

# INVOVATIVE COMPUTING LABORATORY 2017/2018 REPORT





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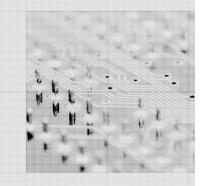
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#### ICL/FROM THE DIRECTOR



I began my director's letter last year by highlighting the striking success that the Innovative Computing Laboratory (ICL) enjoyed with our funded proposals to the Department of Energy's (DOE's) Exascale Computing Project (ECP). Success, of course, has its consequences. This year, many of the highlights of 2017 revolve around our efforts to engage productively in ECP: staffing up to do the work of our seven ECP projects, engaging with ECP's complex management system, setting out our milestones, working to establish the necessary collaborations with other groups, and starting to design and actually write the software we proposed. As the review process that we recently underwent has shown, we are off to a very good start, and so I want to express my thanks to all of you who have contributed to that effort.

Last year I attributed our achievement with ECP funding to two factors: ICL's strong reputation for turning innovative software research into productionquality software, and the sustained improvement over time in our capacity to develop clear and compelling proposals. This year I think that actually working with ECP has brought out another impressive strength of our group—namely, the remarkable level of mature professionalism that we now bring to our collaborations. In the context of ECP, I have seen that professionalism in the way we have been able to scout, evaluate, and recruit the new people we need; in the thoroughgoing preparation for and execution of our management responsibilities; in the mentoring that our senior leadership has provided to our students and new research staff; and—simply—in the general way that ICL people comport themselves in all the different venues and activities in which we are involved. Naturally, I find the many positive comments I get from my colleagues and friends about the quality of our group's professionalism very gratifying.

But even though ECP demanded the lion's share of our attention in 2017, we still managed to have an excellent year in funding for creative new projects with the National Science Foundation (NSF). Our distributed computing group had an especially successful year, picking up two significant additions in the areas of runtime systems and software resilience: the Enhancing the Open MPI Software for Next Generation Architectures and Applications (Evolve) project, a collaboration with ICL alumnus Edgar Gabriel at the University of Houston; and the Cross-layer Application-Aware Resilience at Extreme Scale (CAARES) project, a collaboration with Barbara Chapman from Stony Brook University and Manish Parashar from Rutgers University. Our linear algebra team also made important progress in the critical new area of "batched" algorithms and routines by winning software infrastructure funding for the MAtrix, TEnsor, and Deep-learning Optimized Routines (MATEDOR) project. Finally, with the Highly Parallel Algorithms and Architectures for Convex Optimization for Real-time Embedded Systems (CORES) project, we established a valuable new collaboration with Saeid Nooshabadi of Michigan Tech in the area of performance optimization for embedded systems.

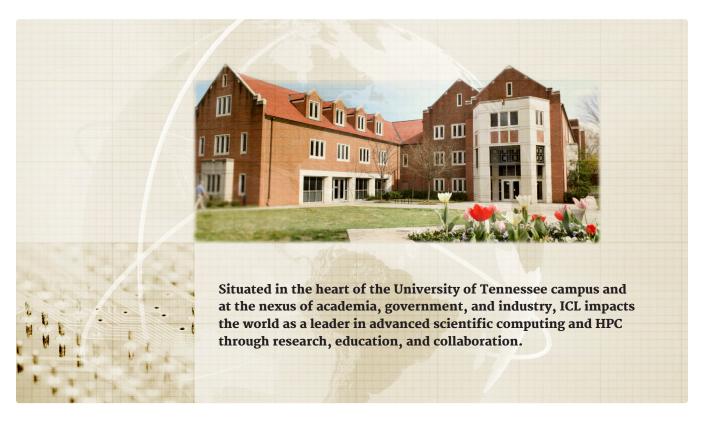
In 2017, we were also able to strengthen our foundation on the University of Tennessee, Knoxville (UTK) campus in two significant ways. First, five of ICL's Research Directors—Jakub Kurzak, George Bosilca, Heike Jagode, Piotr Luszczek, and Stan Tomov—were each raised to the level of Research Assistant Professor. This means, among other things, that they can be authorized to direct theses and dissertations, and we are currently working to establish that authorization for them in 2018. This new mode of productive engagement with UTK students is another sign of ICL's maturity and will clearly be a very positive development for us. Second, with the establishment of the "Jack

Dongarra Endowed Professorship in High-Performance Computing" in UTK's Department of Electrical Engineering and Computer Science this year, we also helped the department recruit Professor Michela Taufer, an outstanding high-performance computing (HPC) researcher from the University of Delaware, to fill it. She will join the Department of Electrical Engineering and Computer Science faculty this summer, and I expect that we will be able to start collaborating with her almost immediately. Her presence at UTK is precisely the kind of development we need to move our work to the next level.

So, given our progress in 2017, we are very much on track to enhance that record and to accomplish great things in 2018 and beyond. Of course, as always, to achieve such goals we will need to work hard—especially by finding productive ways to engage with important ECP application groups. But my sense of our creativity, commitment, and solid professionalism gives me every confidence that we are well positioned to succeed—not only with ECP, but in all those projects that our many sponsors have chosen to support. And as ever, I continue to be amazed at and deeply appreciative of the skill, dedication, and tireless efforts that the researchers, staff, and students of ICL put into their work. They have helped to make ICL and UTK one of the premier centers in the world today for high-performance and scientific computing.

Jack Dongarra
DIRECTOR, ICL

# ICL/INTRODUCTION



The unique challenges of today's computational research are characterized by large datasets and the need for greater performance, energy conservation, and resilience. ICL's cutting-edge efforts, which now span more than 25 years, have evolved and expanded with the agility and focus required to address those challenges. ICL's work encompasses a solid understanding of the algorithms and libraries for multi-core, many-core, and heterogeneous computing, as well as performance evaluation and benchmarking for high-end computing. In addition, ICL's portfolio of expertise includes high-performance parallel and distributed computing, with keen attention to message passing and fault tolerance.

The tools and technologies that ICL designs, develops, and implements play a key role in supercomputing-based discoveries in areas like life sciences, climate science, earthquake prediction, energy exploration, combustion and turbulence, advanced materials science, drug design and more.

#### **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.

#### **PERFORMANCE ANALYSIS** 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 enable 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.

#### DISTRIBUTED COMPUTING



Distributed computing is an integral part of the HPC 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 two decades, and the lab has numerous projects in this arena under active development.

# **ICL/HISTORY**

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 (ORNL). Since then, ICL has grown into an internationally recognized research laboratory, specializing in numerical linear algebra, distributed computing, and performance evaluation and benchmarking.

#### 1989

The Level-3 **Basic Linear Algebra Subprograms (BLAS)** specification was developed to perform assorted matrix-multiplication and triangular-system computations.

The Parallel Virtual Machine (PVM) was a software tool for parallel networking of computers designed to allow a network of heterogeneous Unix and Windows machines to be used as a single distributed parallel processor.

#### 1992

Basic Linear Algebra Communication Subprograms (BLACS) was created to make linear algebra applications easier to program and more portable.

Still developed today, the **Linear Algebra Package (LAPACK)** is a standard software library for numerical linear algebra.

#### 1995

Version 1.0 of the **Scalable LAPACK (ScaLAPACK)** library, which includes a subset of LAPACK routines redesigned for distributed memory multiple instruction, multiple data (MIMD) parallel computers, was released.

#### 1997

Automatically Tuned Linear Algebra Software (ATLAS) was an instantiation of a new paradigm in high-performance library production and maintenance developed to enable software to keep pace with the incredible rate of hardware advancement inherent in Moore's Law.

**NetSolve (GridSolve)** was a clientserver system that enabled users to solve complex scientific problems remotely.

#### 1999

The Heterogeneous Adaptable Reconfigurable Networked SystemS (HARNESS) was a pluggable, lightweight, heterogeneous distributed virtual machine (DVM) environment.

#### 2002

Fault Tolerant MPI (FT-MPI) was an MPI plugin for HARNESS that provided support for fault-tolerant applications crucial for large, long-running simulations.

#### 2003

HPC Challenge was developed for the Defense Advanced Research Projects Agency (DARPA) and consisted of four benchmarks: HPL, Streams, RandomAccess, and PTRANS.

LAPACK for Clusters was developed in the framework of self-adapting numerical software to leverage the convenience of existing sequential environments bundled with the power and versatility of highly tuned parallel codes executed on clusters.

#### 2006

Fault-Tolerant Linear Algebra (FT-LA) is a research effort to develop and implement algorithm-based fault tolerance in commonly used dense linear algebra kernels.

#### 2008

Parallel Linear Algebra Software for Multicore Architectures (PLASMA)

is a dense linear algebra package designed to deliver the highest possible performance from a system of multiple sockets of multi-core processors.

#### 2009

The International Exascale Software Project (IESP) brought together representatives of the global HPC community to plan and create a new software infrastructure for the extremescale systems that represent the future of computational science.

#### 2010

Distributed Parallel Linear Algebra Software for Multicore Architectures (DPLASMA) is a linear algebra package that enables sustained performance for distributed systems, where each node features multiple sockets of multi-core processors and, if applicable, accelerators like GPUs or Intel Xeon Phi.

#### 2011

The Parallel Ultra Light Systolic Array Runtime (PULSAR) project developed a simple programming model for large-scale, distributed-memory machines with multi-core processors and hardware accelerators to automate multithreading, message passing, and multistream multi-GPU programming.

#### 2013

The Big Data and Extreme-scale Computing (BDEC) workshop was initiated to map out and account for the ways in which the major issues associated with Big Data intersect with national (and international) plans being laid out for achieving exascale computing.

The Bench-testing Environment for Automated Software Tuning (BEAST) project enables writing of tunable high-performance kernels by unleashing the

power of heuristic autotuning.

The High Performance Conjugate Gradients (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.

#### 2014

**Argo** is an initiative to develop a new exascale operating system and runtime (OS/R) designed to support extremescale scientific computation.

#### 2015

The **SparseKaffe** project establishes fast and efficient sparse direct methods for platforms with multi-core processors with one or more accelerators.

The Task-based Environment for Scientific Simulation at Extreme Scale (TESSE) used an application-driven design to create a general-purpose software framework focused on programmer productivity and portable performance for scientific applications on massively parallel hybrid systems.

#### 2016

ICL won seven awards through DOE's Exascale Computing Project (ECP) during the fall of 2016 and is the lead institution on four of these projects:

The **Distributed Tasking for Exascale** (**DTE**) project will extend the capabilities of the PaRSEC framework.

The Exascale Performance Application Programming Interface (Exa-PAPI) project builds on PAPI-EX and extends it with performance counter monitoring capabilities for new and advanced ECP

hardware and software technologies.

#### 1993

Now on its 50th list, **TOP500** was launched to improve and renew the Mannheim supercomputer statistics, which—at the time—had been in use for seven years.

#### 1994

Version 1.0 of a standardized and portable message-passing system, called the Message Passing Interface (MPI), was released.

#### 1999

Still in active development, the **Performance Application Programming Interface (PAPI)** is a standardized, easy-to-use interface that provides access to hardware performance counters on most major processor platforms.

#### 2000

High-Performance Linpack (HPL) Benchmark is a benchmark for distributed-memory computers that solves a (random) dense linear system in double-precision (64-bit) arithmetic.

#### 2006

Four institutions merged efforts in the **Open Source Message Passing Interface (Open MPI)**: FT-MPI from UTK/ICL, LA-MPI from Los Alamos National Laboratory, and LAM/MPI from Indiana University, with contributions from the PACX-MPI team at the University of Stuttgart.

#### 2008

Matrix Algebra on GPU and Multicore Architectures (MAGMA) is a linear algebra library that enables applications to exploit the power of heterogeneous systems of multi/many-core CPUs and multi-GPUs/coprocessors.

#### 2012

and Execution Controller (PaRSEC) provides a generic framework for architecture-aware scheduling and management of microtasks on distributed, many-core heterogeneous architectures.

The Parallel Runtime Scheduling

#### 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.

#### 2014

The Rapid Python Deep Learning Infrastructure (RaPyDLI) delivered productivity and performance to the deep learning community by combining high-level Python, C/C++, and Java environments with carefully designed libraries supporting GPU accelerators and Intel Xeon Phi coprocessors.

#### 2015

**PAPI-EX** extends PAPI with measurement tools for changing hardware and software paradigms.

**Data-driven Autotuning for Runtime Execution (DARE)** provides application-level performance tuning capabilities to the end user.

#### 2016

The Production-ready, Exascaleenabled Krylov Solvers for Exascale Computing (PEEKS) project will explore the redesign of solvers and extend the DOE's Extreme-scale Algorithms and Solver Resilience (EASIR) project. The Software for Linear Algebra Targeting Exascale (SLATE) project will converge and consolidate previous ICL efforts with LAPACK and ScaLAPACK into a dense linear algebra library that will integrate seamlessly into the ECP ecosystem.

#### SELECTED ICL ALUMNI

Throughout its history, ICL has attracted numerous postdoctoral researchers and professors from multiple disciplines. Many of these experts came to UTK specifically to work with Dr. Dongarra. This list features ICL alumni who played key roles in the establishment and growth of ICL and went on to build distinguished careers at other organizations and institutions.

Emmanuel Agullo

Ed Anderson
Environmental Protection Agency

Thara Angskun Suranaree University of Technology

> Dorian Arnold Emory University

Zhaojun Bai University of California, Davis

Richard Barrett
Sandia National Laboratories

Adam Beguelin
Sensr.net

Susan Blackford CSP, Inc.

Alfredo Buttari
Institut de Recherche en Informatique
de Toulouse

Henri Casanova University of Hawaii, Manoa

**Zizhong Chen** University of California, Riverside

> Jaeyoung Choi Soongsil University

Andy Cleary
Amazon

David Cronk Leidos

Frederic Desprez

Victor Eijkhout University of Texas, Austin

Graham Fagg

Mathieu Faverge

Karl Fuerlinger Ludwig Maximilian University of Munich

Edgar Gabriel
University of Houston

Sven Hammarling
University of Manchester

Greg Henry

Julien Langou University of Colorado, Denver

Kevin London

Hatem Ltaief
King Abdullah University of Science
and Technology

Bob Manchek Akamai Technologies

Keith Moore
Independent Consultant

Shirley Moore Oak Ridge National Laboratory

Antoine Petitet
Huawei Technologies

Roldan Pozo
National Institute of Standards and
Technology

Yves Robert École normale supérieure de Lyon

Kenneth Roche
University of Washington

Erich Strohmaier Lawrence Berkeley National Laboratory

> Martin Swany Indiana University

Dan Terpstra Living Waters for the World

Françoise Tisseur University of Manchester

Bernard Tourancheau Université Joseph Fourier de Grenoble

Sathish Vadhiyar Indian Institute of Science

Robert van de Geijn University of Texas, Austin

Reed Wade

Vince Weaver University of Maine

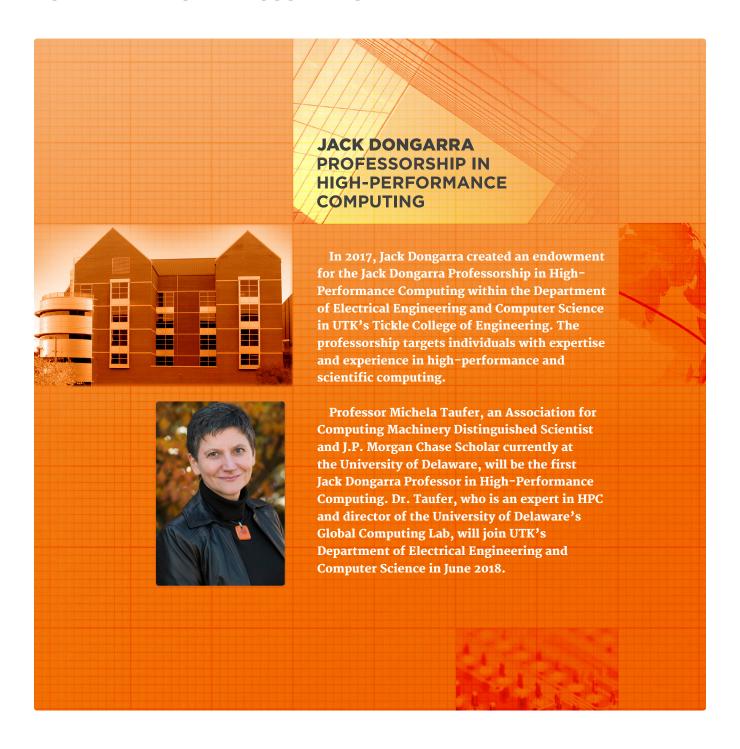
Clint Whaley Indiana University

Felix Wolf
Technische Universität Darmstadt

Haihang You Chinese Academy of Sciences

# **ICL/2017 HIGHLIGHTS**

#### **ACHIEVEMENTS AND ACCOLADES**





#### **BEST PAPER**

On June 2, 2017, ICL Research Scientist Ichitaro Yamazaki traveled to Orlando, Florida to present his paper, "Improving Performance of GMRES by Reducing Communication and Pipelining Global Collectives," at the 18th IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC 2017), where it received the workshop's Best Paper Award.

The work outlined in the paper compared and combined two techniques to improve the parallel scalability of the Krylov subspace projection methods: a communication-avoiding technique and a communication-hiding technique. As the cost of communication continues to increase with scale, such techniques are expected to be critical on emerging extremescale supercomputers. These algorithms are being implemented in ICL's Production-ready, Exascale-Enabled Krylov Solvers for Exascale Computing (PEEKS) effort—part of DOE's ECP—to enable application scientists to take full advantage of exascale supercomputers.

Yamazaki, I., M. Hoemmen, P. Luszczek, and J. Dongarra, "Improving Performance of GMRES by Reducing Communication and Pipelining Global Collectives," The 18th IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC 2017), Best Paper Award, Orlando, FL, June 2017.



## INTEL PARALLEL COMPUTING CENTER

The Intel Parallel Computing Center (IPCC) program—composed of universities, institutions, and labs that are leaders in their field—focuses on modernizing applications to increase parallelism and scalability through optimizations that leverage the cores, caches, threads, and vector capabilities of microprocessors and coprocessors.

As part of this effort, ICL will develop and optimize numerical linear algebra libraries and technologies for emerging HPC applications while also tackling current challenges in Intel® Xeon Phi<sup>™</sup> coprocessor-based HPC applications. In collaboration with Intel's Math Kernel Library (MKL) team, ICL will modernize the LAPACK and ScaLAPACK libraries to run efficiently on current and future many-core architectures and will disseminate the developments through the open-source MAGMA library.



#### NVIDIA GPU CENTER OF EXCELLENCE

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

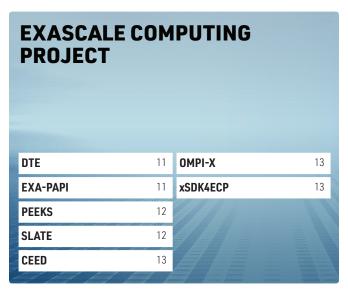
The GPU COE designation also led to the establishment of a productive long-term collaboration between ICL and NVIDIA. As part of the collaboration and GPU COE designation, ICL has continuously received hardware, financial support, and other resources from NVIDIA.

# ICL/RESEARCH

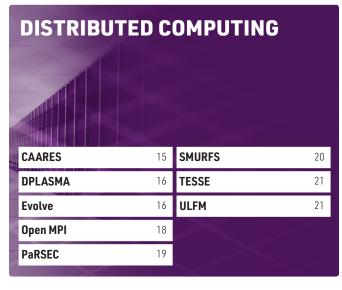
What originally began nearly 30 years ago as in-depth investigations of the numerical libraries that encode the use of linear algebra in software has grown into an extensive research portfolio.

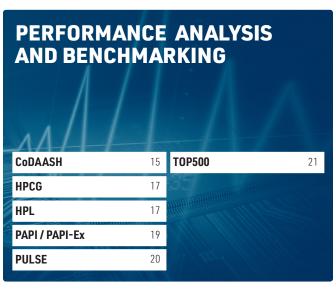
ICL has evolved and expanded our research agenda to accommodate the aforementioned evolution in HPC, which includes a focus on algorithms and libraries for multicore and hybrid computing. As we have gained a solid understanding of the challenges presented in these domains, we have further expanded our scope 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.

In the fall of 2016, ICL won an array of seven awards from the DOE's Exascale Computing Project (ECP). In doing so, ICL earned a place among an elite set of researchers from DOE laboratories who will create the software infrastructure for the nation's first exascale machines. On the following pages, we provide brief summaries of some of our efforts in these areas.











#### **Distributed Tasking for Exascale**

The Distributed Tasking for Exascale (DTE) project will extend the capabilities of ICL's Parallel Runtime and Execution Controller (PaRSEC) project—a generic framework for architecture-aware scheduling and management of microtasks on distributed, manycore, heterogeneous architectures. The PaRSEC environment also provides a runtime component for dynamically executing tasks on heterogeneous distributed systems along with a productivity toolbox and development framework that supports multiple domain-specific languages and extensions and tools for debugging, trace collection, and analysis.

With PaRSEC, applications are expressed as a direct acyclic graph (DAG) of tasks with edges designating data dependencies. This DAG dataflow paradigm attacks both sides of the exascale challenge: managing extreme-scale parallelism and maintaining the performance portability of the code. The DTE award is a vital extension and continuation of this effort and will ensure that PaRSEC meets the critical needs of ECP application communities in terms of scalability, interoperability, and productivity.



#### **Exascale Performance Application Programming Interface**

The Exascale Performance Application Programming Interface (Exa-PAPI) award builds on ICL's Performance Application Programming Interface (PAPI) project and extends it with performance counter monitoring capabilities for new and advanced ECP hardware and software technologies. PAPI provides a consistent interface and methodology for collecting performance counter information from various hardware and software components, including most major CPUs, GPUs and accelerators, interconnects, I/O systems, and power interfaces, as well as virtual cloud environments.

Exa-PAPI extends this effort with performance counter monitoring capabilities for new and advanced ECP hardware and software technologies, fine-grained power management support, and integration capabilities for exascale paradigms like task-based runtime systems. Exa-PAPI also adds events that originate from the ECP software stack, extending the notion of performance events to include not only hardware but also software-based information—all through one consistent interface.

#### ICL/RESEARCH



#### Production-ready, Exascale-Enabled Krylov Solvers for Exascale Computing

The Production-ready, Exascale-Enabled Krylov Solvers for Exascale Computing (PEEKS) project will explore the redesign of solvers and extend the DOE's Extreme-scale Algorithms and Solver Resilience (EASIR) project. Many large-scale scientific applications rely heavily on preconditioned iterative solvers for large linear systems. For these solvers to efficiently exploit extreme-scale hardware, both the solver algorithms and the implementations must be redesigned to address challenges like extreme concurrency, complex memory hierarchies, costly data movement, and heterogeneous node architectures.

The PEEKS effort aims to tackle these challenges and advance the capabilities of the ECP software stack by making the new scalable algorithms accessible within the Trilinos software ecosystem. Targeting exascale-enabled Krylov solvers, incomplete factorization routines, and parallel preconditioning techniques will ensure successful delivery of scalable Krylov solvers in robust, production-quality software that can be relied on by ECP applications.



#### **Software for Linear Algebra Targeting Exascale**

For decades, ICL has applied algorithmic and technological innovations to the process of pioneering, implementing, and disseminating dense linear algebra software—including the Linear Algebra PACKage (LAPACK) and Scalable Linear Algebra PACKage (Scalapack) libraries. The Software for Linear Algebra Targeting Exascale (SLATE) project will converge and consolidate that software into a dense linear algebra library that will integrate seamlessly into the ECP ecosystem.

For context, ScaLAPACK was first released in 1995, some 23 years ago. In the past two decades, HPC has witnessed tectonic shifts in the hardware technology, followed by paradigm shifts in the software technology, and a plethora of algorithmic innovation in scientific computing. At the same time, no viable replacement for ScaLAPACK emerged. SLATE is meant to be this replacement, boasting superior performance and scalability in the modern, heterogeneous, distributed-memory environments of HPC.



#### **CEED Co-Design Center**

The Lawrence Livermore National Laboratory (LLNL)—led Center for Efficient Exascale Discretizations (CEED) co-design effort will develop next-generation discretization software and algorithms—which deliver a significant performance gain over conventional low-order methods—to enable a wide range of DOE and National Nuclear Security Administration (NNSA) applications to run efficiently on future exascale hardware. CEED is a research partnership involving 30+ computational scientists from two DOE labs and five universities, including UTK.

For UTK's part, ICL will be instrumental in identifying, developing, and optimizing tensor contractions that are essential building blocks for these kinds of DOE/NNSA applications. The ICL team will also play an integral role in co-designing application programming interfaces (APIs) with the LLNL scientists, external partners, and vendors, and will deliver a high-performance tensor contractions package through the Matrix Algebra on GPU and Multicore Architectures (MAGMA) library.



# OMPI-X

#### **Open MPI for Exascale**

The Open MPI for Exascale (OMPI-X) project focuses on preparing the Message Passing Interface (MPI) standard—and its implementation in Open MPI—for exascale through improvements in scalability, capability, and resilience. Since its inception, the MPI standard has become ubiquitous in high-performance parallel computational science and engineering, and Open MPI is a widely used, high-quality, open-source implementation of the MPI standard. Despite their history and popularity, however, neither Open MPI nor the MPI standard itself is currently ready for the changes in hardware and software that will accompany exascale computing.

To mitigate this concern, OMPI-X will address a broad spectrum of issues in both the standard and the implementation by ensuring runtime interoperability for MPI+X and beyond, extending the MPI standard to better support coming exascale architectures, improving Open MPI scalability and performance, supporting more dynamic execution environments, enhancing resilience in MPI and Open MPI, evaluating MPI tools interfaces, and maintaining quality assurance.



FIND OUT MORE AT http://www.icl.utk.edu/research/ompi-x/

ECP =

#### Extreme-scale Scientific Software Development Kit

The Extreme-Scale Scientific Software Development Kit for the Exascale Computing Project (xSDK4ECP), a collaboration between Argonne National Laboratory (ANL), ICL, Lawrence Berkeley National Laboratory (LBNL), LLNL, Sandia National Laboratories (SNL), and the University of California at Berkeley (UCB), aims to enable seamless integration and combined use of diverse, independently developed software packages for ECP applications. Currently, this includes a wide range of high-quality software libraries and solver packages that address the strategic needs to fulfill the mission of DOE's Office of Science.

In the first year, ICL's MAGMA and Parallel Linear Algebra Software for Multicore Architectures (PLASMA) projects were integrated into the xSDK 0.3.0 release. To ensure consistency of naming conventions, runtime behavior, and installation procedure, xSDK informs the development process of large projects by providing sets of requirements and guidelines that are influential throughout the software development process. Additionally, as part of the inclusion process—and to lighten the burden on the system administrators and application developers—each package gets a Spack installation script that can be invoked independently or through the installation of the xSDK package itself.



#### ICL/RESEARCH



#### **Asynchronous Iterative Solvers for Extreme-scale Computing**

The Asynchronous Iterative Solvers for Extreme-Scale Computing (AsyncIS) project aims to explore more efficient numerical algorithms by decreasing their overhead. AsyncIS does this by replacing the outer Krylov subspace solver with an asynchronous optimized Schwarz method, thereby removing the global synchronization and bulk synchronous operations typically used in numerical codes.

AsyncIS, a DOE-funded collaboration between Georgia Tech, UTK, Temple University, and SNL, also focuses on the development and optimization of asynchronous preconditioners (i.e., preconditioners that are generated and/or applied in an asynchronous fashion). The novel preconditioning algorithms that provide fine-grained parallelism enable preconditioned Krylov solvers to run efficiently on many-core accelerators like GPUs.



#### **Batched Basic Linear Algebra Subprograms**

The Batched Basic Linear Algebra Subprograms (BBLAS) effort, an international collaboration between INRIA, Rutherford Appleton Laboratory, Umeå University, the University of Manchester, and UTK, will create an API for numerical computing routines that process batches of either uniformly sized or varying-size matrices or vectors. This will go beyond the original Basic Linear Algebra Subprogram (BLAS) standard by specifying a programming interface for modern scientific applications, which produce large numbers of small matrices at once.

Individually, the small sizes of the inputs obviate the potential benefits of using BLAS but are a perfect fit for BBLAS. The BBLAS project will also serve as a working forum for gathering ideas and working out a plan for establishing the consensus for the next official standard that will serve the scientific community and be supported by hardware vendors.



#### **BEAST OpeN Software Autotuning Infrastructure**

The goal of the BEAST OpeN Software Autotuning Infrastructure (BONSAI) project is to develop a software infrastructure for using scalable, parallel hybrid systems to carry out large, concurrent autotuning sweeps in order to dramatically accelerate the optimization process of computational kernels for GPU accelerators and many-core coprocessors. BONSAI is based on Python 2.7 and the Python-based LANquage for Autotuning Infrastructure (LANAI) syntax.

As the name suggests, BONSAI builds on the experiences of the Bench-testing Environment for Automated Software Tuning (BEAST) project, which prototyped and validated an autotuning workflow consisting of generation and pruning of the parameter search space; compilation, benchmarking, and profiling of the kernels that pass the pruning; and collection, analysis, and visualization of the performance data.



#### **Cross-layer Application-Aware Resilience at Extreme Scale**

The Cross-layer Application-Aware Resilience at Extreme Scale (CAARES) project, a collaborative effort between ICL, Rutgers University, and Stony Brook, aims to provide a theoretical foundation for multilevel fault management and a clear understanding of existing obstacles that could obstruct generic and efficient approaches for fault management at scale. This effort is vital for large-scale science, because, as extreme-scale computational power enables new and important discoveries across all science domains, the current understanding of fault rates is casting a grim shadow, revealing a future where failures are not exceptions but are the norm.

By studying a combination of fault tolerance techniques not in isolation from each other, CAARES seizes the opportunity to identify moldable techniques at the frontier of known approaches, a composition of methodologies that will inherit their individual benefits but not exhibit their drawbacks, and techniques able to bridge the gap between fault tolerance ergonomics and efficiency.



#### Cross-layer Application-Aware Resilience at Extreme Scale

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 to achieve efficient implementations for applications in materials science, chemistry, and physics. CoDAASH is a joint effort between UTK, Iowa State University, 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).

ICL's contribution focuses on expressing certain computational chemistry algorithms in the form of a data flow graph and subsequently mapping the DAG representation of the kernels to the hardware platforms. This representation allows for capturing the essential properties of the algorithms (e.g., data dependencies) and computation at extreme scale—in the era of many-core and highly heterogeneous platforms—by utilizing the hardware components (e.g., CPU or GPU) best suited for the type of computational task under consideration. The dataflow-based form of these algorithms makes them compatible with next-generation task scheduling systems like PaRSEC.



#### **Convex Optimization for Realtime Embedded Systems**

The Convex Optimization for Realtime Embedded Systems (CORES) project aims to develop highly efficient real-time convex optimization algorithms and toolsets for solving important engineering problems on hierarchical and heterogeneous embedded system architectures. Though recent advances in optimization solvers have enabled the solution of optimization problems on low-cost embedded systems, the size of the problems that can be solved in real time is still limited.

The CORES project, a collaboration between ICL and Michigan Technological University, works to address this limitation. The ICL team's main responsibility is the design and development of higher-performance, structure-aware linear solvers that would enable us to solve, in real time, the convex optimization problems that have significantly higher performance—and are orders of magnitude greater in size—compared to current state-of-the-art solvers.

#### ICL/RESEARCH



#### **Data-driven Autotuning for Runtime Execution**

The objective of the Data-driven Autotuning for Runtime Execution (DARE) project is to provide application-level performance tuning capabilities to the end user. DARE's development motivation stems from the never-ending hurdles of performance tuning for the PLASMA and MAGMA linear algebra libraries. These hurdles motivated the development of a software architecture that combines three components: hardware analysis, kernel modeling, and workload simulation.

With DARE, the hardware analysis block builds a detailed model of the hardware, its computational resources, and its memory system. The kernel modeling block builds accurate performance models for the computational kernels involved in the workload, and the workload simulation block rapidly simulates a large number of runs to find the best execution conditions while relying on the information provided by the other two blocks. The ultimate objective of DARE is to arrange the blocks in a continuous refinement loop that can serve as a framework for optimizing applications beyond the field of dense linear algebra.



#### Distributed Parallel Linear Algebra Software for Multicore Architectures

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 multi-core processors and, if available, accelerators like GPUs or Intel Xeon Phi coprocessors. DPLASMA achieves this objective by deploying PLASMA algorithms on distributed-memory systems using the state-of-the-art PaRSEC runtime.

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



Evolve, a collaborative effort between ICL and the University of Houston, expands the capabilities of Open MPI to support the NSF's critical software infrastructure missions. Core challenges include: extending the software to scale to 10,000–100,000 processes; ensuring support for accelerators; enabling highly asynchronous execution of communication and I/O operations; and ensuring resilience. Part of the effort involves careful consideration of modifications to the MPI specification to account for the emerging needs of application developers on future extreme-scale systems.

For 2017, Evolve efforts revolved around exploratory research in improving the performance of multithreaded programs using MPI. Collective operations based on events have been investigated and have demonstrated a clear advantage in terms of aggregate bandwidth in heterogeneous (shared-memory + network) systems. User-Level Failure Mitigation (ULFM) fault-tolerance was released based on the latest Open MPI. Counters and performance profiling of internal Open MPI events are now exposed, which has enabled the team to discover and eliminate important performance limitations in the MPI implementation.



#### **High Performance Conjugate Gradients**

The High Performance Conjugate Gradients (HPCG) benchmark is designed to measure performance that is representative of modern scientific applications. It does so by exercising the computational and communication patterns commonly found in real science and engineering codes, which are often 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.

The HPCG 3.0 reference code was released on November 11, 2015 for the SC15 conference in Austin, TX. In addition to bug fixes, this release positions HPCG to even better represent modern partial differential equation (PDE) solvers and aids in running HPCG on production supercomputing installations. The reference version is accompanied by binary releases from Intel and NVIDIA that are carefully optimized for the vendors' respective hardware platforms. The current HPCG performance list was released at SC17 and now features over 100 supercomputing sites. The HPCG score has also been tracked by the TOP500 list since June 2017.



#### **High Performance LINPACK**

The High Performance LINPACK (HPL) benchmark solves a dense linear system in double precision (64-bit) arithmetic on distributed-memory computers. HPL is written in a portable ANSI C and requires an MPI implementation and either BLAS or the Vector Signal and Image Processing Library (VSIPL). HPL is often one of the first programs to run on large HPC installations, producing a result that can be submitted to the TOP500 list of the world's fastest supercomputers.

The major focus of HPL 2.2, released in 2016, was to improve the accuracy of reported benchmark results and ensure scalability of the code on large supercomputer installations with 100,000+ cores. HPL now features detailed time-of-run accounting to better assess power requirements at run time, a metric which is reported on the TOP500 and also highlighted on the Green500. The LINPACK app for iOS achieves over 4 gigaFLOP/s on the iPad Air and iPad Pro. For the November 2017 TOP500 list, an optimized version of the HPL code ran on a machine with over 10,000,000 cores.



#### The Linear Algebra PACKage

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 multi-core BLAS library. ScaLAPACK is parallel, distributed, and relies on the BLAS, LAPACK, MPI, and BLACS libraries.

LAPACK 3.8.0, released in November 2017, includes level-3 BLAS communication-avoiding, symmetric-indefinite factorizations with Aasen's triangular tridiagonalization using the two-stage algorithm. 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. ScaLAPACK 2.0.0, which includes the multiple relatively robust representations (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.

#### ICL/RESEARCH



#### Matrix Algebra on GPU and Multicore Architectures

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 enables applications to fully exploit the power of current heterogeneous systems of many-core CPUs and multi-GPUs/coprocessors to deliver the fastest possible time to accurate solution within given energy constraints.

MAGMA 2.3 features LAPACK-compliant routines for multi-core CPUs enhanced with NVIDIA GPUs (including the Volta V100). MAGMA now includes more than 400 routines, covering one-sided dense matrix factorizations and solvers, and two-sided factorizations and eigen/singular-value problem solvers, as well as a subset of highly optimized BLAS for GPUs. A MagmaDNN package was launched to provide high-performance data analytics, including functionalities for machine learning applications that use MAGMA as their computational backend. The MAGMA Sparse and MAGMA Batched packages were added with the MAGMA 1.6 release and continuously extended and improved with each release.



#### MAtrix, TEnsor, and Deep-learning Optimized Routines

The MAtrix, TEnsor, and Deep-learning Optimized Routines (MATEDOR) project will perform the research required to define a standard interface for batched operations and to provide a performance-portable software library that demonstrates batching routines for a significant number of kernels. This research is critical, given that the performance opportunities inherent in solving many small batched matrices often yield more than a 10× speedup over the current classical approaches.

Working closely with affected application communities, along with ICL's Batched BLAS initiative, MATEDOR will define modular, optimizable, and language-agnostic interfaces that can work seamlessly with a compiler. This modularity will provide application, compiler, and runtime system developers with the option to use a single call to a routine from the new batch operation standard and would allow the entire linear algebra community to collectively attack a wide range of small matrix or tensor problems.



#### **Open-Source Message Passing Interface**

The Open MPI Project is an open-source Message Passing Interface (MPI) implementation 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 3.1-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.



#### Performance Application Programming Interface

The Performance Application Programming Interface (PAPI) supplies a consistent interface and methodology for collecting performance counter information from various hardware and software components, including most major CPUs, GPUs and accelerators, interconnects, I/O systems, and power interfaces, as well as virtual cloud environments. Industry liaisons with Bull, Cray, Intel, IBM, NVIDIA, and others ensure seamless integration of PAPI with new architectures at or near their release. As the PAPI component architecture becomes more populated, performance tools that interface with PAPI automatically inherit the ability to measure these new data sources.

In 2015, ICL, together with the University of Maine, began work on PAPI-EX to build support for performance counters available in recent generations of CPUs and GPUs, develop support for system-wide hardware performance counter monitoring, create a sampling interface in PAPI, and incorporate a user-facing command line tool for PAPI. PAPI-EX will also incorporate a counter inspection toolkit designed to improve understanding of low-level hardware events. At the end of 2016, ICL was awarded funding for the ECP Exa-PAPI project, which will augment PAPI-EX.



#### Parallel Runtime Scheduling and Execution Controller

The Parallel Runtime Scheduling and Execution Controller (PaRSEC) is a generic framework for architecture-aware scheduling and management of microtasks on distributed many-core heterogeneous architectures. Applications considered are expressed as a DAG of tasks with edges designating the 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 orchestrates the execution of an algorithm on a particular set of resources, assigns computational threads to the cores, overlaps communications and computations, and uses a dynamic, fully distributed scheduler. PaRSEC includes a set of tools to generate the DAGs and integrate them into legacy codes, a runtime library to schedule the microtasks on heterogeneous resources, and tools to evaluate and visualize the efficiency of the scheduling. Many dense and sparse linear algebra extensions have been implemented, as well as chemistry and seismology applications, which produced significant speedup in production codes.



#### **Parallel Linear Algebra Software for Multicore Architectures**

The Parallel Linear Algebra Software for Multicore Architectures (PLASMA) package implements a set of fundamental linear algebra routines using the Open Multi-Processing (OpenMP) standard. PLASMA includes, among others, routines for solving linear systems of equations, linear least square problems, parallel BLAS, and parallel matrix norms.

Over the last decade, PLASMA—which has been deployed on a variety of systems using Intel processors (including Xeon Phi coprocessors), IBM POWER processors, and ARM processors—has served as a tremendous research vehicle for the design of new dense linear algebra algorithms and has paved the way for new developments, including the new ECP SLATE project, which will ultimately deliver these capabilities at exascale.

#### ICL/RESEARCH



#### PAPI Unifying Layer for Software-defined Events

The PAPI Unifying Layer for Software-defined Events (PULSE) project focuses on enabling cross-layer and integrated monitoring of whole application performance by extending PAPI with the capability to expose performance metrics from key software components found in the HPC software stack. Up to this point, the abstraction and standardization layer provided by PAPI has been limited to profiling information generated by hardware only. Information about the behavior of the underlying software stack had to be acquired either through low-level binary instrumentation or through custom APIs.

To overcome this shortfall, PULSE will extend the abstraction and unification layer that PAPI has provided for hardware events to also encompass software events. On one end, PULSE will provide a standard, well-defined and well-documented API that high-level profiling software can utilize to acquire and present to application developers performance information about the libraries used by their application. On the other end, it will provide standard APIs that library and runtime writers can utilize to communicate to higher software layers information about the behavior of their software.



#### Simulation and Modeling for Understanding Resilience and Faults at Scale

The Simulation and Modeling for Understanding Resilience and Faults at Scale (SMURFS) project seeks to acquire the predictive understanding of the complex interactions of a given application, a given real or hypothetical hardware and software environment, and a given fault-tolerance strategy at extreme scale.

SMURFS is characterized by two facets: (1) medium- and fine-grained predictive capabilities and (2) coarse-grained fault tolerance strategy selection. Accordingly, ICL plans to design, develop, and validate new analytical and system component models that use semi-detailed software and hardware specifications to predict application performance in terms of time to solution and energy consumption. Also, based on a comprehensive set of studies using several application benchmarks, proxies, full applications, and several different fault tolerance strategies, ICL will gather valuable insights about application behavior at scale.



The Sparse direct methods via Run-time Scheduling and Execution of Kernels with Auto-tunable and Frequency-scaling Features for Energy-aware computing on heterogeneous architectures (SparseKaffe) project creates fast and efficient sparse direct methods for platforms with multi-core processors with one or more accelerators (e.g., GPUs or Xeon Phi coprocessors). SparseKaffe spans the platform pyramid, from desktop machines to extreme-scale systems consisting of multiple heterogeneous nodes connected through a high-speed network, with the goal of achieving orders of magnitude gains in computational performance while also paying careful attention to energy requirements.

The SparseKaffe project is a collaboration between UTK, the University of Florida, and Texas A&M University. ICL's work on the project concentrates on kernel designs and performance tuning, as well as on dynamic runtime scheduling using a dataflow model. This work will leverage—and be a natural extension of—ICL's work on runtimes as part of the MAGMA, PLASMA, and PaRSEC projects. The autotuning of the algorithm-specific computational kernels will apply the principles behind ICL's DARE project.



#### Task-based Environment for Scientific Simulation at Extreme Scale

The goal of the Task-based Environment for Scientific Simulation at Extreme Scale (TESSE) is to use an application-driven design to create a general-purpose, production-quality software framework that attacks the twin challenges of programmer productivity and portable performance for advanced scientific applications on massively-parallel, hybrid, many-core systems of today and tomorrow.

The TESSE team is composed of researchers from Stony Brook, Virginia Tech, and UTK, who have designed a system that uses DAG-based data flow as the basis of the software. This capability, with the extensions being explored by the TESSE team, will provide significant potential advantages in ease of composition, performance, and ease of migration to future architectures for irregular parallel applications. The TESSE team's next major goal is the ubiquitous existence of a powerful DAG-based data flow tool that complements, and is completely interoperable with, mainstream standard parallel programming models such as OpenMP and MPI.



#### Ranking the 500 fastest computers in the world

With more than two decades of tracking supercomputing progress, the TOP500 list continues to provide a reliable historical record of supercomputers around the world. The list clearly lays out critical HPC metrics across all 500 machines and draws a rich picture of the state of the art in terms of performance, energy consumption, and power efficiency. The TOP500 now features an HPCG ranking, which benchmarks a machine's performance using irregular accesses to memory and fine-grain recursive computations—factors which dominate real-world, large-scale scientific workloads.

In November 2017, the 50th TOP500 list showed China overtaking the United States in the number of ranked systems—with 202 Chinese machines to 143 US machines. With these numbers in play, China now has more machines in the TOP500 than they ever have previously, while the number of US machines drops to a 25-year low. As far as the rankings themselves, China's Sunway TaihuLight system, installed at the National Supercomputing Center in Wuxi, maintains its number one ranking for the fourth time, with an HPL run of 93.01 petaFLOP/s.



#### **User Level Failure Mitigation**

User Level Failure Mitigation (ULFM) is a set of new interfaces for MPI that enables message passing applications to restore MPI functionality affected by process failures. The MPI implementation is spared the expense of internally taking protective and corrective automatic actions against failures. Instead, it can prevent any fault-related deadlock situation by reporting 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. A wide range of application types and middlewares are already building on top of ULFM to deliver scalable and user-friendly fault tolerance, notable recent additions include the CoArray Fortran language, and SAP databases. ULFM software is available in recent versions of both MPICH and Open MPI.

#### **ICL/PUBLICATIONS**

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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# **ICL/EVENTS**

Every year, members of our research staff 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. Participating in the intellectual life of the scientific community in this way is an essential part of the research process.

January 9 / Trieste, Italy  Master in HPC Advanced  Programming and Software  Optimization	Feb 27-Mar 2 / Portland, OR <b>MPI Forum</b>		June 5-9 / Riverhead, NY <b>2017 GPU Hackathon</b>
January 10 / Argonne, IL ECP CEED Meeting	Feb 27-Mar 3 / Atlanta, GA SIAM Conference on Computational Science and Engineering	April 28 / Wuxi, China ASC17 Student Supercomputer Challenge	June 12-22 / Zurich, Switzerland The International Conference on Computational Science (ICCS17)
January 24–26 / San Jose, CA Open MPI Developers Meeting		May 8-11 / San Jose, CA NVIDIA's GPU Technology Conference (GTC)	June 19-22 / Frankfurt, Germany ISC High Performance (ISC17)
Jan 30-Feb 2 / Knoxville, TN ECP All-Hands Meeting	March 9-10 / Wuxi, China  Workshop on Big Data and Extreme-scale Computing (BDEC)	May 11-12 / Toulouse, France CERFACS 30-Year Conference	
February 4 / Austin, TX Principles and Practice of Parallel Programming (PPoPP)	Mar 29-30 / Heidelberg, Germany <b>Parallel 2017</b>		June 23 / Frankfurt, Germany VI-HPS 10th Anniversary Workshop
February 4-5 / Austin, TX GPGPU-10 Workshop	April 4-5 / Atlanta, GA Future Online Analysis Platform	May 24-26 / Knoxville, TN The 12th Scheduling for Large Scale Systems Workshop	July 5-8 / Schloss Ringberg, Germany Power-Aware Computing (PACO2017)
February 23-25 / Atlanta, GA Workshop on Batched, Reproducible, and Reduced Precision BLAS		May 29-Jun 1 / Orlando, FL International Parallel & Distributed Processing Symposium (IPDPS)	Jun 26-28 / Lugano, Switzerland Platform for Advanced Scientific Computing (PASC17)

July 10-14 / Pittsburgh, PA
2017 SIAM Annual Meeting

Sep 12-14 / Waltham, MA
IEEE High Performance
Extreme Computing
Conference (HPEC)

Jul 17-19 / Urbana, IL **7th JLESC Workshop** 

Sep 13-15 / Los Angeles, CA Linux Plumbers Conference 2017

Aug 15-17 / Livermore, CA
CEED First Annual Meeting



Aug 27-30 / Dagstuhl, Germany Dagstuhl Seminar 17352: Analysis and Synthesis of Floating-Point Programs Sep 25-28 / Chicago, IL **EuroMPI/USA 2017** 

Aug 29-31 / Gatlinburg, TN
Smoky Mountains
Computational Sciences &
Engineering Conference
(SMC17)



Sep 5-8 / Atlanta, GA

DOE Async IS Project

Meeting

Nov 12-17 / Denver, CO
The International
Conference for High
Performance Computing,
Networking, Storage and
Analysis (SC17)

Sep 11-12 / Dresden, Germany 11th Parallel Tools Workshop Dec 11-14 / Boston, MA
2017 IEEE International
Conference on Big Data



The International Conference for High Performance Computing Networking, Storage, and Analysis (SC), established in 1988, is a staple of ICL's November itinerary. SC is vital to the growth and evolution of HPC 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.

SC17 was held in Denver, Colorado, on November 12–17. 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. Since the University of Tennessee did not have a booth at SC this year, ICL leveraged an online "virtual booth" through which interested parties could keep tabs on ICL-related events at SC, including a list of attendees and detailed schedule of talks.



FIND OUT MORE AT http://www.icl.utk.edu/sc17/

# **ICL/PARTNERSHIPS**

Since its inception in 1989, ICL has fostered relationships with many academic institutions and research centers and has proactively built enduring collaborative partnerships with HPC vendors and industry leaders in the United States and abroad. In this section, we recognize many of those partners and collaborators, most of whom we continue to work with today.

GOVERNMENT AND ACADEMIC	Argonne Argonal Laboratory	EMORY	Georgia Tech <u>⊌</u>	<b>Ψ</b> INDIANA UNIVERSITY
Joint Institute for Computational Sciences	BERKELEY LAB	Lawrence Livermore National Laboratory	• Los Alamos NATIONAL LABORATORY EST. 1943	Massachusetts Institute of Technology
Michigan Technological University	NC5A	NIGHT IN THE CONTINUE LEAST	NORTHWESTERN UNIVERSITY	OAK RIDGE National Laboratory
Pacific Northwest NATIONAL LABORATORY	<b></b>	THE STATE UNIVERSITY OF NEW JERSEY RUTGERS	SDSC San Diego Supercomputer Center	Sandia National Laboratories
Stony Brook University	STANFORD UNIVERSITY	TEXAS A&M	Berkeley UNIVERSITY OF CALIFORNIA	UCRIVERSITY OF CALIFORNIA
University of Colorado Denver	UNIVERSITY of FLORIDA	UNIVERSITY of HOUSTON	I L L I N O I S  LINVERSITY OF ALMOIS AT LIBRADA CHAMPMON	THE UNIVERSITY OF IOWA
MAINE	THE UNIVERSITY OF NEW MEXICO	USC University of Southern California	WASHINGTON	<b>"</b> VirginiaTech

# INDUSTRY AMDE Atos FUITS FUITS Mathworks Mathworks Mathworks Mathworks Mathworks Mathworks Mathworks Mathworks Mathworks Mathworks

## 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 United States to identify and prototype revolutionary technology opportunities, and exchange expertise in various fields of HPC.

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 coprocessor. 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.

# INTERNATIONAL COLLABORATIONS

Barcelona Supercomputing Center Barcelona, Spain

Central Institute for Applied Mathematics Jülich, Germany

Doshisha University Kyoto, Japan

École Normale Supérieure de Lyon Lyon, France

École Polytechnique Federale de Lausanne Lausanne, Switzerland

ETH Zurich
Zurich, 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

Hokkaido University Sapporo, Japan

> INRIA France

Karlsruhe Institute of Technology Karlsruhe, Germany

Kasetsart University Bangkok, Thailand

King Abdullah University of Science and Technology Thuwal, Saudi Arabia

Laboratoire d'Informatique de Paris 6 Paris, France

Moscow State University
Moscow, Russia

National Institute of Advanced Industrial Science and Technology Tsukuba, Japan

Parallel and HPC Application Software Exchange Tsukuba, Japan

Prometeus GmbH Mannheim, Germany

Regionales
Rechenzentrum Erlangen
Erlangen, Germany

**RIKEN** Wako, Japan

Rutherford Appleton Laboratory Oxford, England

Soongsil University Seoul, South Korea

Technische Universitaet Wien Vienna, Austria

Technische Universität Dresden Dresden, Germany

> Tokyo Institute of Technology Tokyo, Japan

Umeå University Umeå, Sweden

Université Claude Bernard Lyon 1 Lyon, France

University of Bordeaux Bordeaux, France

University of Cape Town Cape Town, South Africa

University of Manchester Manchester, England

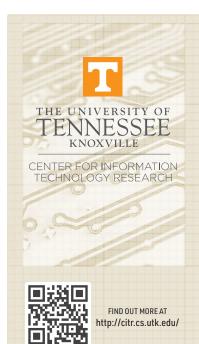
University of Paris-Sud Paris, France

University of Picardie Jules Verne Amiens, France

University of Tsukuba Tsukuba, Japan

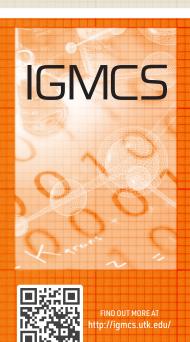
# **ICL/LEADERSHIP**

While leading-edge research and high-impact software are hallmarks of the ICL mission, the lab also cultivates a strong core of leadership. To this end, ICL actively engages the HPC and computational research communities through impactful efforts like those outlined below.



The Center for Information Technology Research (CITR) was established in 2001 to drive the growth and development of leading-edge information technology research at UTK. CITR's primary objective is to develop a thriving, well-funded community in basic and applied information technology research 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 UTK 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 UTK 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.



# INTERDISCIPLINARY GRADUATE MINOR IN COMPUTATIONAL SCIENCE

Addressing the need for a new educational strategy in computational science, 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 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. Through the IGMCS, graduate students can augment their graduate work in their chosen field with courses from other disciplines that are specifically tailored to round out their education in computational science. The IGMCS curriculum, requirements, and policies are governed by a program committee composed of faculty members from participating IGMCS academic units and departments.





BDEC China Group Photo / MARCH 2017

In the past several years, the United States, the European Union, Japan, and China have each moved aggressively to develop their own plans for achieving exascale computing in the next decade. Such concerted planning by the traditional leaders of HPC speaks eloquently about both the substantial rewards that await the success of such efforts, and about the unprecedented technical obstacles that apparently block the path upward to get there. But while these exascale initiatives, including the International Exascale Software Project (IESP), have understandably focused on the big challenges of exascale for hardware and software architectures, the relatively recent emergence of the phenomena of "big data" in a wide variety of scientific fields represents a tectonic shift that is transforming the entire research landscape on which all plans for exascale computing must play out.

The workshop series on Big Data and Extreme-scale Computing (BDEC) marks a distinctly new phase for the work of the IESP community and is premised on the idea that we must begin to systematically map out and account for the ways in which the major issues associated with big data intersect with, impinge upon, and potentially change the national (and international) plans that are now being laid out for achieving exascale computing.

In 2017, ICL was instrumental in organizing and staging the fifth BDEC workshop in Wuxi, China.

Along with Jack Dongarra, and following through with work they began with the IESP and the first four BDEC meetings in Charleston, Fukuoka, Barcelona, and Frankfurt, several members of ICL's CITR staff—including Terry Moore, Tracy Rafferty, and David Rogers—played essential roles in making the fifth BDEC workshop a major success.

A follow-up BDEC BoF was held in Denver, Colorado during SC17. This meeting marked the release of the BDEC "Pathways to Convergence" report, which examines the progress toward (or potential for) convergence of HPC and emerging high-end data analysis at three different levels: (1) large-scale scientific applications, (2) large-scale HPC platforms, and (3) next generation distributed services.

The next BDEC workshop is planned for the spring of 2018. 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://www.exascale.org/



# ICL/PEOPLE



#### STAFF AND STUDENTS

As the HPC landscape continues to evolve rapidly, 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 highly motivated and hardworking students.

In 2017, five members of ICL earned their degrees from UTK under the guidance and mentorship of Prof. Dongarra and ICL's research scientists.

- · Chongxiao Cao, PhD in Computer Science, May 2017
- · Heike Jagode, PhD in Computer Science, May 2017
- · Khairul Kabir, PhD in Computer Science, May 2017
- Sangamesh Ragate, MS in Computer Science, May 2017
- Wei Wu, PhD in Computer Science, May 2017



WEI WU, CHONGXIAO CAO, GEORGE BOSILCA, AND HEIKE JAGODE



Ahmad Abdelfattah RESEARCH SCIENTIST I



Hartwig Anzt RESEARCH SCIENTIST I



Matthew Bachstein
GRADUATE RESEARCH ASSISTANT



George Bosilca RESEARCH ASST. PROFESSOR



Aurelien Bouteiller RESEARCH DIRECTOR



**Qinglei Cao** GRADUATE RESEARCH ASSISTANT



Earl Carr PROGRAM ADMINISTRATOR



Sam Crawford
INFORMATION SPECIALIST II



Anthony Danalis RESEARCH DIRECTOR



Jack Dongarra
UNIVERSITY DISTINGUISHED
PROFESSOR / DIRECTOR OF ICL



David Eberius
GRADUATE RESEARCH ASSISTANT



Teresa Finchum ADMINISTRATIVE SPECIALIST II



Jamie Finney SOFTWARE ENGINEER



Mark Gates
RESEARCH SCIENTIST II



Damien Genet RESEARCH SCIENTIST I



Azzam Haidar RESEARCH SCIENTIST II



Hanumantharayappa GRADUATE RESEARCH ASSISTANT



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Thomas Herault RESEARCH DIRECTOR



Reazul Hoque GRADUATE RESEARCH ASSISTANT



Harry Hughes GRADUATE RESEARCH ASSISTANT



**Heike Jagode** RESEARCH ASST. PROFESSOR



Cindy Knisley
FINANCIAL SPECIALIST



Jakub Kurzak RESEARCH ASST. PROFESSOR

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Terry Moore
ASSOCIATE DIRECTOR



Phil Mucci RESEARCH CONSULTANT



Thananon Patinyasakdikul GRADUATE RESEARCH ASSISTANT



Yu Pei GRADUATE RESEARCH ASSISTANT



Tracy Rafferty PROGRAM MANAGER



Gerald Ragghianti
RESEARCH LEADER



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Frank Winkler CONSULTANT



Panruo Wu POST DOCTORAL RESEARCH ASSOCIATE



Ichitaro Yamazaki RESEARCH SCIENTIST I



Asim YarKhan RESEARCH SCIENTIST II



**Dong Zhong** GRADUATE RESEARCH ASSISTANT

#### **ICL/VISITORS**

Since its founding, ICL has had a tradition of hosting many visitors from around the world. Some stay only briefly to give insightful seminars or presentations; others remain with us for as long as a year to collaborate, teach, and learn. Our connection to these researchers enables us to leverage an immense array of intellectual resources and work with the best and brightest people in the HPC community.



**Dorian Arnold** EMORY UNIVERSITY



Camille Coti UNIVERSITE PARIS 13, FRANCE



Chris Davis OAK RIDGE NATIONAL LABORATORY



Markus Eisenbach OAK RIDGE NATIONAL LABORATORY



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Nuria Losada UNIVERSITY OF A CORUÑA, SPAIN



Hatem Ltaief KING ABDULLAH UNIVERSITY OF SCIENCE AND TECHNOLOGY



Samuel Mabakane CENTRE FOR HIGH PER-FORMANCE COMPUTING, SOUTH AFRICA



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Arvind Ramanathan OAK RIDGE NATIONAL LABORATORY



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Sophie Voisin OAK RIDGE NATIONAL LABORATORY



Kwai Wong JOINT INSTITUTE FOR COMPUTATIONAL SCIENCES



Dmitry Zaitsev
INTERNATIONAL
HUMANITARIAN UNIVERSITY
UKRAINE

## **ICL/ALUMNI**

Since its inception, ICL has attracted many research scientists and students from a variety of backgrounds and academic disciplines. Many of these experts came to UTK 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.

Maksims Abalenkovs	Bonnie Browne	Simplice Donfack	Adriana Garties
Carolyn Aebischer	Cynthia Browne	Tingxing "Tim" Dong	Peter Gaultney
Sudesh Agrawal	Murray Browne	Leon Dong	Christoph Geile
Bivek Agrawal	Giuseppe Bruno	Nick Dongarra	Jean Patrick Gelas
Emmanuel Agullo	Antonin Bukovsky	David Doolin	Boris Gelfend
Jennifer Allgeyer	Greg Bunch	Joe Dorris	Jonathan Gettler
Wes Alvaro	Alfredo Buttari	Andrew Downey	Scott Gibson
Ed Anderson	Anthony Canino	Mary Drake	Eric Greaser
Daniel Andrzejewski	Domingo Gimenez Canovas	Julio Driggs	Stan Green
Thara Angskun	Chongxiao "Shawn" Cao	Brian Drum	Alice Gregory
Papa Arkhurst	Henri Casanova	Peng Du	Amina Guermouche
Dorian Arnold	Cedric Castagnede	Eduardo Echavarria	Jason Gurley
Cedric Augonnet	Ramkrishna Chakrabarty	Victor Eijkhout	Bilel Hadri
Marc Baboulin	Sharon Chambers	Brett Ellis	Hunter Hagewood
Zhaojun Bai	Zizhong Chen	Shawn Ericson	Christian Halloy
Ashwin Balakrishnan	Jaeyoung Choi	Zachary Eyler-Walker	Sven Hammarling
Richard Barrett	Wahid Chrabakh	Lisa Ezzell	J. Mike Hammond
Alex Bassi	Eric Clarkson	Christoph Fabianek	Satomi Hasegawa
David Battle	Andy Cleary	Graham Fagg	Hidehiko Hasegawa
Micah Beck	Michelle Clinard	Mathieu Faverge	Chris Hastings
Daniel Becker	Vincent Cohen-Addad	Diana Fayad	Blake Haugen
Dulceneia Becker	Matthias Colin	Shengzhog Feng	David Henderson
Adam Beguelin	Charles Collins	Don Fike	Greg Henry
Annamaria Benzoni	Stephanie Moreaud Cooper	Salvatore Filippone	Julien Herrmann
Tom Berry	Tom Cortese	Anna Finchum	Holly Hicks
Vincent Berthoux	Camille Coti	Mike Finger	Alexandra Hicks-Hardiman
Scott Betts	Jason Cox	Markus Fischer	Sid Hill
Nikhil Bhatia	David Cronk	Len Freeman	Tomoyuki Hiroyasu
Noel Black	Javier Cuenca	Xiaoquan Fu	George Ho
Laura Black	Manoel Cunha	Erika Fuentes	Josh Hoffman
Susan Blackford	Yuanshun (Shaun) Dai	Karl Fuerlinger	Jeff Horner
Wesley Bland	Cricket Deane	Megan Fuller	Mitch Horton
Kartheek Bodanki	Remi Delmas	Edgar Gabriel	Yan Huang
David Bolt	Frederic Desprez	Tracy Gangwer	Aurelie Hurault
Fernando Bond	Ying Ding	Lynn Gangwer	Chris Hurt
Carolyn Bowers	Jun Ding	Nathan Garner	Paul Jacobs
Barry Britt	Jin Ding	Kelley Garner	Emmanuel Jeannot
Randy Brown	Martin Do	Tina Garrison	Weizhong Ji

Yulu Jia Nuria Losada Tim Poore Joe Thomas Weicheng Jiang **Hatem Ltaief** Roldan Pozo John Thurman Song Jin **Daniel Lucio** Farzona Pulatova Francoise Tisseur Richard Luczak Patrick Johansson Martin Quinson **Jude Toth** 

Matt JohnsonTeng MaTammy RaceBernard TourancheauAral JohnsonSticks MabakaneSangamesh RagateVolodymyr Turchenko

Sean Jolly Robert Manchek James Ralph Lauren Vaca Jan Jones **Gabriel Marin** Sathish Vadhiyar **Ganapathy Raman** Kim Jones Tushti Marwah Kamesh Ramani Robert van de Geijn Mei Ran Vijay Joshi Theo Mary Chad Vawter

Khairul Kabir Ian Masliah Arun Rattan Eugene Vecharynski Venkata Kakani Donald McCasland Sheri Reagan Scott Venckus Ajay Kalhan Paul McMahan Mike Reynolds Antoine Vernois

Mike Reynolds **Antoine Vernois** Balajee Kannan Eric Meek George Rhinehart Reed Wade Madhuri Kasam James Meyering Jon Richardson Michael Walters Kiran Kumar Kasichayanula Jeremy Millar Ken Roche Mike Waltz **Ajay Katta** Michelle Miller **Andrew Rogers** Robert Waltz

Tom Rothrock

Zhiao Shi

**Thomas Spencer** 

Jerzy Wasniewski

Felix Wolf

Jin Yi

**Cindy Mitchell** 

**Matthew Nabity** 

Caroline Papadopoulos

**David Katz** 

Tilman Kuestner

Valentin Le Fevre

Joshua Kelly **Stuart Monty** Tom Rowan Vince Weaver Supriya Kilambi Erik Moore Narapat (Ohm) Saengpatsa Scott Wells Myung Ho Kim **Keith Moore** Kiran Sagi David West Youngbae Kim **Shirley Moore Evelyn Sams** R. Clint Whaley Jenya Kirshtein Robert Morgan Ken Schwartz Jody Whisnant Michael Kolatis Kishan Motheramgari **Keith Seymour** James White Moritz Kreutzer Steven Moulton Farial Shahnaz Scotti Whitmire Chandra Krintz Daichi Mukunoki **Brian Sheely** Susan Wo

Krerkchai Kusolchu Shankar Narasimhaswami Sergei Shinkarev Stephen Wood Rajib Nath Majed Sidani Coire Kyle Jiayi Wu Amanda Laake Fernando Navarro Shilpa Singhal Wei Wu John Nelson Matt Skinner Qiu Xia **Xavier Lacoste** Julien Langou Donnie Newell Peter Soendergaard Tinghua Xu **Jeff Larkin** Peter Newton Raffaele Solca **Tao Yang Brian LaRose** Jonas Nilsson **Gwang Son** Erlin Yao Frank Lauer Kevin Ye Jakob Oestergaard **Fengguang Song** 

Tracy Lee Leelinda Parker Jeffrey Steill Haihang You DongWoo Lee **Thibault Parpaite Erich Strohmaier** Lamia Youseff Pierre Lemarinier Dilip Patlolla Xiaobai Sun **Brian Zachary Todd Letsche Andy Pearson** Martin Swany **Dmitry Zaitsev Sharon Lewis** Paul Peltz Daisuke Takahashi Omar Zenati Yinan Li Theresa Pepin Judi Talley Yuanlei Zhang **Antoine Petitet** Weiran Li Ronald Tam Junlong Zhao Xiang Li Peter Pham Chunyan Tang Yong Zheng Chaoyang Liu **Gregoire Pichon** Yuan Tang Min Zhou **Kevin London** Vlado Pjesivac Yusuke Tanimura Luke Zhou

Matt LongleyJelena Pjesivac-GrbovicKeita TeranishiFlorent LopezJames S. PlankDan Terpstra

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The main source of support has been federal agencies that are charged with allocating public research funding. Therefore, we acknowledge the following agencies for supporting our efforts, both past and present:











In addition to the support of the federal government, we have solicited strong support from private industry, which has also played a significant role in our success and growth. We gratefully acknowledge the following vendors for their generosity and support:















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