic recovery technique, and can achieve both goals of enabling applications to resume communication after failure and maintaining extreme communication performance outside of recovery periods.

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Evidence of our research and our contributions to the HPC community might be best exemplified by the numerous publications we produce every year. Here is a listing of our most recent papers, including journal articles, book chapters, and conference proceedings. Many of these are available for download from our website.

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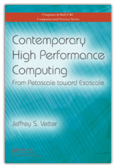

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2013 EVENTS

Every year, various members of our research staff regularly attend national and international conferences, workshops, and seminars. These meetings provide opportunities to present our research, share our knowledge, and exchange ideas with leading computational science researchers from around the world. Showing the work we have done and participating in the intellectual life of the scientific community in this way is an essential part of the research process. The following pages contain a list of events we have participated in over the past year.

JANUARY 25-27
Numerical Methods for PDEs
College Station, Texas

JANUARY 28-29
First ISTC Retreat
Santa Clara, CA

JANUARY 31
PetaApps Annual Meeting
Nashville, TN

FEBRUARY 25-1
SIAM CSE 2013
Boston, MA

MARCH 4-5
G8 ESC meeting
Boulder, CO

MARCH 5-6
ISAT Resilient Computing Frameworks Workshop
San Francisco, CA

MARCH 11-14
MPI Forum
Chicago, IL

MARCH 18-21
GPU Technology Conference (GTC) 2013
San Jose, CA

APRIL 1-5
Parallel Computational Technologies
Chelyabinsk, Russia

APRIL 4-5
SUPER All-hands Meeting
Houston, TX

APRIL 9-11
EASC2013: Solving Software Challenges for Exascale
Edinburgh, UK

APRIL 29 - MARCH 1
Big Data and Extreme-scale Computing (BDEC)
Charleston, SC

MAY 13-14
1st International Workshop on OpenCL (IWOCL)
Atlanta, GA

MAY 14-15
Thirty Years of Parallel Computing at Argonne: A Symposium
Chicago, IL

MAY 20-24
IEEE International Parallel and Distributed Processing Symposium (IPDPS)
Boston, MA

MAY 28-29
ExaOSR/Argo
Chicago, IL

JUNE 3-7
MPI Forum
San Jose, CA

JUNE 10-14
International Conference on Supercomputing
Eugene, OR

JUNE 16-20
2013 International Supercomputing Conference (ISC13)
Leipzig, Germany

JULY 17-18
VMware Academic Research Symposium
Palo Alto, CA

JULY 18-19
Code and Data Interoperability Workshop
Blacksburg, VA

JULY 20-21
MuMMI Annual Status Meeting
San Diego, CA

JULY 22-25
XSEDE 13 Conference
San Diego, CA

JULY 24-26
SciDAC-3 PI Meeting
Rockville, MD

AUGUST 22-23
MuMMI all-hands project meeting
Knoxville, TN

AUGUST 26
EuroPar 2013
Aachen, Germany

SEPTEMBER 8-11
10th International Conference on Parallel Processing and Applied Mathematics (PPAM 2013)
Warsaw, Poland

SEPTEMBER 14-15
CSCS-USI Autumn School on GPU-enabled Numerical Libraries
Lugano, Switzerland

SEPTEMBER 15
Algorithms and Scheduling Techniques for Exascale Systems
Wadern, Germany

SEPTEMBER 15-18
EuroMPI
Madrid, Spain

SEPTEMBER 18-19
SUPER All-hands meeting
Oakland, CA

SEPTEMBER 29
Automatic Application Tuning for HPC Architectures
Wadern, Germany

OCTOBER 1-4
International Conference on Parallel Processing (ICPP 2013)
Lyon, France

OCTOBER 9-11
Extreme Scale Research PI Meeting
Washington, DC

NOVEMBER 9
Drupal Camp Chattanooga 2013
Chattanooga, TN

NOVEMBER 17-20
Supercomputing 2013 (SC13)
Denver, CO

DECEMBER 5
Intel Big Data ISTC Year 2 Retreat
Santa Clara, CA

DECEMBER 9
MPI Forum Meeting
Chicago, IL

DECEMBER 9-12
2013 NLA-HPC
Hsinchu, Taiwan

Jack Dongarra at SC13
PHOTO Courtesy of Dirk Van den Poel

SC13
Denver, CO 2013

The annual **ACM/IEEE Supercomputing Conference (SC)**, established in 1988, is a staple of ICL's November itinerary. SC is vital to the growth and evolution of high performance computing in the United States because it is the only US event that elicits substantial participation from all segments of the HPC community, including hundreds of users, developers, vendors, research institutions, and representatives of government funding agencies. Such a talent-rich gathering enables participants to discuss challenges, share innovations, and coordinate relationships and collaborations with some of the best minds in scientific and high performance computing.

In November 2013, SC was held in scenic Denver, Colorado. As usual, ICL had a significant presence at SC, with faculty, research staff, and students giving talks, presenting papers, and leading "Birds-of-a-Feather" sessions. ICL's director and UT Distinguished Professor, Jack Dongarra, received the ACM-IEEE Ken Kennedy Award at SC13 for his extensive work and leadership in the HPC community.

The University of Tennessee's SC booth, which was organized and led by the National Institute for Computational Sciences, made a return trip for 2013, and was visually designed with the help of ICL/CITR staff, manned with support from ICL researchers attending SC, and featured the lab's research projects in the booth's kiosks.

COMPUTATIONAL RESOURCES

Titan, Cray XK7
OAK RIDGE NATIONAL LABORATORY

Kraken, Cray XT5
NATIONAL INSTITUTE FOR COMPUATIONAL SCIENCES

CAMPUS RESOURCES

To meet these challenges, ICL has access to multiple state-of-the-art heterogeneous systems in house. In fact, our hardware industry partners, including AMD, Intel, and NVIDIA, provide us with bleeding edge hardware resources (often under NDA and prior to public release) which we use to upgrade and maintain the lab's infrastructure. Our research staff also has access to other campus resources, including UTK's Newton Cluster.

Newton Cluster
UNIVERSITY OF TENNESSEE

As the new GPU hybrid computing paradigm leads the evolution of computational hardware into Petascale computing, computing architectures are increasingly changing. However, the programming tools, applications, and algorithms that form the backbone of the ever growing need for greater performance are equally as important. Such myriad hardware/software configurations present unique challenges that require testing and development of applications that are often unique to the platform on which they reside. For this reason, it is imperative that we have access to a wide range of computing resources in order to conduct our cutting-edge research.

LOCAL RESOURCES

ICL has access to many local resources in East Tennessee to help keep us at the forefront of enabling technology research, including some machines that are regularly found on the TOP500 list of the world's fastest supercomputers. The recent modernization of the DOE's National Center for Computational Sciences (NCCS), just 30 minutes away at the Oak Ridge National Laboratory (ORNL), has enabled us to leverage our ORNL collaborations to take advantage of what has become one of the world's fastest scientific computing facilities.

ORNL houses Titan, a Cray XK7 supercomputer, which currently holds the number two spot on the TOP500 at 17.59 petaflop/s. The National Institute for Computational Sciences (NICS), a joint UT/ORNL computing facility in Oak Ridge, houses Kraken, UT's Cray XT5 system which is one of the world's fastest open-science supercomputers. NICS is also home to Beacon, an Appro Xtreme-X Supercomputer which topped the Green500 list in November 2012, and held the number three spot in June 2013, making it one of the most energy efficient supercomputers in the world.

GRID RESOURCES

With the continuing trend of high performance grid and cloud computing, it is important for ICL to have access to these types of infrastructures in order to test and implement our software packages on grid hardware and virtualized environments. In keeping with this goal, research staff members at ICL have access to grid resources all over the US, as well as in Europe, including XSEDE, Grid5000, and FutureGrid.

Keeneland System Integrated with XSEDE
GEORGIA TECH

PARTNERSHIPS

Since 1989, ICL has fostered relationships with many other academic institutions and research centers. We have also aggressively sought to build lasting, collaborative partnerships with HPC vendors and industry research leaders, both here and abroad. Together with these partners, we have built a strong portfolio of shared resources, both material and intellectual. In this section, we recognize many of the partners and collaborators that we have worked with over the years, most of whom we are still actively involved with.

INDUSTRY

Vendors and industry research leaders are an integral part of our partnerships, contributing significantly to our efforts to be a world leader in computational science research. Many have utilized our work, including our linear algebra libraries and performance analysis tools. As a result of these exchanges, we maintain close working relationships with many industry leaders.

The Innovative Computing Laboratory (ICL) joins a very small and select group of labs given a **CUDA Center of Excellence** designation. UTK's CCOE focuses on the development of numerical linear algebra libraries for CUDA-based hybrid architectures. ICL's work on the Matrix Algebra on GPU and Multicore Architectures (MAGMA) project further enables and expands our CUDA-based software library efforts, especially in the area of high-performance scientific computing.

The CCOE designation also led to the establishment of a productive long-term collaboration between ICL and NVIDIA. As part of the collaboration and CCOE designation, ICL has continuously received hardware, financial support, and other resources from NVIDIA.

ICL joined the SciDB project of the **Intel Science and Technology Center (ISTC) for Big Data**, one of a series of research collaborations that Intel is establishing with universities in the U.S. to identify and prototype revolutionary technology opportunities, and exchange expertise in various fields of high performance computing.

In the case of ICL, the lab will help improve the efficiency of large scale data analytics by providing efficient codes for linear algebra on the Intel Xeon Phi. The lab will also provide expertise on fault tolerance to help make the compute intensive portion of data management more resilient, which is essential given the large databases used in Big Data applications. Finally, the distributed nature of large data processing calls for optimal data distribution and redistribution operations, which has long been one of ICL's core strengths.

GOVERNMENT & ACADEMIC

Our relationships with academic and government research institutions also play a pivotal role in our success. By exchanging ideas, expertise, and personnel, ICL becomes more dynamic with each new collaboration. Our lab routinely develops relationships with researchers whose primary focus is on other scientific disciplines, such as biology, chemistry, and physics, which makes many of our collaborations truly multidisciplinary.

Argonne NATIONAL LABORATORY
Georgia Tech
INDIANA UNIVERSITY
IOWA STATE UNIVERSITY
JICS Joint Institute for Computational Sciences
Lawrence Livermore National Laboratory
Los Alamos NATIONAL LABORATORY EST. 1943
LSU
NCSA
NICS NATIONAL INSTITUTE FOR COMPUTATIONAL SCIENCES
NIST
OAK RIDGE National Laboratory
RICE
SDSC SAN DIEGO SUPERCOMPUTER CENTER
Sandia National Laboratories
TEXAS A&M UNIVERSITY
Berkeley UNIVERSITY OF CALIFORNIA
UC RIVERSIDE UNIVERSITY OF CALIFORNIA
University of Colorado Denver
USC University of Southern California
UTEP
VirginiaTech

COLLABORATING INTERNATIONAL INSTITUTIONS

Barcelona Supercomputing Center
Barcelona, Spain

Central Institute for Applied Mathematics
Jülich, Germany

Consiglio Nazionale delle Ricerche
Rome, Italy

Danish Computing Center for Research and Education
Lyngby, Denmark

Doshisha University
Kyoto, Japan

École Normale Supérieure de Lyon
Lyon, France

École Polytechnique Federale de Lausanne
Lausanne, Switzerland

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

European Exascale Software Initiative
European Union

Forschungszentrum Jülich
Jülich, Germany

High Performance Computing Center Stuttgart
Stuttgart, Germany

INRIA
France

Institut ETH Zentrum
Zurich, Switzerland

Kasetsart University
Bangkok, Thailand

King Abdullah University of Science and Technology
Saudi Arabia

National Institute of Advanced Industrial Science and Technology (AIST)
Tsukuba, Japan

Parallel and HPC Application Software Exchange
Tsukuba, Japan

RIKEN
Wako, Japan

Rutherford Appleton Laboratory
Oxford, England

Soongsil University
Seoul, South Korea

Technische Universitaet Wien
Vienna, Austria

Tokyo Institute of Technology
Tokyo, Japan

Universität Mannheim
Mannheim, Germany

Université Claude Bernard de Lyon
Lyon, France

University of Manchester
Manchester, England

University of Umeå
Umeå, Sweden

LEADERSHIP

In addition to the development of tools and applications, ICL is regularly engaged in other activities and efforts that include our leadership at conferences and workshops, as well as our teaching and outreach. Having a leadership role in the HPC arena requires that ICL be engaged with the community, and actively share our vision for the exciting future of high performance computing. This section contains some of the activities in which we are participating or have a taken a leadership role.

CITR
CENTER FOR INFORMATION TECHNOLOGY RESEARCH

IGMCS

Addressing the need for a new educational strategy in Computational Science, the Center for Information Technology Research (CITR) worked with faculty and administrators from several departments and colleges in 2007 to help establish a new university-wide program that supports advanced degree concentrations in this critical new field across the curricula. Under the **Interdisciplinary Graduate Minor in Computational Science** (IGMCS), students pursuing advanced degrees in a variety of fields of science and engineering are 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.

Computational Science integrates elements that are normally studied in different parts of the traditional curriculum, but which are not fully covered or combined by any one of them. As computational power continues to increase and data storage costs decrease, the potential for new discoveries using Computational Science is greater than ever. And as more academic disciplines begin to realize and exploit the incredible benefits Computational Science provides, the IGMCS program is expected to grow by adding new disciplines, new courses, and new faculty. As of late 2013, there are 18 departments from four UT colleges contributing more than 130 courses to the program.

> FIND OUT MORE AT http://igmcs.utk.edu/

10^{18} BDEC
BIG DATA AND EXTREME-SCALE COMPUTING

The **Center for Information Technology Research** was established in 2001 to drive the growth and development of leading edge information technology research at the University of Tennessee. CITR's first objective is to build up a thriving, well-funded community in basic and applied information technology research at UT in order to help the university capitalize on the rich supply of research opportunities that now exist in this area. As part of this goal, CITR staff members currently provide primary administrative and technical support for ICL, helping maintain the lab's status as a world leader in high performance and scientific computing research. CITR has also provided secondary support for other UT research centers.

CITR's second objective is to grow an interdisciplinary Computational Science program as part of the university curriculum. To this end, CITR helped establish the Interdisciplinary Graduate Minor in Computational Science (IGMCS) to offer UT graduate students an opportunity to acquire the balanced package of knowledge and skills required for today's computationally intensive research methods. CITR is also the sole provider of administrative support for the IGMCS.

> FIND OUT MORE AT http://citr.cs.utk.edu/

This year, ICL was instrumental in organizing and staging the first **Big Data and Extreme-scale Computing** (BDEC) workshop, which took place at the end of April in Charleston, SC. This workshop, the first in a series, marks a distinctly new phase for the work of the International Exascale Software Project (IESP) community, which ICL also helped to organize and lead. Through four years and eight international workshops, the IESP brought together leaders from the HPC software research community in order to produce a plan for the IESP Roadmap for a common, high quality computational environment that future exascale supercomputers will require. Guided in some degree by the work of the IESP, the United States, the European Union, and Japan have, in the past three years, moved aggressively to develop their own plans for achieving exascale computing in the next decade. Now, with the launch of the BDEC, this same community turns its attention to the unprecedented problems of the emerging era of "Big Data," when every major field of science and engineering is producing and needs to analyze truly extraordinary amounts of data. The BDEC shares the general mission of the IESP—the co-design of software infrastructure for extreme scale science drawing on international cooperation—but it reframes the problems involved to fully take account of challenging workflow patterns that different research communities must create to work with both data and computing resources that are unprecedented in their scale. All the imposing design and development issues of creating an exascale-capable software stack remain. But the supercomputers that need this stack must now be viewed as the nodes (albeit the largest and most important nodes) in a very large network of computing resources that will be required to generate, collect, manipulate, transform, analyze, and collaboratively explore gigantic mountains of data.

BDEC Charleston Group Photo
APRIL 2013

Along with Jack, and following through with work they began with the IESP, several members of ICL's CITR staff, including Terry Moore, Tracy Rafferty, Teresa Finchum, and David Rogers, played essential roles in making the first BDEC workshop a major success. The next workshop is scheduled for Fukuoka, Japan, in late February. Given the ever increasing emphasis that science, government, and industry continue to place on both big data and extreme-scale computing, this example of ICL's community leadership seems likely to become more and more prominent.

> FIND OUT MORE AT http://exascale.org/

ICL Group
FALL 2013

PEOPLE

As the landscape in high performance computing continues to rapidly evolve, remaining at the forefront of discovery requires great vision and skill. To address this evolution and to remain a leader in innovation, we have assembled a staff of top researchers from all around the world who apply a variety of novel and unique approaches to the challenges and problems inherent in world-class scientific computing.

As part of an engineering college at a top 50 public research university, we have a responsibility to combine exemplary teaching with cutting-edge research. As such, we regularly employ bright and motivated graduate and undergraduate students. We have been, and will continue to be, very proactive in securing internships and assistantships for students who are hardworking and willing to learn.

CURRENT STAFF AND STUDENTS

Hartwig Anzt
POST DOCTORAL RESEARCH ASSOCIATE

George Bosilca
RESEARCH ASSISTANT PROFESSOR

Aurelien Bouteiller
RESEARCH SCIENTIST II

Chongxiao Cao
GRADUATE RESEARCH ASSISTANT

Sam Crawford
INFORMATION SPECIALIST I

Anthony Danalis
RESEARCH SCIENTIST II

Simplice Donfack
POST DOCTORAL RESEARCH ASSOCIATE

Tingxing Dong
GRADUATE RESEARCH ASSISTANT

Jack Dongarra
UNIVERSITY DISTINGUISHED PROFESSOR

Don Fike
IT SPECIALIST III

Teresa Finchum
ADMINISTRATIVE SPECIALIST II

Mark Gates
RESEARCH SCIENTIST I

Peter Gaultney
GRADUATE RESEARCH ASSISTANT

Azzam Haidar
RESEARCH SCIENTIST I

Blake Haugen
GRADUATE RESEARCH ASSISTANT

Thomas Herault
RESEARCH SCIENTIST II

Reazul Hoque
GRADUATE RESEARCH ASSISTANT

Yulu Jia
GRADUATE RESEARCH ASSISTANT

Khairul Kabir
GRADUATE RESEARCH ASSISTANT

Cindy Knisley
FINANCIAL SPECIALIST

CURRENT STAFF AND STUDENTS

Jakub Kurzak
RESEARCH DIRECTOR

Julie Langou
RESEARCH LEADER

Piotr Luszczek
RESEARCH DIRECTOR

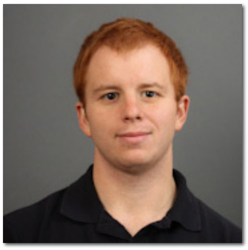
Gabriel Marin
RESEARCH SCIENTIST II

Heike McCraw
RESEARCH SCIENTIST II

Terry Moore
ASSOCIATE DIRECTOR

Thananon Patinyasakdikul
GRADUATE RESEARCH ASSISTANT

Tracy Rafferty
PROGRAM MANAGER



James Ralph
RESEARCH ASSOCIATE II

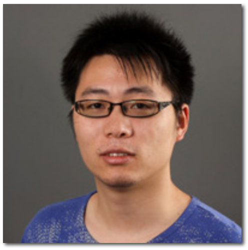
Yves Robert
VISITING SCHOLAR

David Rogers
IT SPECIALIST III

Leighanne Sisk
ADMINISTRATIVE SPECIALIST I

Dan Terpstra
RESEARCH LEADER II

Stanimire Tomov
RESEARCH DIRECTOR



Wei Wu
GRADUATE RESEARCH ASSISTANT

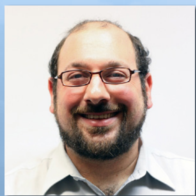
Ichitaro Yamazaki
RESEARCH SCIENTIST I

Asim YarKhan
SENIOR RESEARCH ASSOCIATE

2013 VISITORS

Since ICL was founded, we have routinely hosted many visitors, some who stay briefly to give seminars or presentations, and others who remain with us for as long as a year collaborating, teaching, and learning. By collaborating with researchers from around the globe, we are able to leverage an immense array of intellectual resources. For this reason, our list of research collaborators and partners continues to grow. These relationships present enormous opportunities to host and work with top minds within the global HPC community.

Emmanuel Agullo
INRIA
FRANCE



Vincent C. Betro
NICS

Mark Dean
EECS, UTK

Joseph Dobson
NAG
UK

Mathieu Faverge
UNIVERSITY OF BORDEAUX
FRANCE

Salvatore Filippone
UNIVERSITY OF ROME
TOR VERGATA, ITALY

Julien Herrmann
ENS-LYON
FRANCE

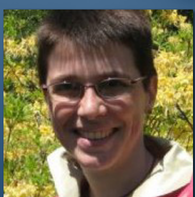
Matt Johnson
GARMIN

Rainer Keller
UNIVERSITY OF
STUTTGART, GERMANY

Julien Langou
UNIVERSITY OF COLORADO,
DENVER

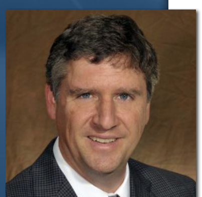
Jeff Larkin
NVIDIA

Dong Li
ORNL



Alisa Meador
CIE, UTK

Shirley Moore
UTEP



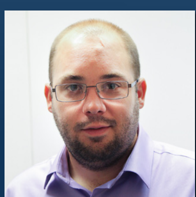
James Plank
EECS, UTK

Bhanu Rekepalli
NICS

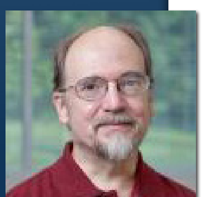
Amy Szczepanski
EECS/NICS

Michela Taufer
UNIVERSITY OF DELAWARE

Volodymyr Turchenko
TERNOPIL NATIONAL ECONOMIC
UNIVERSITY, UKRAINE



Jean-Chales Vasnier
ORNL



Patrick Worley
ORNL

Erlin Yao
CHINESE ACADAMY OF
SCIENCES, CHINA

Christal Yost
NICS

Haihang You
NICS

ALUMNI

Since its inception, ICL has attracted many students, post-doctoral researchers, and professors from a variety of backgrounds and academic disciplines. Many of these experts came to UT specifically to work with Dr. Dongarra, beginning a long list of top research talent to pass through ICL and move on to make exciting contributions at other institutions and organizations.

Carolyn Aebischer 1990-1993
Bivek Agrawal 2004-2006
Sudesh Agrawal 2004-2006
Emmanuel Agullo 2009
Ahmad Abdelfattah Ahmad 2012
Jennifer Allgeyer 1993
Wes Alvaro 2007-2011
Ed Anderson 1989-1991
Daniel Andrzejewski 2007
Thara Angskun 2003-2007
Hartwig Anzt 2011
Papa Arkhurst 2003
Dorian Arnold 1996-2001
Cedric Augonnet 2010
Marc Baboulin 2008
Zhaojun Bai 1990-1992
Ashwin Balakrishnan 2001-2002
Richard Barrett 1992-1994
Alex Bassi 2000-2001
David Battle 1990-1992
Micah Beck 2000-2001
Daniel Becker 2007
Dulceneia Becker 2010-2012
Adam Beguelin 1991
Annamaria Benzoni 1991
Tom Berry 1991
Vincent Berthoux 2010
Scott Betts 1997-1998
Nikhil Bhatia 2003-2005
Noel Black 2002-2003
Laura Black 1996
Susan Blackford 1989-2001
Kartheek Bodanki 2009
David Bolt 1991
Fernando Bond 1999-2000
Carolyn Bowers 1992
Barry Britt 2007-2009
Randy Brown 1997-1999
Cynthia Browne 2005
Murray Browne 1998-1999
Bonnie Browne 2011-2012
Antonin Bukovsky 1998-2003
Greg Bunch 1995
Alfredo Buttari 2004-2007
Giuseppe Bruno 2001
Anthony Canino 2012
Domingo Gimenez Canovas 2001
Henri Casanova 1995-1998
Cedric Castagnede 2012
Ramkrishna Chakrabarty 2005
Sharon Chambers 1998-2000
Zizhong Chen 2001-2006
Jaeyoung Choi 1994-1995
Wahid Chrabakh 1999
Eric Clarkson 1998
Andy Cleary 1995-1997
Michelle Clinard 1989-1991
Vincent Cohen-Addad 2012
Matthias Colin 2004
Charles Collins 2012
Stephanie Cooper 2011-2013
Tom Cortese 2002-2009
Camille Coti 2007
Jason Cox 1993-1997
David Cronk 1999 - 2010
Javier Cuenca 2003
Manoel Cunha 2006
Yuanshun Dai 2007-2013
Cricket Deane 1998-1999
Remi Delmas 2006
Frederic Desprez 1994-1995
Jin Ding 2003
Jun Ding 2001-2003
Ying Ding 2000-2001
Martin Do 1993-1994
Leon Dong 2000-2001
Nick Dongarra 2000
David Doolin 1997
Andrew Downey 1998-2003
Mary Drake 1989-1992
Julio Driggs 2002-2004
Brian Drum 2001-2004
Peng Du 2005-2012
Eduardo Echavarria 2005
Victor Eijkhout 1992-2005
Brett Ellis 1995-2005
Shawn Ericson 2004
Zachary Eyler-Walker 1997-1998
Lisa Ezzell 2003-2004
Christoph Fabianek 2003
Graham Fagg 1996-2006
Mathieu Faverge 2010-2012
Shengzhog Feng 2005-2006
Salvatore Filippone 2004
Anna Finchum 2010
Mike Finger 1997
Markus Fischer 1997-1998
Len Freeman 2009
Xiaoquan Fu 2003-2004
Erika Fuentes 2003-2007
Karl Fuerlinger 2006-2008
Megan Fuller 2006
Edgar Gabriel 2003-2004
Tracy Gangwer 1992-1993
Lynn Gangwer 2000-2001
Nathan Garner 2001-2006
Kelley Garner 1998
Tina Garrison 1991
Adriana Garties 2011
Christoph Geile 2008
Jean Patrick Gelas 2001
Boris Gelfend 1993
Jonathan Gettler 1996
Eric Greaser 1993
Stan Green 1992-1996
Alice Gregory 2004-2006
Jason Gurley 1997-1998
Bilel Hadri 2008-2009
Hunter Hagewood 2000-2001
Christian Halloy 1996-1997
Sven Hammarling 1996-1997
J. Mike Hammond 1994-1995
Satomi Hasegawa 1995-1996
Hidehiko Hasegawa 1995-1996
Chris Hastings 1996
David Henderson 1999-2001
Greg Henry 1996
Julien Herrmann 2011-2012
Holly Hicks 1993-1994
Alexandra Hicks-Hardiman 2009
Sid Hill 1996-1998
Tomoyuki Hiroyasu 2002-2003
George Ho 1998-2000
Josh Hoffman 2008-2010
Jeff Horner 1995-1999
Mitch Horton 2010-2012
Yan Huang 2000-2001
Aurelie Hurault 2009
Chris Hurt 2002
Paul Jacobs 1992-1995
Emmanuel Jeannot 2001-2006
Weizhong Ji 1999-2000
Weicheng Jiang 1992-1995
Song Jin 1997-1998
Patrick Johansson 2001
Aral Johnson 2009
Matt Johnson 2011-2013
Sean Jolly 1997-1998
Jan Jones 1992-2008
Kim Jones 1996-1997
Vijay Joshi 2011-2013
Venkata Kakani 2007
Ajay Kalhan 1995
Balajee Kannan 2001
Madhuri Kasam 2007-2008
Kiran Kasichayanula 2010-2012
Ajay Katta 2010
David Katz 2002
Joshua Kelly 2000-2001
Supriya Kilambi 2008

Myung Ho Kim 2005-2006
Youngbae Kim 1992-1996
Jenya Kirshtein 2008
Michael Kolatis 1993-1996
Chandra Krintz 1999-2001
Tilman Kuestner 2010
Krerkchai Kusolchu 2010
Coire Kyle 2005
Amanda Laake 2003-2004
Xavier Lacoste 2012
Julien Langou 2003-2006
Jeff Larkin 2003-2005
Brian LaRose 1990-1992
Frank Lauer 2010
DongWoo Lee 2000-2002
Tracy Lee 1996-2012
Klaudia Leja 2008
Pierre Lemarinier 2008-2010
Todd Letsche 1993-1994
Sharon Lewis 1992-1995
Xiang Li 2001
Yinan Li 2006-2008
Weiran Li 2002
Chaoyang Liu 2000
Kevin London 1996-2005
Matt Longley 1999
Hatem Ltaief 2008-2011
Daniel Lucio 2008
Richard Luczak 2000-2001
Teng Ma 2006-2012
Robert Manchek 1990-1996
Tushti Marwah 2004
Donald McCasland 1994
Paul McMahan 1994-2000
Eric Meek 2003-2006
James Meyering 1991-1992
Jeremy Millar 1998-2002
Michelle Miller 1999-2003
Cindy Mitchell 2001-2002
Stuart Monty 1993
Eric Moore 2000
Keith Moore 1987-2007
Shirley Moore 1993-2012
Robert Morgan 1990-1991
Kishan Motheramgari 1997
Steven Moulton 1991-1993
Phil Mucci 1994-2004
Daichi Mukunoki 2012
Matthew Nabity 2008
Shankar Narasimhaswami 2004-2005
Rajib Nath 2008-2010
Fernando Navarro 2009
Donnie Newell 2010
John Nelson 2011-2013
Peter Newton 1994-1995
Jonas Nilsson 2001
Jakob Oestergaard 2000
Caroline Papadopoulos 1997-1998
Leelinda Parker 2002
Dilip Patlolla 2007-2008
Andy Pearson 1989-1991
Paul Peltz 2003-2013
Theresa Pepin 1994
Antoine Petitet 1993-2001
Peter Pham 2012
Vlado Pjesivac 2008
Jelena Pjesivac-Grbovic 2003-2007
James S. Plank 1991-1992
Ciara Proctor 2008
Tim Poore 2009
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