



# INNOVATIVE COMPUTING LABORATORY *2023/24 REPORT*

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# ICL 2023/24 REPORT

**2** FROM THE DIRECTOR

**4** INTRODUCTION

**6** HISTORY

## 2023 HIGHLIGHTS

**8** ECP RETROSPECTIVE

**12** CONFERENCE HIGHLIGHTS

**14** CONGRATULATIONS

**15** SOFTWARE RELEASES

**16** VISITING RESEARCHERS

**18** ICL SEMINAR SERIES

**18** RESEARCH

**26** 2023 CONFERENCES ATTENDED

**28** 2023 PUBLICATIONS

**30** ICL STAFF & STUDENTS

**32** ICL ALUMNI

**34** PARTNERSHIPS

**36** ACKNOWLEDGMENTS

## FROM THE DIRECTOR



Hartwig Anzt

**REFLECTING ON** this year, we recognize that 2023 will be remembered in ICL history as a year packed with success, change, new initiatives, and the culmination of 7 years of work on the Department of Energy's Exascale Computing Project (ECP). We could finally demonstrate (and debug!) our software on the first exascale machine, Frontier, at Oak Ridge National Laboratory.

ICL was fortunate to have had or contributed to 8 projects within ECP:

SLATE developed distributed, GPU-accelerated dense linear algebra; Ginkgo developed GPU-accelerated sparse linear algebra; heFFTe provided distributed, GPU-accelerated 3D FFT; Exa-PAPI developed novel performance metrics and monitoring capabilities; Open MPI developed distributed communication; PaRSEC for distributed runtime scheduling; xSDK focused on math library interoperability and concentrated efforts on batched sparse and mixed precision functionality; and CEED served as a center for high-order finite-element tensor computations. At the end of ECP, several of ICL's software products and standardization efforts had become integral components of multiple high-profile ECP application projects, including plasma physics simulations in the WarpX and XGC projects, chemistry simulations in NWChemEX, molecular dynamics in LAMMPS, material science in MEUMAPPS-SS, particle simulations through CoPA, finite element simulations in MFEM, nonlinear solvers in SUNDIALS, sparse-direct solvers in STRUMPACK, and advancing the MPI communication standard. I am thankful for all ICL members contributing to ECP, and I am sure this gives ICL a headstart in future DOE initiatives.

We started 2023 with a well-attended winter reception that offered the opportunity to bid farewell to ICL's Assistant Director, Joan Snoderly. With Joan's retirement from ICL, we merged the ICL administrative support group and the ICL technical support group to become one team, the ICL operations group, reporting directly to the director.

With the end of ECP in sight, we organized an ICL directors' retreat in February to develop a strategy for post-ECP ICL. Team building activities helped us to identify challenges and opportunities ahead of us.

Later in the spring, we held an ICL/ORNL workshop to strengthen that partnership and create new collaborations. The summer brought the traditional ICL retreat at Park Vista. A new format based on breakout

sessions initiated numerous new initiatives and demonstrated ICL's adaptability to new research fields.

Fall 2023 brought a long list of visitors to ICL, including Veronica Montanaro, Andy Adelman, Sonali Mayani, Brieuc Nicolas, Lisa Gaedke-Merzhäuser, Thomas Grützmacher, You Wu, Terry Cojean, Tobias Ribizel, Mike Tsai, Albert Njoroge Kahira, and Yves Robert. International research exchange has always been a hallmark of ICL, and I am thankful for all the visitors and ICL members who helped make the research visits successful.

The Sparse BLAS Workshop just before SC23 started a new initiative at ICL to define a standard for sparse linear algebra operations. Attendees from academic institutions, national laboratories, and major industry partners, including ARM, NVIDIA, AMD, Intel, and MathWorks, discussed different approaches and held hackathons to develop a reference implementation.

The end of ECP was a bittersweet moment. We celebrate all the work accomplished over seven years. Unfortunately, with the end of ECP, ICL also shrank, and we said goodbye to many people. As has been true throughout the history of ICL, people come to obtain training as graduate students, post-docs, and research scientists and then go out into industry and academia to advance their careers and contribute to cutting-edge HPC. Many ICL alumni continue to work in the same field and help to ensure that the ideas developed here spread and thus have a broad impact. We look forward to continuing collaborations with the ICL alumni.

The end of the year is also the end for me in the office of the ICL Director. Although I am very grateful for the position, trust, and support that has been shown to me, it is with a heavy heart that I have decided to take on a new role at the Technical University of Munich in Germany, beginning in 2024. I am sure that ICL is well-positioned to thrive and grow over the next few years, and I will continue to contribute to ICL's success as much as it is still in my power!

Hartwig ANZT  
ICL DIRECTOR, 2022-2023



Mark Gates

*WE ARE* sad to say goodbye to Hartwig Anzt, who directed ICL for the past 18 months through the completion of ECP. We will continue collaborating with Hartwig through the Ginkgo project, which has seen an uptake in several DOE applications and math libraries, the sparse BLAS standardization, and undoubtedly other efforts.

Starting in 2024, I am taking on the role of Interim ICL Director during the transition period until the next permanent ICL Director. I came to ICL in 2011 as a post-doc after graduating from the University of Illinois, Urbana-Champaign, never dreaming that I would spend over 12 years here and have the opportunity to lead ICL. It has been an honor to work with the many people at ICL.

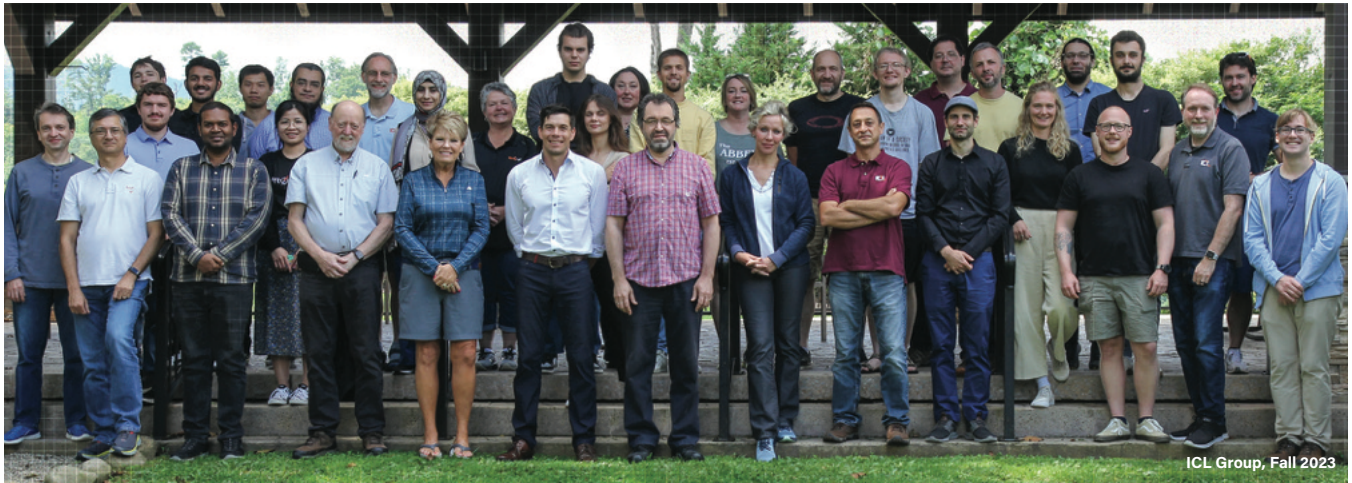
Looking forward to the coming year, we will continue to sustain and leverage our successes in ECP, foster collaborations with applications using ICL software, and look for new opportunities. Artificial Intelligence (AI) dominates the current market, and ICL is well-positioned to contribute to AI software through our linear algebra libraries and performance analysis utilities. Our Surrogates project is advancing the state-of-the-art in neural networks. We have several newly funded projects using AI for computational science, including AI for Environmental Remediation, Biochar Enhanced Ecosystems for Energy, Critical Minerals, and the newly awarded Consortium for Nuclear Forensics (CNF).

Our recent involvement in AI applications and computational science, building upon our historical leadership in HPC, uniquely positions us to lead advances in many areas of science and engineering.

*Mark Gates*

**Mark GATES**  
 INTERIM ICL DIRECTOR

## INTRODUCTION



### ENABLING TECHNOLOGIES FOR HIGH-PERFORMANCE COMPUTING SINCE 1989

**THE INNOVATIVE COMPUTING LABORATORY (ICL)** is a computer science research and development group in the Department of Electrical Engineering and Computer Science (EECS), situated in the heart of the University of Tennessee's Knoxville campus. ICL has a rich history that has spanned over 30 years of advancements in high-performance computing. These advancements have brought ever-increasing demands for parallelism, data management, energy efficiency, and resilience to the field.

ICL's work, which has evolved and expanded to address these challenges, 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-performance computing. In addition, ICL's portfolio of expertise includes high-performance parallel and distributed computing—with a focus on 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 such as life sciences, climate science, earthquake prediction, energy exploration, combustion and turbulence, advanced materials science, and drug design, among others.

FIND OUT MORE AT [icl.utk.edu/](https://icl.utk.edu/)

## AREAS OF RESEARCH



*THE NUMERICAL LINEAR* algebra libraries that serve as the backbone of scientific computing applications also serve as the strong basis of ICL's research expertise. As hardware architectures and computing trends change over time, it is essential that these libraries also be improved and modernized to achieve high levels of performance and efficiency on new platforms. ICL has a long history of developing and standardizing these libraries in this way, and it has multiple projects under development in this arena.



*AS THE NUMBER* of cores, nodes, and other components in HPC systems continues to grow, applications require runtime systems that can exploit greater levels of parallelism. Moreover, as the number of components increases, it becomes more difficult to detect and recover from failures and protect the integrity of data. These challenges must be addressed with fault-tolerant software and hardware, and the escalating communication traffic that they generate necessitates smarter and more efficient message passing standards and practices.

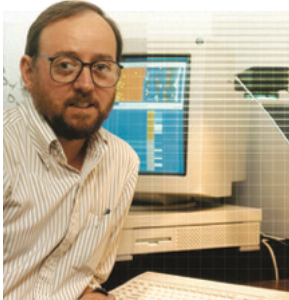


*ICL'S PERFORMANCE EVALUATION* tools enable programmers to see correlations between the structure and performance of their code. These correlations are important for performance tuning, optimization, debugging, and finding and correcting performance bottlenecks. Similarly, ICL's benchmark software is 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.



*THE PURSUIT OF* the world's most pioneering research demands the integration of the most sophisticated computational expertise available. Over recent years, ICL has become more involved in the emerging field of computational science. This inherently interdisciplinary field combines high-performance computing expertise with domain-specific knowledge to tackle complex scientific challenges in a wide range of areas like climate modeling, biomedical research, and materials science.

# HISTORY



**JACK DONGARRA ESTABLISHED** ICL in 1989 when he received a dual appointment as a Distinguished Professor at UTK and as a Distinguished Scientist at Oak Ridge National Laboratory. Over three decades, ICL has established itself as an internationally recognized research laboratory in advanced scientific and high-performance computing. The following timeline highlights just some of the significant projects and initiatives from ICL that have significantly influenced the landscape of high-performance and scientific computing.

## 1990

The **Level-3 Basic Linear Algebra Subprograms (BLAS)** specification extended earlier BLAS versions, introducing more complex and efficient routines for matrix-matrix operations, which significantly enhanced computational performance for high-level scientific and engineering applications.

## 1992

The **Basic Linear Algebra Communication Subprograms (BLACS)** project was created to make linear algebra applications easier to program and more portable. BLACS provided a standard communication layer critical for the development and performance optimization of distributed matrix computations.

Still developed today, the **Linear Algebra Package (LAPACK)** is a foundational software library for numerical linear algebra. It provides routines for solving systems of linear equations, eigenvalue problems, and singular value decomposition, building on the legacy of BLAS. LAPACK's significance lies in its efficiency on shared-memory processors, greatly influencing computational methods in various scientific and engineering applications.

## 1989

**Parallel Virtual Machine (PVM)** was a parallel networking tool that enabled a user to leverage a network of heterogeneous Unix and Windows machines as a single distributed parallel processor. Widely used in the 1990s and early 2000s, PVM played a significant role in the development of distributed computing techniques and applications and was awarded with a R&D 100 Award in 1994.

## 1993

The **TOP500** list ranks the world's 500 most powerful supercomputers. It serves as a benchmark for tracking the development of supercomputing technology and its evolution over time, reflecting shifts in computing power, architecture, and geopolitical dominance in high-performance computing. The list, updated biannually, has become a key indicator of technological and scientific progress in the field of computing.



**1994**  
PVM becomes ICL's first R&D 100 Award winner. Often referred to as the "Oscars of Invention," an R&D 100 Award signifies a significant contribution to science and technology and is seen as a mark of excellence in innovation.

## 1994

Version 1.0 of a standardized and portable message-passing system, the **Message Passing Interface (MPI)**, was released. MPI has become the *de facto* standard for communication among processes in a distributed memory system. The development of MPI is guided by the **MPI Forum**, a group comprised of representatives from academia, industry, and government institutions. ICL was one of the founding members and still participates in MPI Forum meetings.

## 1995

The **Scalable LAPACK (ScaLAPACK)** library extended the LAPACK library for high-performance distributed-memory architectures, providing routines for solving linear equations, eigenvalue problems, and singular value problems. ScaLAPACK's design reflects the shift in computational science towards parallel processing. Together, LAPACK and ScaLAPACK form foundational technologies for high-performance computing.

## 1996

**NetSolve** was a client-server system that enabled users to solve complex scientific problems using remote resources. NetSolve envisioned scientists, engineers, research professionals, and students working with the powerful and flexible toolset provided by their familiar desktop computing environment and yet being able to easily draw on the vast, shared resources of the Grid for exceptional computational resource needs.

## 1997

**Automatically Tuned Linear Algebra Software (ATLAS)** is a software library for linear algebra that automatically optimized itself for specific hardware configurations to maximize performance, a pioneering approach that greatly influenced subsequent software development in high-performance computing.

## 1999

ICL's flagship performance analysis tool, the **Performance Application Programming Interface (PAPI)**, is a standardized, easy-to-use interface that provides a consistent methodology for collecting performance data from a variety of hardware counters on most major processor platforms. PAPI received an R&D 100 Award in 2002 and is still developed and widely used today. The PAPI team released version 7.1.0 in December 2023.



**1999**  
ATLAS and NetSolve each received R&D 100 Awards.



**2000**  
ICL moved from Ayres Hall to the newly-built Claxton building on UTK campus.

## 2000

**High-Performance Linpack (HPL)** is a benchmark for distributed-memory computers that solves a (random) dense linear system in double-precision (64-bit) arithmetic. HPL is often one of the first programs to run on large HPC machines, producing a result that can be submitted to the TOP500 list of the world's fastest supercomputers.



**2002**  
PAPI was recognized with an R&D 100 Award.

## 2002

**Fault Tolerant MPI (FT-MPI)** extended the standard MPI by adding fault tolerance capabilities. This innovation allows programs to continue functioning despite node failures, enhancing parallel applications' robustness and resilience. FT-MPI was later merged with LA-MPI, LAM/MPI, and PACX-MPI to form the Open MPI project.

## 2003

The **HPC Challenge (HPCC)** benchmark suite provided a comprehensive set of tests to evaluate the performance of HPC systems. HPCC extended beyond the capabilities of the LINPACK benchmark, offering a broader assessment of memory bandwidth, computational speed, and network communication to better understand the varied performance aspects of HPC systems across a range of complex computational tasks.



**2004**

In 2004, four institutions merged efforts in the **Open Source Message Passing Interface (Open MPI)**: FT-MPI from UTK/ICL, LA-MPI from LANL, and LAM/MPI from Indiana University, with contributions from PACX-MPI at the University of Stuttgart. Open MPI is an open-source implementation of the Message Passing Interface (MPI) standard that is fundamentally centered around component concepts.

**2012**

The **Parallel Runtime Scheduling and Execution Controller (PaRSEC)** provides a generic framework for architecture-aware scheduling and management of microtasks on distributed, many-core heterogeneous architectures. PaRSEC's innovative approach optimizes dataflow and dependencies in parallel applications, significantly improving performance and scalability in modern HPC environments, particularly for dynamic and irregular computations.

**2013**

The **High Performance Conjugate Gradients (HPCG)** benchmark was designed as a complement to the HPL benchmark that drives the TOP500. HPCG focuses on iterative methods and data access patterns more representative of real-world applications, providing a more comprehensive view of a system's computational capabilities, particularly in memory-bound operations. HPCG awards are now presented in conjunction with TOP500 awards biannually.



**2016**  
At SC16, Clint Whaley and Jack Dongarra's 1998 paper on ATLAS was recognized with a Test of Time Award, which "recognizes an outstanding paper that has deeply influenced the HPC discipline."

**2019**

The **Ecosystem for Programming and Executing eXtreme Applications (EPEXA)** team is creating a production-quality, open-source software ecosystem to allow rapid composition of advanced scientific applications for modern distributed memory heterogeneous platforms. A key outcome of EPEXA is the **Template Task Graph (TTG)** programming model, which facilitates an intuitive expression of parallelism in algorithms handling irregular and uneven data sets that are poorly served by current models on modern HPC systems.

**2008**

ICL initiated two projects in response to the evolving landscape of HPC hardware architectures. **Matrix Algebra on GPU and Multi-core Architectures (MAGMA)** is a linear algebra library that enables applications to exploit the power of heterogeneous systems of multi-core CPUs and multiple GPUs or coprocessors. **Parallel Linear Algebra Software for Multi-core Architectures (PLASMA)** is a dense linear algebra package designed to deliver the highest possible performance from a system of multiple sockets of multi-core CPUs.

**2012**

**User Level Failure Mitigation (ULFM)** is an extension of the MPI standard, designed to enhance fault tolerance in parallel computing environments. ULFM provides mechanisms for detecting and recovering from failures at the user level, allowing applications to continue operation despite node or process failures, thereby improving resilience and reliability in large-scale high-performance computing systems.



**2016**  
ICL landed seven awards through the Exascale Computing Project (ECP) and was the lead institution on four projects focused on enabling technologies for exascale computing.

**2017**

The **Batched BLAS (BBLAS)** effort was initiated to create an API for efficiently handling multiple independent BLAS operations simultaneously (in batch), and to serve as a working forum for establishing this strategy as the next official BLAS standard. This approach is particularly useful for optimizing performance when dealing with a large number of small-sized matrix or vector operations, which is common in many scientific and engineering applications.

**2020**

The **Surrogate Benchmark Initiative (Surrogates)** for short) aims to provide benchmarks and tools for assessing deep neural network "surrogate" models, which can imitate part or all of a simulation and produce the same outcomes while requiring fewer resources, enabling faster simulations and predictions while maintaining a high level of accuracy. Tools developed under Surrogates will evaluate these models to measure progress and inform the co-design of new HPC systems to support their use.

**2009**

The **International Exascale Software Project (IESP)** was a global series of workshops spanning three years that brought together representatives of the international HPC community focused on developing a cohesive software infrastructure for exascale computing. At the end of the series, the *IESP Roadmap* was published, a strategic plan outlining the necessary steps to successfully create such an infrastructure.



**2013**  
Jack Dongarra was awarded with the ACM/IEEE Ken Kennedy Award "for his leadership in designing and promoting standards for mathematical software used to solve numerical problems common to high-performance computing."

**2016**

**Distributed Tasking for Exascale (DTE)** extended the capabilities of PaRSEC for exascale architectures.

**Exascale Performance Application Programming Interface (Exa-PAPI)** built on PAPI and extended it with performance counter monitoring capabilities for advanced ECP hardware and software technologies.

**2018**

The **ECP Fast Fourier Transform (ECP-FFT)** project was tasked with designing and implementing a fast and robust 2-D and 3-D fast Fourier transform (FFT) library that targets large-scale heterogeneous systems with multi-core processors and hardware accelerators and to do so as a co-design activity with other ECP application developers. The resulting library, known as **heFFT**e, delivers highly efficient FFTs for exascale computing.



**2021**  
Jack Dongarra received the 2021 ACM A.M. Turing Award "for pioneering contributions to numerical algorithms and libraries that enabled high performance computational software to keep pace with exponential hardware improvements for over four decades."



**2013**

Building upon the work of the IESP, the **Big Data and Extreme-scale Computing (BDEC)** workshop series was initiated to tackle the emerging challenges and opportunities at the nexus of large-scale data analysis and exascale computing. A follow-up series, **BDEC2**, later extended the effort through 2020 and culminated in the publication of the "Pathways to Convergence" strategic roadmap, a comprehensive guide outlining the future direction for integrating these emerging technological fields.

The **Production-ready, Exascale-enabled Krylov Solvers for Exascale Computing (PEEKs)** effort aimed to advance the capabilities of the ECP software stack by making new scalable algorithms accessible within the **Ginkgo** software ecosystem.

**Software for Linear Algebra Targeting Exascale (SLATE)** was designed to provide fundamental dense linear algebra capabilities to the ECP software ecosystem, building a new modern version of the venerable **ScalLAPACK** library.

**2019**

Now known as **HPL-MxP**, a new benchmark initiative was introduced in 2019 to highlight the emerging convergence of high-performance computing and artificial intelligence (AI) workloads. Machine learning methods that fuel advances in AI can deliver results that utilize much lower precision compared to the requirements in traditional HPC fields.

**2023**

As high-performance computing expertise becomes more crucial in scientific research, ICL has become increasingly involved in more interdisciplinary projects in the field of Computational Science.

ICL leads the HPC/AI cross-cutting focus area within the new **Consortium for Nuclear Forensics (CNF)**. Sponsored by the National Nuclear Security Administration (NNSA), the CNF comprises 16 Universities and 7 National Laboratories that contribute to important research fields within nuclear forensics.

## 2023 HIGHLIGHTS

# ECP RETROSPECTIVE

THE Exascale Computing Project (ECP) marked a monumental shift in the computational science landscape. The program was initiated in 2016 by the U.S. Department of Energy (DOE) and the National Nuclear Security Administration (NNSA) with the ambitious goal of developing the technologies required to support a computing ecosystem capable of breaking through the exascale barrier, a benchmark of computing performance exceeding a quintillion ( $10^{18}$ ) calculations per second. This leap represents not just a quantitative enhancement in computing speed, but a qualitative transformation in computational capabilities, enabling unprecedented scientific research and innovation.

The ECP's goals included not only building the hardware required to reach these computational speeds but also developing the software, applications, and tools necessary to run efficiently on exascale systems. This comprehensive strategy was designed to tackle some of the most complex challenges in various domains, including energy sustainability, environmental science, materials engineering, and more. By pushing computational frontiers, ECP aspired to unlock new realms of scientific inquiry, simulating intricate processes and phenomena with unmatched precision and scale.

ICL played a prominent role in the ECP, having contributed multiple projects in the program's Software Technologies and Application Development thrusts. These projects spanned ICL's core research areas of Numerical Linear Algebra, Distributed Computing, and Performance Analysis, demonstrating the foundational importance of ICL's expertise in high-performance computing.

The ECP proved triumphant when the *Frontier* supercomputer at Oak Ridge National Laboratory officially broke the exascale barrier. This achievement marked a new era in computational science, opening up new possibilities for scientific discovery and technological innovation.



ICL members in attendance at the 2023 ECP Annual Meeting in Houston, Texas



Hear a conversation with Jack Dongarra about the ECP on episode 105 of the *Let's Talk Exascale* podcast

[tiny.utk.edu/ecp-podcast](https://tiny.utk.edu/ecp-podcast)



## CEED

ICL LEAD

Stanimire Tomov

FIND OUT MORE AT

[ceed.exascaleproject.org/](http://ceed.exascaleproject.org/)

**“THE CENTER FOR Efficient Exascale Discretizations (CEED) is a focused team effort within the U.S. Department of Energy Exascale Computing Project that aims to develop the next-generation discretization software and algorithms to enable a wide range of finite element applications to run efficiently on future hardware.”** – [EXASCALEPROJECT.ORG](http://EXASCALEPROJECT.ORG)

The Lawrence Livermore National Laboratory (LLNL)–led **Center for Efficient Exascale Discretizations (CEED)** co-design effort developed 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 NNSA applications to run efficiently on 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 is instrumental in identifying, developing, and optimizing tensor contractions that are essential building blocks for these kinds of DOE/NNSA applications. The ICL team also plays an integral role in co-designing application programming interfaces (APIs) with the LLNL scientists, external partners, and vendors. It delivers a high-performance tensor contractions package through the Matrix Algebra on GPU and Multicore Architectures (MAGMA) library.

## CLOVER

ICL LEADS

Hartwig Anzt

Mark Gates

Stanimire Tomov

**“SCIENTIFIC APPLICATIONS NEED to apply efficient and scalable implementations of numerical operations, such as matrix–vector products and Fourier transforms, in order to simulate their phenomena of interest. Software libraries are powerful means of sharing verified, optimized numerical algorithms and their implementations. The CLOVER project is delivering scalable, portable numerical algorithms to facilitate efficient simulations.”** – [EXASCALEPROJECT.ORG](http://EXASCALEPROJECT.ORG)

The ECP **CLOVER** project focused on developing three advanced, vendor-agnostic GPU-accelerated numerical libraries. This project addressed the need for efficient computational tools that are compatible across various GPU platforms, catering to the diverse and evolving landscape of high-performance computing.

Each of the three libraries in CLOVER has a distinct focus: **SLATE** is dedicated to dense linear algebra computations, offering optimized performance for these tasks on GPU systems. **Ginkgo** specializes in sparse linear algebra, providing efficient solutions for computations involving sparse matrices. Lastly, **heFFTe** focuses on multidimensional Fast Fourier Transforms, a

critical component in many scientific calculations, ensuring accelerated performance on GPUs.

By spearheading the development of these three libraries, CLOVER positioned itself as a cornerstone in the realm of GPU-accelerated distributed computing. This initiative represents a significant stride in the ongoing journey to harness the full potential of GPU technologies, underscoring the importance of adaptable, cross-platform solutions in high-performance computing.

## 2023 HIGHLIGHTS

ECP  
RETROSPECTIVE**DTE**

ICL LEAD

George Bosilca

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[icl.utk.edu/dte](http://icl.utk.edu/dte)

**“ONE DIFFICULTY ASSOCIATED with programming exascale systems is expressing the tasks comprising a scientific simulation and then mapping them to the heterogenous computational resources on that system, while achieving high performance. PaRSEC supports the development of domain-specific languages and tools to simplify and improve the productivity of scientists when using a task-based system and provides a low-level runtime.” – EXASCALEPROJECT.ORG**

The **Distributed Tasking for Exascale (DTE)** project has extended the capabilities of ICL’s Parallel Runtime and Execution Controller (PaRSEC)—a generic framework for architecture-aware scheduling and management of microtasks on distributed, many-core, heterogeneous architectures. The PaRSEC environment 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 (DSLs) and extensions and tools for debugging, trace collection, and analysis.

PaRSEC also enables fast prototyping DSLs to express the dependencies between tasks. It provides a stable, scalable, and efficient distributed runtime so they can run on any execution platform at any scale. The underlying dataflow paradigm attacks both sides of the exascale challenge: managing extreme-scale parallelism and maintaining the performance portability of the code. The DTE project has been a vital extension and continuation of this effort. It has ensured that PaRSEC meets the critical needs of ECP application communities regarding scalability, interoperability, and productivity.

**Exa-PAPI**

ICL LEADS

Heike Jagode  
Anthony Danalis

FIND OUT MORE AT

[icl.utk.edu/exa-papi](http://icl.utk.edu/exa-papi)

**“UNDERSTANDING THE PERFORMANCE characteristics of exascale applications is necessary in order to identify and address the barriers to achieving performance goals. This becomes more difficult as the architectures become more complex. The Performance Application Programming Interface (PAPI) provides both library and application developers with generic and portable access to low-level performance counters found across the exascale machine.” – EXASCALEPROJECT.ORG**

The **Exa-PAPI** project has expanded PAPI’s capabilities in performance counter monitoring, incorporating support for power management across cutting-edge hardware and software technologies. This includes performance and power monitoring for AMD GPUs through integration with AMD ROCm and ROCm-SMI, Intel Ponte Vecchio GPUs via Intel’s oneAPI Level Zero, and NVIDIA GPUs through the Perfworks API. Additionally, PAPI is compatible with interconnects, the latest CPUs, and ARM chips. These enhancements have been implemented while preserving the standard PAPI interface and methodology for utilizing low-level performance counters in CPUs, GPUs, on/off-chip memory, interconnects, and the I/O system, encompassing energy and power management. To strengthen PAPI’s sustainability, ECP has facilitated its integration into the Spack package manager and the Extreme-scale Scientific Software Stack (E4S), ensuring software robustness through continuous integration and continuous deployment. In addition

to hardware counter-based data, PAPI now supports the registration and monitoring of Software-Defined Events. This exposes the internal behavior of runtime systems and libraries like PaRSEC, SLATE, MAGMA, and Ginkgo to applications utilizing those libraries, broadening the scope of performance events to include software-based information. Additionally, PAPI has been expanded with the Counter Analysis Toolkit, aiding in native performance counter disambiguation through micro-benchmarks. These micro-benchmarks probe various essential aspects of modern chips, contributing to the classification of raw performance events.

In summary, the Exa-PAPI project has enabled PAPI to add comprehensive counter analysis capabilities, advanced performance and power monitoring support for exascale hardware components, and broadened the scope of performance events to encompass not only hardware-related metrics but also software-based information.

## OMPI-X

### ICL LEADS

George Bosilca  
Joseph Schuchart

FIND OUT MORE AT  
[icl.utk.edu/ompi-x](http://icl.utk.edu/ompi-x)

**“THE MESSAGE PASSING Interface (MPI) is a community standard for inter-process communication and is used by the majority of DOE’s parallel scientific applications running on pre-exascale systems. The MPI standard can be implemented on all the large systems. The OMPI-X project ensures that the MPI standard and its specific implementation in Open MPI meet the needs of the ECP community in terms of performance, scalability, and capabilities.”** – [EXASCALEPROJECT.ORG](http://EXASCALEPROJECT.ORG)

The **Open MPI for Exascale (OMPI-X)** project focused on preparing the 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. Open MPI is a widely used, high-quality, open-source implementation of the MPI standard. However, despite their history and popularity, neither Open MPI nor the MPI standard itself were ready for the changes in hardware and software that has accompanied exascale computing.

To mitigate this concern, OMPI-X addressed 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.

## xSDK

### ICL LEAD

Piotr Luszczek

FIND OUT MORE AT  
[xsdk.info/ecp/](http://xsdk.info/ecp/)

**“THE LARGE NUMBER of software technologies being delivered to the application developers poses challenges, especially if the application needs to use more than one technology at the same time, such as using a linear solver from the PETSc/TAO mathematics library in conjunction with a time integrator from the SUNDIALS library. The xSDK project is an effort to create a value-added aggregation of mathematics and scientific libraries, to increase the combined usability.”** – [EXASCALEPROJECT.ORG](http://EXASCALEPROJECT.ORG)

The **Extreme-Scale Scientific Software Development Kit (xSDK)** was a collaborative effort between Argonne National Laboratory, ICL, Karlsruhe Institute of Technology, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Sandia National Laboratories, and the University of California, Berkeley. The project aimed to enable seamless integration and combined use of diverse, independently developed software packages for ECP applications. This includes a wide range of high-quality software libraries, solver packages, and two applications that address the strategic requirements of DOE’s Office of Science.

xSDK streamlined processes for system administrators and application developers by standardizing naming conventions, runtime behavior, and installation procedures through its community policies. Each xSDK package provides a Spack installation script that can be invoked independently or through the installation of xSDK’s Spack package. In addition, xSDK ships with a set of curated examples showing potential package integrations into application exemplars. ICL’s MAGMA, PLASMA, SLATE, Ginkgo, and heFFTe libraries were included in the latest release of xSDK versioned as 1.0.

# 2023 HIGHLIGHTS

## CONFERENCE HIGHLIGHTS



## SC23

The International Conference for High Performance Computing, Networking, Storage, and Analysis returned to Denver in 2023, November 12th–17th. This year's conference General Chair was ICL alumnus Dorian Arnold. ICL was once again well represented at the conference. ICL's Associate Director, Deborah Penchoff, served as SC23's Plenary Productions Chair, and ICL members led and participated in workshops, tutorials, and Birds of a Feather sessions, demonstrating their leadership in the field.



The annual ICL Alumni Dinner was held at Henry's Tavern in Denver on November 15th, and gathered around 40 past and present ICL members. It was a vibrant evening fostering connections and re-connections among attendees, embodying the collaborative spirit fundamental to ICL's legacy.

## AWARDS

### BEST PAPER FINALIST

ICS 2023 International Conference on Supercomputing  
Orlando, FL, June 2023

Lindquist, N., P. Luszczek, and J. Dongarra  
**Using Additive Modifications in LU Factorization Instead of Pivoting**

### BEST POSTER

29th International European Conference on Parallel and Distributed Computing (Euro-Par)  
Limassol, Cyprus, August 2023

Cojean, T., F. Göbel, and H. Anzt  
**BDDC Preconditioning in the Project MICROCARD**

### BEST PAPER FINALIST

37th IEEE International Parallel & Distributed Processing Symposium (IPDPS)  
St. Petersburg, FL, May 2023

Sid-Lakhdar, W., S. Cayrols, D. Bielich, A. Abdelfattah, P. Luszczek, M. Gates, S. Tomov, H. Johansen, D. Williams-Young, T. Davis, J. Dongarra, and H. Anzt  
**PAQR: Pivoting Avoiding QR factorization**

### BEST STUDENT POSTER

IEEE International Conference on Cluster Computing 2023  
Sante Fe, NM, October 2023

Mishler, D., J. Ciesko, S. Olivier and G. Bosilca  
**Performance Insights into Device-initiated RMA using Kokkos Remote Spaces**

## HOSTED WORKSHOPS & COLLABORATIONS



### ICL/ORNL COLLABORATION MEETING

On May 1, ICL hosted a group of researchers from ORNL for a one-day workshop with ICL members. The event was organized by ICL's George Bosilca as an effort to foster collaboration between the two East Tennessee area HPC research groups.



### LARGE SCALE SYSTEMS WORKSHOP

ICL hosted the 16th Scheduling for Large Scale Systems Workshop from May 22 through May 24. The workshop featured thematic half-day sessions focused on topics related to scheduling and algorithms for large-scale systems. George Bosilca and Yves Robert organized the event, which attracted 25 researchers from around the globe, including ICL alumni Mathieu Faverge and Amina Guermouche.



### AI-ENVIRONMENT KICK-OFF MEETING

In July, ICL hosted the formal Kick-off meeting for the AI for Environmental Remediation project, which aims to spearhead the design of novel AI-driven solutions to reduce environmental contamination involving REEs and actinides through HPC-exascale enabling capabilities. Joining ICL's George Bosilca, Deborah Penchoff, and Stan Tomov were Niki Labbe from the UT Institute of Agriculture, Charles Sims from UTK's Howard H. Baker Jr. School of Public Policy and Public Affairs, Vasileios Anagnostopoulos from University of Central Florida, and Charles Peterson from University of California, Los Angeles.



### SPARSE BLAS WORKSHOP

ICL hosted a Sparse BLAS Workshop November 7-9, 2023. The workshop brought together scientists from major research institutions and industry partners, including AMD, ARM, Intel, MathWorks, and NVIDIA, and focused on developing a common understanding and interface for basic operations on sparse linear algebra objects.

## 2023 HIGHLIGHTS

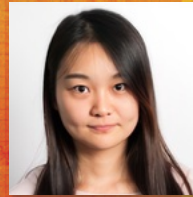
### CONGRATULATIONS

#### 2023 Graduates

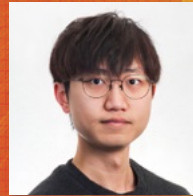
ICL provides an excellent environment for students to gain knowledge and experience, working alongside its expert research staff. In 2023, ICL celebrated the graduation of three students. Neil Lindquist completed his PhD in Computer Science, advised by Jack Dongarra and Piotr Luszczek, focusing on *Reducing Communication in the Solution of Linear Systems*. Jiali Li, under the guidance of Dongarra and George Bosilca, earned her PhD with her dissertation titled *Optimizing Collective Communication for Scalable Scientific Computing and Deep Learning*. Patrick Hon Man Lau earned his Master's in Computer Science, advised by Stanimire Tomov and Hartwig Anzt.



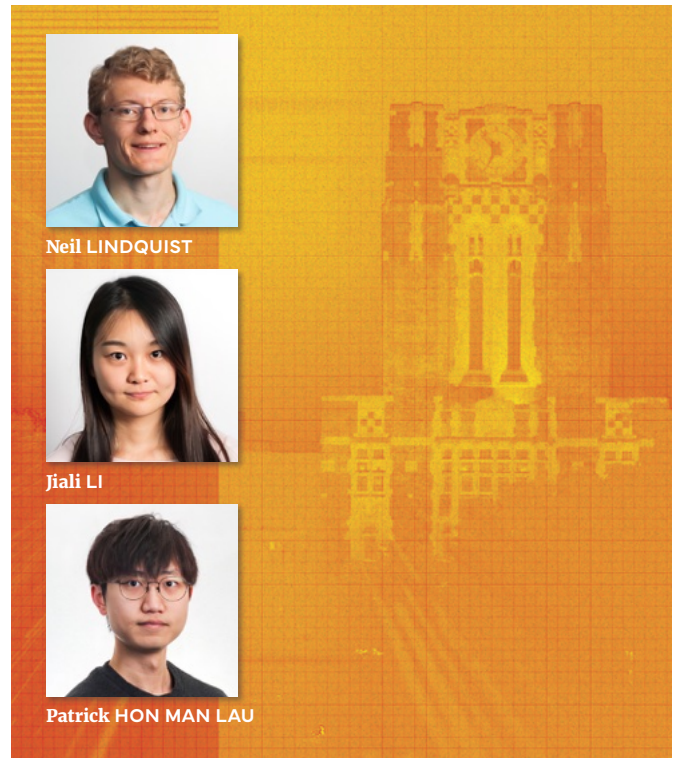
Neil LINDQUIST



Jiali LI

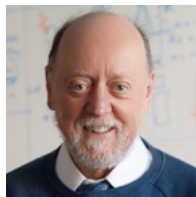


Patrick HON MAN LAU



#### Jack Dongarra Elected to the National Academy of Sciences

In May 2023, ICL founder Jack Dongarra was elected to the National Academy of Sciences. This prestigious recognition is a testament to his contributions to the field of computer science and high-performance computing. Dongarra has been at the forefront of developing numerical algorithms, software libraries, and performance analysis tools that are widely used in scientific and engineering applications.



#### TCE Commitment to Inclusive Community Award

In April 2023, ICL Associate Director Deborah Penchoff was awarded with the Tickle College of Engineering Commitment to Inclusive Community Award. The award recognizes an individual within the college who has demonstrated a commitment to diversity and inclusion in consideration of affordability, ability, identity, and access. The Commitment to Inclusive Community Award recipient demonstrates an exceptional understanding of diversity and inclusiveness beyond the call of duty.



## SOFTWARE RELEASES



### **Ginkgo 1.7**

Ginkgo is a high-performance linear algebra library for GPU systems, with a focus on solution of sparse linear systems. Version 1.7 was released in November 2023.

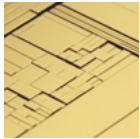
AVAILABLE AT  
[ginkgo-project.github.io/](https://github.com/ginkgo-project/ginkgo)



### **heFFTe 2.4.0**

Version 2.4.0 of the heFFTe software library was released in October 2023. heFFTe is focused on providing highly efficient and scalable FFT computations on distributed GPU architectures, designed specifically to meet the demands of exascale computing.

AVAILABLE AT  
[github.com/icl-utk-edu/heffte/](https://github.com/icl-utk-edu/heffte/)



### **LAPACK 3.12.0**

First released in 1992, the LAPACK software library for numerical linear algebra is a foundational HPC technology used in systems worldwide. Version 3.12.0 was released in November 2023, featuring new features, performance improvements, and bug fixes.

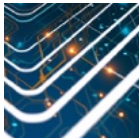
AVAILABLE AT  
[www.netlib.org/lapack/](https://www.netlib.org/lapack/)



### **MAGMA 2.7.2**

MAGMA is a collection of next-generation dense linear algebra libraries that is designed for heterogeneous architectures, such as multiple GPUs and multi- or many-core CPUs. MAGMA had two releases in 2023, with the latest version, 2.7.2, in August.

AVAILABLE AT  
[icl.utk.edu/magma](https://icl.utk.edu/magma)



### **Open MPI 5.0.1**

The Open MPI Project is an open-source Message Passing Interface implementation that is developed and maintained by a consortium of academic, research, and industry partners, including ICL's Distributed Computing team. The latest major version, v5, was released in 2023.

AVAILABLE AT  
[www.open-mpi.org](https://www.open-mpi.org)



### **PAPI 7.1.0**

ICL's flagship performance analysis tool, PAPI, provides a consistent interface and methodology for collecting performance counter information from various hardware and software components. The latest major version, 7.1.0, was released in December 2023.

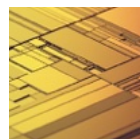
AVAILABLE AT  
[icl.utk.edu/papi](https://icl.utk.edu/papi)



### **PLASMA 23.8.2**

PLASMA is a dense linear algebra package at the forefront of multicore computing, designed to deliver the highest possible performance from a system of multiple sockets of multi-core CPUs. Version 23.8.2 was released in August 2023.

AVAILABLE AT  
[github.com/icl-utk-edu/plasma](https://github.com/icl-utk-edu/plasma)



### **SLATE 2023.11.05**

SLATE is a distributed, GPU-accelerated, dense linear algebra library targeting current and upcoming extreme-scale high-performance computing systems.

AVAILABLE AT  
[github.com/icl-utk-edu/slate/](https://github.com/icl-utk-edu/slate/)

## 2023 HIGHLIGHTS

VISITING  
RESEARCHERS

*THE SPIRIT OF* collaboration is fundamental to ICL's approach to research. The following researchers visited ICL in 2023, each bringing their unique expertise and perspectives to the group.



**Andreas ADELMANN**  
PAUL SCHERRER INSTITUTE  
VILGIGEN, SWITZERLAND



**Terry COJEAN**  
KARLSRUHE INSTITUTE OF TECHNOLOGY  
KARLSRUHE, GERMANY



**Lisa GAEDKE-MERZHÄUSER**  
UNIVERSITÀ DELLA SVIZZERA ITALIANA  
LUGANO, SWITZERLAND



**Thomas GRÜTZMÄCHER**  
KARLSRUHE INSTITUTE OF TECHNOLOGY  
KARLSRUHE, GERMANY



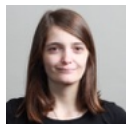
**Sascha HUNOLD**  
VIENNA UNIVERSITY OF TECHNOLOGY  
VIENNA, AUSTRIA



**Albert KAHIRA**  
JÜLICH SUPERCOMPUTING CENTRE  
JÜLICH, GERMANY



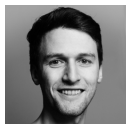
**Sonali MAYANI**  
PAUL SCHERRER INSTITUTE  
VILGIGEN, SWITZERLAND



**Veronica MONTANARO**  
ETH ZÜRICH  
ZÜRICH, SWITZERLAND



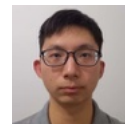
**Briec NICOLAS**  
ENSEIRB-MATMECA  
TALENCE, FRANCE



**Tobias RIBIZEL**  
KARLSRUHE INSTITUTE OF TECHNOLOGY  
KARLSRUHE, GERMANY



**Yves ROBERT**  
ENS LYON  
LYON, FRANCE



**Yu-Hsiang MIKE TSAI**  
KARLSRUHE INSTITUTE OF TECHNOLOGY  
KARLSRUHE, GERMANY



**Robert UNDERWOOD**  
ARGONNE NATIONAL LABORATORY



**You WU**  
ETH ZÜRICH  
ZÜRICH, SWITZERLAND



## ICL SEMINAR SERIES

**FRIDAY LUNCH TALKS** are a long-standing tradition at ICL that offer further opportunities to foster collaborations and bring new ideas to the group. ICL's 2023 Seminar Series featured a distinguished group of invited speakers from UTK and ORNL to other groups around the globe.



JAN 27

**David ICOVE**  
UL Professor of Practice  
UTK EECS



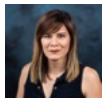
FEB 10

**Slaven PELES**  
Senior Computational Scientist  
ORNL



FEB 17

**Jakob LUETTGAU**  
Research Assistant Professor  
UTK Global Computing Lab



FEB 24

**Andrea DELGADO**  
Distinguished Staff Fellow  
ORNL



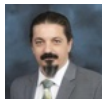
MAR 3

**Corey AHL**  
PhD Student  
UTK Nuclear Engineering



MAR 10

**Rafael FERREIRA DA SILVA**  
Senior Research Scientist  
ORNL



MAR 17

**Vincent PAQUIT**  
Section Head, Secure & Digital  
Manufacturing  
ORNL



MAR 24

**Mathieu FAVERGE**  
Assistant Professor  
Bordeaux Institute of Technology



MAR 31

**Sascha HUNOLD**  
Associate Professor  
Vienna University of Technology



APR 14

**Robert HARRISON**  
Professor / Director of Institute for  
Advanced Computational Science  
Stony Brook University



APR 21

**Reza ABEDI**  
Associate Professor  
UT Space Institute



APR 28

**Suzanne PARETE-KOON**  
HPC Engineer  
ORNL



MAY 5

**Nicholas PETERS**  
Section Head &  
Distinguished R&D Staff  
ORNL



MAY 12

**Sunita CHANDRASEKARAN**  
Associate Professor  
University of Delaware



AUG 25

**Briec NICOLAS**  
Computer Science Engineering  
Student  
ENSEIRB-MATMECA



SEP 7

**Devina SANJAYA**  
Assistant Professor  
UTK MABE Department



SEP 8

**Rinkle JUNEJA**  
R&D Associate  
ORNL



SEP 22

**Lisa GAEDKE-MERZHÄUSER**  
PhD Student  
Università della Svizzera italiana



SEP 29

**Steffen SCHOTTHOEFER**  
Householder Fellow  
ORNL



OCT 6

**Fabrizio BISETTI**  
Associate Professor  
University of Texas at Austin



OCT 13

**Thomas GILLIS**  
Postdoctoral Appointee  
Argonne National Laboratory



OCT 20

**Cory HAUCK**  
Applied Mathematician  
ORNL



OCT 27

**Yaohung (MIKE) TSAI**  
Research Scientist  
Meta



NOV 10

**Tobias RIBIZEL**  
Research Software Engineer  
Karlsruhe Institute of Technology



DEC 8

**Yves ROBERT**  
Professor  
ENS Lyon

## RESEARCH

### AI-Environment

ICL LEAD

Deborah Penchoff

FIND OUT MORE AT

[icl.utk.edu/ai-env](http://icl.utk.edu/ai-env)

The **AI For Environmental Remediation** Project is funded by the AI Tennessee Initiative, and it focuses on applying AI-driven tools to reduce environmental toxicity stemming from nuclear and radiochemical processes. The project contributes to the University's mission of leading research and development efforts to increase sustainability. The goal of the project is to design AI-driven solutions (1) to reduce environmental contamination from anthropogenic sources and (2) to develop environmentally friendly separations of Rare Earth Elements (REEs).

The team includes members from The University of Tennessee Knoxville, the UT Institute for Agriculture, the University of Central Florida, and the University of California, Los Angeles.

### BALLISTIC

ICL LEAD

Piotr Luszczyk

FIND OUT MORE AT

[icl.utk.edu/ballistic](http://icl.utk.edu/ballistic)

**Basic ALgebra Libraries for Sustainable Technology with Interdisciplinary Collaboration (BALLISTIC)** is an NSF-funded effort to create new software components capable of running at every level of the hardware pyramid by delivering seamless access to the most up-to-date algorithms, numerics, and performance via familiar Linear Algebra PACKage (LAPACK) and Scalable Linear Algebra PACKage (ScaLAPACK) interfaces. BALLISTIC makes advanced algorithms, numerics, and performance capabilities available through new interface extensions and by providing a well-engineered conduit for channeling new developments to science and engineering applications that depend on high-performance, high-quality linear algebra libraries.

Scientific software libraries have long provided a large and growing resource for high-quality, reusable software components upon which applications from science and engineering can be rapidly constructed. The BALLISTIC project will introduce tools to simplify the transition to the next generation of extreme-scale computer architecture.

### Batched BLAS

ICL LEAD

Stanimire Tomov

FIND OUT MORE AT

[icl.utk.edu/bblas](http://icl.utk.edu/bblas)

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 simultaneously produce large numbers of small matrices.

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 establishing the consensus for the next official standard that will serve the scientific community and ensure support from hardware vendors.

### Batched Sparse Linear Algebra

ICL LEAD

Piotr Luszczyk

Batched sparse linear algebra solvers form the new frontier for algorithmic development and performance engineering. Many applications require simultaneous solutions of small linear systems of structurally sparse equations. In order to move towards higher hardware utilization, it is essential to provide these applications with appropriate interfaces to efficient batched sparse solvers running on modern hardware accelerators.

The **Batched Sparse Linear Algebra** effort developed batched kernels for small tensor operations for unassembled matrix-free iterative solvers, batched solvers for partially assembled operators, and batched solvers with support for various sparse formats. Participants included representatives from ECP's numerical libraries, scientific applications, and hardware vendors. The project milestones were sets of interfaces to batched sparse linear algebra solvers running on hardware accelerators for use in ECP libraries and applications. Other noteworthy outcomes included the development of sparse batched kernels, solvers/preconditioners, and the creation of interoperability in xSDK libraries with sparse and dense batched functions to benefit ECP applications.

### BIOCHAR

ICL LEAD

Deborah Penchoff

The **Biochar Enhanced Ecosystem Services for Energy Crop Systems in the Southeast** project is sponsored by the Department of Energy Office of Energy Efficiency and Renewable Energy. The project focuses on decarbonization strategies in the supply chain to decrease the carbon intensity of sustainable aviation fuel (SAF) through the application of biochar, a carbon-rich soil enhancer made from organic waste. Biochar contributes to carbon sequestration and fertilization and allows for pathways in a circular system. ICL's contribution to the project focuses on applying HPC and AI-driven strategies to predict biochar properties to optimize its utilization in SAF production systems in the southeast.

Team members are from The University of Tennessee, Knoxville; The University of Tennessee Institute of Agriculture; Tennessee State University; Mississippi State University; Oak Ridge National Laboratory; and industry partners Kolmar-Americas and Genera Inc.

## CETOP

ICL LEADS  
Hartwig Anzt  
Natalie Beams

FIND OUT MORE AT  
[icl.utk.edu/cetop](http://icl.utk.edu/cetop)

ICL will participate in the **Center for Edge of Tokamak Optimization (CETOP)**, a new SciDAC effort led by the Princeton Plasma Physics Laboratory (PPPL). In addition to PPPL and UTK, the project brings together researchers from universities (Columbia, Utah State), national labs (Lawrence Livermore, Oak Ridge, Brookhaven, Argonne, National Renewable Energy Lab), and industry (Fiat Lux, General Atomics). CETOP aims to advance the current understanding of transient edge-localized modes (ELMs) in burning plasmas. ELMs are a key risk factor in tokamak fusion reactors, and controlling them is vital to creating a tokamak capable of deployment in a practical fusion power plant. Harnessing the power of HPC, CETOP will create new high-fidelity-based ELM stability maps and also perform stability analyses for some non-ELMing regimes. An AI/ML thrust will extrapolate from databases to guide ELM-free design optimization. ICL's main contribution to CETOP will focus on improving GPU-capable preconditioning of solvers in the plasma physics codes and will make use of the Ginkgo library.

## Consortium for Nuclear Forensics

ICL LEAD  
Deborah Penchoff

FIND OUT MORE AT  
[icl.utk.edu/cnf](http://icl.utk.edu/cnf)

The **Consortium for Nuclear Forensics (CNF)** is the latest consortium sponsored by the US Department of Energy's National Nuclear Security Administration (NNSA). It focuses on nuclear forensics research and education involving rapid turnaround forensics, advanced analytical methods, ultrasensitive measurements, signature discovery, and prompt effects. These efforts are achieved through combined expertise in radiochemistry, geochemistry, analytical chemistry, nuclear material science, shock physics, quantum-enabling sensing, HPC, data science, and AI.

The CNF team includes members from the University of Florida; the University of Tennessee; the University of California, Berkeley; the University of Central Florida; the City University of New York; Clemson University; George Washington University; Iowa State University; the University of Michigan; the University of Nevada, Las Vegas; North Carolina State University; the University of Notre Dame; Oregon State University; Penn State; Lawrence Berkeley National Laboratory; Lawrence Livermore National Laboratory; Los Alamos National Laboratory; Oak Ridge National Laboratory; Pacific Northwest National Laboratory; Sandia National Laboratory; and Savannah River National Laboratory.

## CORE-CM

ICL LEAD  
Deborah Penchoff

The **Carbon Ore, Rare Earth and Critical Minerals (CORE-CM)** initiative for the U.S. Basins is funded by the Department of Energy Fossil Energy & Carbon Management Office of Resource Sustainability. Our project within this program focuses on applying HPC and AI to optimize processes to advance the manufacturing of valuable coal-derived products in southern Appalachia.

REEs are essential in applied technologies that include communications, computing, medical capabilities, green energy, and defense. Our project in CORE-CM seeks to develop HPC/AI-driven optimized strategies to extract REEs from coal ash ponds. This benefits society by providing potential alternatives to increase internal production of REEs while providing uses for coal ash. The team includes participants from The University of Tennessee, the Institute for Advanced Composites Manufacturing Innovation (IACMI), Oak Ridge National Laboratory, the University of Alabama, Southern Company, Roane State Community College, the Tennessee Geological Survey, and the Geological Survey of Alabama.

## CORES

ICL LEAD  
Stanimire Tomov

FIND OUT MORE AT  
[icl.utk.edu/corecs](http://icl.utk.edu/corecs)

The **Convex Optimization for Real-time 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 enable us to solve, in real-time, convex optimization problems with significantly higher performance—and orders of magnitude greater size—compared to current state-of-the-art solvers.

## DPLASMA

ICL LEADS  
George Bosilca  
Aurelien Bouteiller

FIND OUT MORE AT  
[icl.utk.edu/dplasma](http://icl.utk.edu/dplasma)

The **Distributed Parallel Linear Algebra Software for Multi-core Architectures (DPLASMA)** package is the leading implementation of a dense linear algebra package for distributed heterogeneous systems. DPLASMA is designed to deliver sustained performance for distributed systems, where each node features multiple sockets of multi-core processors and, if available, accelerators like NVIDIA, AMD, or Intel GPUs. DPLASMA achieves this objective by deploying PLASMA tile-based 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.

## RESEARCH

### EPEXA

ICL LEADS

George Bosilca  
Joseph Schuchart  
Thomas Herault

FIND OUT MORE AT  
[icl.utk.edu/epexa](http://icl.utk.edu/epexa)

A collaborative project involving Virginia Tech, Stony Brook, and ICL, **Ecosystem for Programming and Executing eXtreme Applications (EPEXA)** aims to create a software framework that implements high-performance methods for irregular and dynamic computations that are poorly supported by current programming paradigms. Employing science-driven co-design, the EPEXA team hardens a successful research prototype into an accessible, production-quality programming model that leverages domain-specific languages (DSLs) to improve accessibility and accelerate the adoption of high-performance tools for computer scientists and domain scientists.

The project bridges the so-called “valley of death” between a successful proof of concept and an implementation with enough quality, performance, and community support to motivate application scientists and other researchers to adopt and push for its community use. Specifically, the new powerful data-flow programming model and associated parallel runtime directly address multiple challenges scientists face as they leverage rapidly changing computer technologies—including current massively parallel, hybrid, and many-core systems.

### Evolve

ICL LEAD

George Bosilca

**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.

Evolve efforts have involved exploratory research for improving different performance aspects of the Open MPI library. Notably, this has improved efficiency in multi-threaded programs using MPI in combination with other thread-based programming models (e.g., OpenMP). A novel collective communication framework with event-based programming and data dependencies was investigated. It demonstrated a clear advantage regarding aggregate bandwidth in heterogeneous (shared memory + network) systems. Support for MPI resilience following the User-Level Failure Mitigation (ULFM) fault-tolerance proposal was released and has been fully integrated into Open MPI.

### F-block Elements Separations

ICL LEAD

Deborah Penchoff

The project “**Membrane separations of f-block elements utilizing rhamnolipid-based chelants. A joint experimental and computational investigation**” is funded by the Department of Energy Small Business Technology Transfer (STTR), and it focuses on using machine learning to design better membranes to enable REE separations.

This effort is within technology areas relevant to the DOE Office of Science seeking to optimize selectivity and rate of extraction or rejection using AI/ML methodology membrane synthesis design, experimental design, and data analytics. The R&D is intended to lead to hybrid models that incorporate fundamental mechanisms and lead to feasible material structures that would be readily synthesizable for large-scale processes and complex systems.

The team includes The University of Tennessee and GlycoSurf, LLC.

### Ginkgo

ICL LEAD

Hartwig Anzt

FIND OUT MORE AT  
[ginkgo-project.github.io/](https://ginkgo-project.github.io/)

In the **Ginkgo** project, we develop high performance numerical linear algebra functionality reflecting the parallelism of modern HPC platforms. The focus is on GPU-accelerated systems, and Ginkgo can currently be used on AMD GPUs, Intel GPUs, and NVIDIA GPUs using backends written in the respective vendor languages. Ginkgo features a variety of Krylov solvers, sparse direct solvers, sophisticated preconditioners exposing fine-grain parallelism, including incomplete factorizations, incomplete sparse approximate inverses, and algebraic multigrid technology, mixed precision algorithms, and preconditioned batched iterative solvers.

Ginkgo is implemented in modern C++ and is used by several popular simulation frameworks, including MFEM, SUNDIALS, deal.ii, HyTeg, openCARP, XGC, NEK5000, and OpenFOAM. Scalability of the Ginkgo backend to up to thousands of GPUs has been demonstrated on the *Frontier* and *Perlmutter* Supercomputers. The Ginkgo library is open source under the 3-clause BSD license.

### Greening the Southeast

ICL LEAD

Deborah Penchoff

The **Advancing Carbon-Neutral Crop Technologies to Develop Sustainable Consumer Goods (AL, GA, NC, TN)** (“Greening the Southeast” for short) is an NSF Engines Development Award in the Advanced Agriculture Topic and targets the BioTech, Advanced Materials, and Quantum Tech focus areas.

The NSF Engine Development Awards will help regional partners collaborate to advance technologies, address societal challenges, and create economic opportunities.

The team includes The University of Tennessee, HudsonAlpha Institute for Biotechnology, and other partners.

## heFFTe

ICL LEAD

Stanimire Tomov

FIND OUT MORE AT  
[icl.utk.edu/fft](http://icl.utk.edu/fft)

The fast Fourier transform (FFT) is used in many domain applications—including molecular dynamics, spectrum estimation, fast convolution and correlation, signal modulation, and wireless multimedia applications—but previous FFT libraries were not scalable on large heterogeneous machines with many nodes.

The main objective of the ECP FFT project was to design and develop a **Highly Efficient FFTs for Exascale** (heFFTe) library that provided fast and robust multidimensional FFTs for large-scale heterogeneous systems with multi-core processors and hardware accelerators. HeFFTe collects and leverages existing FFT capabilities while building a sustainable FFT library that minimizes data movements, optimizes MPI communications, overlaps computations with communications, and autotunes performance on various architectures and large-scale platforms. The current heFFTe v2.4 release achieves very good scalability on exascale systems and performance close to 90% of the roofline peak.

## HPCG

ICL LEAD

Piotr Luszczyk

FIND OUT MORE AT  
[hpcg-benchmark.org/](http://hpcg-benchmark.org/)

The **High Performance Conjugate Gradients** (HPCG) benchmark is designed to measure performance representative of modern scientific applications relying on discretizations of Partial Differential Equations (PDEs). It does so by exercising the computational and communication patterns commonly found in real science and engineering codes, often based on sparse iterative solvers with complex multi-level preconditioners. HPCG exhibits the same irregular accesses to the main memory and fine-grain recursive computations that dominate large-scale scientific workloads to simulate complex physical phenomena.

The HPCG 3.1 reference code was released in March 2019. This release positioned HPCG to represent modern PDE solvers better and made it easier to run HPCG on production supercomputing installations. The reference version is accompanied by multiple binary or source code releases from AMD, ARM, Intel, and NVIDIA, which are carefully optimized for these vendors' respective hardware platforms. The current HPCG performance list was released at SC23 and features over 100 entries across the supercomputing landscape that are also tracked by TOP500, giving a unique opportunity to compare the bookend performance levels of these machines.

## HPFFT

ICL LEAD

Stanimire Tomov

The new **High Performance FFT** (HPFFT) benchmarking effort aims to comprehensively measure the performance of a variety of parallel FFT implementations for the ECP and its rich application ecosystem. Many scientific applications of strategic importance to DOE need multidimensional Discrete Fourier transforms, implemented by ICL's own heFFTe project. Over the course of the CLOVER project and, more specifically, its heFFTe component, the need for comparing FFT implementations became apparent in order to understand how tradeoffs made by developers affect floating-point performance and mitigate communication overheads.

In its current incarnation, the HPFFT project released a technical report, ICL-UT-21-03, to provide an interim update on comprehensive testing and measuring of various aspects of the FFT implementations for three-dimensional transforms on high-performance systems that may include hardware accelerators. The results from the report reveal significant differences in functionality, performance, and supported hardware and give the ECP application community a much better appreciation of the available software choices.

## HPL

ICL LEADS

Piotr Luszczyk

Jack Dongarra

FIND OUT MORE AT  
[icl.utk.edu/hpl](http://icl.utk.edu/hpl)

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 Vector Signal and Image Processing Library (VSIBL). HPL is often the first program to run on large HPC machines. Carefully optimized versions of HPL are available from major HPC hardware vendors.

The primary focus of HPL 2.3, released in 2018, was to improve the accuracy of reported benchmark results and ensure easier configuration and building on modern HPC platforms. HPL is now hosted on GitHub and features more detailed reporting of the solution's scaled residual and the achieved performance number. Another addition is a software configuration tool based on GNU Autotools and the removal of deprecated MPI functions. The LINPACK app for iOS reached over 8 Gflop/s on the iPhone X. For the November 2021 TOP500 list, an optimized version of the HPL code achieved over 440 Pflop/s on the *Fugaku* supercomputer at RIKEN, Japan, and in June 2022, achieved 1.1 Eflop/s on *Frontier* at Oak Ridge National Laboratory and was further improved by almost 10% for June 2023.

## HPL-MxP

ICL LEADS

Piotr Luszczyk

Jack Dongarra

FIND OUT MORE AT  
[hpl-mxp.org/](http://hpl-mxp.org/)

The **HPL-MxP** benchmark seeks to highlight the emerging convergence of HPC and artificial intelligence workloads. While traditional HPC focused on simulation runs for modeling phenomena in physics, chemistry, biology, and so on, the mathematical models that drive these computations require, for the most part, 64-bit accuracy. On the other hand, the machine learning methods that fuel advances in AI achieve desired results at 32-bit and even lower floating-point precision formats. This lesser demand for accuracy fueled a resurgence of interest in new hardware platforms that deliver a mix of unprecedented performance levels and energy savings to achieve the classification and recognition fidelity afforded by higher-accuracy formats. HPL-MxP strives to unite these two realms by delivering a blend of modern algorithms and contemporary hardware while simultaneously connecting to the solver formulation of the decades-old HPL framework of benchmarking the largest supercomputing installations in the world.

## RESEARCH

### LAPACK/ ScaLAPACK

#### ICL LEADS

Julie Langou  
Piotr Luszczek  
Jack Dongarra

#### FIND OUT MORE AT

[netlib.org/lapack](https://netlib.org/lapack)  
[netlib.org/scalapack](https://netlib.org/scalapack)

**Linear Algebra PACKage (LAPACK)** and **Scalable LAPACK (ScaLAPACK)** are foundational libraries for solving dense linear algebra problems. ICL has contributed to the development and maintenance of these two packages. LAPACK is single node and relies on a multi-core BLAS library for parallelism. ScaLAPACK is parallel and distributed and depends on the BLAS, LAPACK, MPI, and BLACS libraries.

The latest major release of LAPACK, version 3.12.0, was released in November 2023. This version added a number of improvements along with bug fixes. Highlights include the dynamic mode decomposition (DMD), truncated QR with column pivoting, reciprocal vector scaling, improvements in the 64-bit API, and a revised online documentation structure.

### MAGMA

#### ICL LEAD

Stanimire Tomov

#### FIND OUT MORE AT

[icl.utk.edu/magma](https://icl.utk.edu/magma)

**Matrix Algebra on GPU and Multi-core Architectures (MAGMA)** is a collection of next-generation linear algebra libraries for heterogeneous computing. MAGMA supports interfaces for current linear algebra packages and standards (e.g., LAPACK and BLAS) to enable computational scientists to easily port any linear algebra-reliant software component to heterogeneous computing systems. MAGMA enables applications to fully exploit the power of current hybrid systems of many-core CPUs and multi-GPUs/coprocessors to deliver the fastest possible time to accurate solutions within given energy constraints.

MAGMA features LAPACK-compliant routines for multi-core CPUs enhanced with NVIDIA or AMD GPUs. MAGMA 2.7.2 now includes more than 400 routines that cover 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. A MagmaDNN package has been added and further enhanced to provide high-performance data analytics, including functionalities for machine learning applications that use MAGMA as their computational back end. The MAGMA Sparse and MAGMA Batched packages have been included since MAGMA 1.6.

### MAGMA-Edge

#### ICL LEAD

Stanimire Tomov

**MAGMA-Edge** is a fast deep learning (DL) library which aims to become the *de facto* standard DL framework for running AI applications on commodity edge devices. Edge devices such as the Raspberry Pi, NVIDIA Jetson Nano, or embedded processors from Intel and AMD are widely used in many common applications or appliances. These devices, when equipped with various sensors, provide efficient and economical Internet of Things (IoT) solutions for many common commercial needs and operations, most obviously on the food delivery bot seen around the UTK campus. Unlike traditional IoT devices that exchange data and instructions with a cloud server, the latest generation of edge devices is capable of performing data analytics and providing real-time AI solutions for a spectrum of designated tasks. MAGMA-Edge has been built on a set of fast linear algebra kernels for tensor operations extended from the MAGMA and MagmaDNN libraries.

### MATEDOR

#### ICL LEAD

Stanimire Tomov

The **MATrix, TENSOR, and Deep-learning Optimized Routines (MATEDOR)** project is performing the research required to define a standard interface for batched operations and provide a performance-portable software library demonstrating 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 defines modular, optimizable, and language-agnostic interfaces that can work seamlessly with a compiler. This modularity provides application, compiler, and runtime system developers with the option to use a single call to a routine from the new batch operation standard and allows the entire linear algebra community to collectively attack a wide range of small matrix or tensor problems.

### Mixed- Precision Numerical Computing

#### ICL LEAD

Piotr Luszczek

With the rapidly expanding landscape of mixed- and multi-precision methods, the ongoing cross-pollination between HPC and machine learning or generative artificial intelligence is leading to intelligent computational steering of large-scale simulations. As these disparate scientific fields share hardware platforms, exploiting their wide range of computational modes has led to a proliferation of multiple representations of floating-point data. Taking full advantage of them is this effort's main goal.

Against this backdrop, ICL's high-performance libraries (also those produced by internet-scale companies, hardware vendors, national laboratories, and academic institutions) spearhead the recent algorithmic progress in exploiting multiple precisions for increased efficiency in achieved performance, required communication, or optimized storage needs. The techniques used in this effort employ floating-point representations such as limited precision, quantized integers, and modular precision ecosystems, among others. Note that the lossless or lossy compression approaches can independently benefit HPC codes as their algorithmic and accuracy advances are developed in parallel to the mixed-precision aspects.



## oneAPI

ICL LEAD

Hartwig Anzt

oneAPI is an industry initiative to create a single, unified, cross-architecture programming model for CPUs and accelerator architectures. Based on industry standards and its open development approach, the initiative will help streamline software development for high-performance computers, increase performance, and provide specifications for efficient and diverse architecture programming.

In the **oneAPI Center of Excellence**, Intel teams up with ICL to spearhead the development of numerical linear algebra functionality in the oneAPI ecosystem by deploying SYCL kernels in the Ginkgo linear algebra library. This allows running Ginkgo and applications that use Ginkgo's functionality on any hardware supporting the oneAPI industry standard, including Intel high-performance GPUs that are powering the *Aurora* supercomputer at Argonne National Laboratory.

## Open MPI

ICL LEADS

George Bosilca  
Joseph Schuchart

FIND OUT MORE AT  
[open-mpi.org](https://open-mpi.org)

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 one process's address space to another through cooperative operations on each process. Open MPI integrates technologies and resources from several other projects (e.g., HARNESS/FT-MPI, LA-MPI, LAM/MPI, and PACX-MPI) to build the best MPI library available.

A completely new MPI 4.1-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 next-generation exascale challenges.

## PAPI

ICL LEADS

Heike Jagode  
Anthony Danalis

FIND OUT MORE AT  
[icl.utk.edu/papi](https://icl.utk.edu/papi)

The **Performance Application Programming Interface (PAPI)** offers a universal interface and methodology for gathering performance counter information from diverse hardware and software components. This includes major CPUs, GPUs, accelerators, interconnects, I/O systems, power interfaces, and even virtual cloud environments. Collaborations with industry leaders like AMD, Cray/HPE, IBM, Intel, NVIDIA, and others ensure seamless integration of PAPI with new architectures as they are introduced or come close to release. As the PAPI component architecture expands, 3rd-party performance tools interfacing with PAPI gain the capability to measure data from these emerging architectures.

In 2023, PAPI released versions 7.0.1 and 7.1.0. These provide enhanced performance counter monitoring capabilities, extending support now to Intel Sapphire Rapids, AMD Zen4 CPUs, and ARM Neoverse V1 and V2 architectures. The ROCm component has been significantly refactored, enabling efficient monitoring of multiple GPUs in sampling mode and laying the foundation for future ROCm tools support. The ROCm SMI component was also expanded to include GPU-to-GPU XGMI event support, offering a wider range of monitoring capabilities. Furthermore, the CUDA component has also undergone significant refactoring and now provides multi-thread and multi-GPU support.

## PaRSEC

ICL LEADS

George Bosilca  
Thomas Herault

FIND OUT MORE AT  
[icl.utk.edu/parsec](https://icl.utk.edu/parsec)

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 directed acyclic graph (DAG) of tasks with edges designating the data dependencies. DAGs are represented in a compact format that can be queried to discover data dependencies in a distributed and scalable fashion—a drastic shift from today's programming models, which are based on the replicated 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.

## PESA

ICL LEAD

Stanimire Tomov

Emerging HPC systems require innovations in existing infrastructure to deliver the best performance for science domains. The MPI 4.0 standard has also brought forward new opportunities for co-designing applications. These include partitioned point-to-point and collective operations and neighborhood collectives. Recent developments in GPU-based compression techniques provide an attractive option to optimize communication. With these advances, there is a critical need to update the commonly used tools and libraries that form the basis for the NSF's HPC cyberinfrastructure. The **Performance Engineering Scientific Applications with MVAPICH and TAU using Emerging Communication Primitives (PESA)** project undertakes this challenge and pursues new performance engineering avenues – by exploiting a co-design approach using the MPI\_T API – in the MVAPICH2 and TAU libraries with scientific applications. PESA focuses on two popular HPC applications: Anelastic Wave Propagation (AWP-ODC) and Highly efficient FFTs for Exascale (heFFTe). AWP-ODC is a highly scalable parallel finite-difference application with point-to-point operations that enables 3D earthquake calculations. HeFFTe, dominated by collective operations, is a massively parallel application that provides a scalable and efficient implementation of the widely used Fast Fourier Transform (FFT) operations.

## RESEARCH

### PLASMA

ICL LEAD

Piotr Luszczyk

FIND OUT MORE AT

[icl.utk.edu/plasma](http://icl.utk.edu/plasma)

**Parallel Linear Algebra Software for Multicores and Accelerators (PLASMA)** implements a set of fundamental linear algebra routines using the latest updates to the OpenMP standard, including advanced tasking and GPU offload pragmas. PLASMA includes, among others, LAPACK-equivalent routines for solving linear systems of equations, linear least square problems, parallel BLAS, and parallel matrix norms.

Over the last decade, PLASMA has been used on various systems using Intel CPUs and coprocessors as well as AMD, IBM POWER, and ARM processors. As a research vehicle, PLASMA is an example of a modern design for new dense linear algebra algorithms. At the same time, PLASMA benefits from the continuous evolution of the OpenMP standard, which now includes offloading functionality and enables porting to hardware accelerators. The latest PLASMA release, version 23.8.2 from August 2023, added a tighter integration with vendor libraries, convenience scripts for easier configuration, and other general bug fixes and integration with external projects such as the ECP-sponsored Spack package manager.

### RHE-HPC

ICL LEAD

Deborah Penchoff

The **Numerically-Exact Relativistic Many-Body Electronic Structure of Heavy Elements (RHE-HPC)** for short project is a collaborative effort focused on the development of a completely new and novel computational tool that enables, for the first time, fully predictive calculations on molecules containing f-block elements. This effort includes high-performance distributed and heterogeneous computing to assist with tuning the implementation of novel methods for execution on large-scale HPC platforms, including exascale machines.

RHE-HPC enables advances in global needs involving f-block elements, with a special focus on actinium-225, a highly promising radiotherapeutic to treat cancer. The team includes members from The University of Tennessee, Stony Brook University, and Virginia Tech.

### ScaRT

ICL LEAD

George Bosilca

The **Scalable Run Time for Highly Parallel, Heterogeneous Systems (ScaRT)** project aimed to increase the scientific throughput of existing and future cyberinfrastructure platforms by reducing communication overheads, improving the match between modern, parallel-computing frameworks and the applications upon which they run, and by better matching the functionality of the underlying communication library to the capabilities of modern communication adapters.

To this end, ScaRT brought together a multidisciplinary team to design and implement a communication library with new communication primitives, accelerate multiple task-based runtimes (e.g., Legion and ParSEC) and communication libraries (e.g., MPI and GasNET), port key components to a programmable NIC, and deliver improvements and extensions to mainstream communication libraries to provide the new functionality.

### SLATE

ICL LEAD

Mark Gates

FIND OUT MORE AT

[icl.utk.edu/slate](http://icl.utk.edu/slate)

For decades, ICL has applied algorithmic and technological innovations to pioneer, implement, and disseminate dense linear algebra software—including the LAPACK and ScaLAPACK libraries. The **Software for Linear Algebra Targeting Exascale (SLATE)** project is the next iteration of our linear algebra libraries, using modern C++ technologies and targeting modern GPU-accelerated computer architectures to integrate into the ECP ecosystem.

For context, ScaLAPACK was first released in 1995, nearly 30 years ago. In the past three decades, HPC has witnessed tectonic shifts in hardware and software technology, as well as many algorithmic innovations in scientific computing. SLATE was conceived to be a replacement for ScaLAPACK, with new algorithms and boasting superior performance and scalability in HPC's modern, heterogeneous, distributed-memory environments.

### SPADE

ICL LEADS

Heike Jagode  
Anthony Danalis

ICL is breaking new ground with SPADE, an NSF-funded "Frameworks" project titled "**Scalable Performance and Accuracy analysis for Distributed and Extreme-scale systems (SPADE)**." ICL leads this collaborative project with Heike Jagode as the PI and Anthony Danalis as co-PI. The project also involves partnerships with the University of Maine and the University of Texas, El Paso. Spanning four years, the project started on September 15th, 2023, with a total budget of \$3.5M (ICL's share is \$2.1M).

The SPADE project is dedicated to enhancing monitoring, optimization, evaluation, and decision-making functions for extreme-scale systems, catering to the needs of the HPC and scientific applications communities. As HPC resources evolve towards extreme scale, there's a growing necessity for integrated frameworks to tackle performance and reliability issues. Through extending support for heterogeneity and scalability across various computing platforms, and employing the established PAPI performance monitoring library, SPADE aims to provide the necessary software and APIs to effectively address the demands of scientific and machine learning applications while exploring new accuracy versus performance trade-offs with low-precision floating-point types.

## STEP

ICL LEAD

Heike Jagode

FIND OUT MORE AT  
[ascr-step.org/](https://ascr-step.org/)

The **Software Tools Ecosystem Project** (STEP) is a DOE ASCR-funded initiative, with ICL's Heike Jagode as one of the co-PIs. As part of its efforts, STEP organized a series of three town hall meetings throughout the summer of 2023. The primary objective of these meetings has been to formulate a strategic action plan for DOE/ASCR, with a specific focus on the long-term stewardship and advancement of the HPC tools ecosystem.

As part of the STEP initiative, the PAPI project will receive five years of funding totaling \$1.375M. The project aims to develop monitoring capabilities for emerging hardware technologies and create innovative abstractions for software-defined events. PAPI follows sustainable software practices and collaborates with stakeholders to meet the specific needs of the HPC community.

## Surrogates

ICL LEAD

Piotr Luszczyk

FIND OUT MORE AT  
[icl.utk.edu/surrogates](https://icl.utk.edu/surrogates)

The DOE-funded **Surrogate Benchmark Initiative** (Surrogates) is a collaborative effort involving Indiana University, UTK/ICL, the University of Virginia, and Rutgers University to provide new benchmarks and tools for assessing "surrogate" models based on deep neural networks. When trained on data produced by ensemble runs of a given HPC simulation, a surrogate model can imitate—with high fidelity—part or all of that simulation and produce the same outcomes for a given set of inputs while requiring far less time and energy.

At present, however, there are no accepted benchmarks to evaluate these surrogate models, and there is no easy way to measure progress or inform the codesign of new HPC systems to support their use. Surrogates aims to address this fundamental problem by creating a community repository and a Findable, Accessible, Interoperable, and Reusable (FAIR) data ecosystem for HPC application surrogate benchmarks, including data, code, and all relevant collateral artifacts that the science and engineering community needs to use and reuse these data sets and surrogates.

## Sustainable Energy Ecosystems

ICL LEAD

Deborah Penchoff

The **UTEC-UTK Collaboration for Sustainable Energy Ecosystems in Southern Cone** project focuses on accelerating workforce development, knowledge sharing, and climate action through international collaboration in the field of sustainable energy. The project is funded by the CAF Development Bank of Latin America, the U.S. Department of State (DOS), the Bureau of Western Hemisphere Affairs, and the U.S. Embassy in Chile, and involves higher education institutions in the United States and Argentina, Chile, Paraguay, and Uruguay. This effort aligns with the DOS goal to create a greener, more inclusive, and prosperous Hemisphere through enhanced regional education cooperation.

Participating institutions include The University of Tennessee, the UT Institute for Agriculture, and the Technological University of Uruguay.

## TOP500

ICL LEAD

Jack Dongarra

FIND OUT MORE AT  
[top500.org/](https://top500.org/)

With over three decades of tracking the progress of high performance computing, the **TOP500** lists continue to provide a reliable historical record of supercomputers worldwide. The lists lay out critical HPC metrics across all of its 500 machines and draw 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 measures machines' performance using irregular accesses to memory and fine-grain recursive computations—the very factors that dominate real-world, large-scale scientific workloads.

In November 2023, the 62nd TOP500 list was unveiled during SC23, which was held in Denver, Colorado. Yet again, the U.S. took the crown with *Frontier*, with a mix of AMD CPUs and GPUs featuring a Cray Slingshot 11 interconnect and built by HP Enterprise. The system's mix of nearly 9 million cores propelled Frontier into the exascale era. It achieved nearly 1.2 Efllop/s in HPL, making it the fastest supercomputer in the world by more than a twofold factor over Japan's Fugaku machine, a CPU-only ARM system. Frontier has now held the first spot for four consecutive lists. The second place finally saw Argonne National Lab's *Aurora* system, but running only at about half of its capacity.

## ULFM

ICL LEADS

George Bosilca  
Aurelien Bouteiller

FIND OUT MORE AT  
[fault-tolerance.org/](https://fault-tolerance.org/)

**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 wherein failures rendered the completions impossible.

Using the constructs defined by ULFM, applications and libraries drive the recovery of the parallel application and execution environment state. Consistency issues resulting from failures are addressed according to an application's needs, and the recovery actions are limited to MPI communication objects. Many application types and middleware are built on top of ULFM to deliver scalable fault tolerance. Notable additions include the CoArray Fortran language and SAP databases. ULFM software is available in recent versions of MPICH and Open MPI.

## 2023 CONFERENCES ATTENDED



**JAN 16-21 HOUSTON, TX**  
ECP Annual Meeting



**JAN 18-19 WASHINGTON, DC**  
Energy, Mobility, and Environment



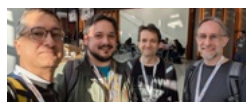
**FEB 1-8 VIRTUAL**  
MPI Forum



**FEB 2-3 NEW YORK, NY**  
EPEXA Meeting



**FEB 15-18 BATON ROUGE, LA**  
WAMTA 2023  
Workshop on Asynchronous Many-Task Systems and Applications



**FEB 26 - MAR 3 AMSTERDAM**  
SIAM CSE23  
Conference on Computational Science and Engineering



**MAR 13-16 VIRTUAL**  
MPI Forum



**MAR 21-23 BORDEAUX, FRANCE**  
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**MAR 26-30 INDIANAPOLIS, IN**  
American Chemical Society Spring 2023



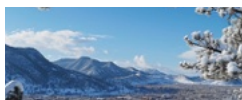
**MAR 29-31 PARIS, FRANCE**  
Scheduling Variable Capacity Resources for Sustainability



**APR 10 YORKTOWN HEIGHTS, NY**  
IBM Quantum Lab visit



**APR 13-15 KNOXVILLE, TN**  
American Nuclear Society 2023 Student Conference



**APR 16-20 COPPER MOUNTAIN, CO**  
Copper Mountain Conference on Multigrid Methods



**APR 20-21 ROANOKE, VA**  
EPEXA Project Meeting



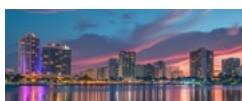
**APR 24-28 GLENEDEN BEACH, OR**  
Salishan HPC Conference



**APR 26-27 GAINESVILLE, FL**  
DOE NNSA Consortium for Nuclear Forensics Kick-off Meeting



**MAY 2-5 VIRTUAL**  
MPI Forum



**MAY 15-19 ST. PETERSBURG, FL**  
IPDPS 2023  
IEEE International Parallel and Distributed Processing Symposium Workshops



**MAY 21-24 KNOXVILLE, TN**  
USPLF 2023  
U.S. Precision Livestock Farming Conference



**MAY 21-25 HAMBURG, GERMANY**  
ISC High Performance 2023



**JUN 6-9 YORKTOWN HEIGHTS, NY**  
STEP Town Hall Meeting



**JUN 6-9 LEMONT, IL**  
PESO Community Workshop



**JUN 17 ORLANDO, FL**  
CSC 2023  
Correctness and Resiliency at Scale in Scientific Computing



**JUN 18-22 LAKE TAHOE, CA**  
Scalable Tools Workshop



**JUN 21-23 ORLANDO, FL**  
ICS 2023  
ACM International Conference on Supercomputing



**JUN 26-28** DAVOS, SWITZERLAND  
**PASC 2023**  
 The Platform for Advanced Scientific Computing



**JUL 3-7** BERLIN, GERMANY  
**Berlin Summit for EVE**  
 Earth Virtualization Engines



**JUL 10-12** BUCHAREST, ROMANIA  
**ISPC 2023**  
 22nd IEEE International Symposium on Parallel and Distributed Computing



**JUL 11-12** AMES, IA  
**STEP Midwest Town Hall**



**AUG 1-3** LIVERMORE, CA  
**ECP CEED Annual Meeting**



**AUG 9-10** WASHINGTON, DC  
**Systems and Applications Challenges for the Emerging Bazaar of Accelerators Workshop**



**AUG 13-17** SAN FRANCISCO, CA  
**American Chemical Society Fall 2023 Meeting**



**AUG 20-25** TOKYO, JAPAN  
**ICIAM 2023**  
 10th International Congress on Industrial and Applied Mathematics



**AUG 21-23** COLUMBUS, OH  
**11th Annual MVAPICH User Group (MUG) Conference**



**AUG 21-24** MONTEREY, CA  
**Monterey Data Conference**



**AUG 29-31** KNOXVILLE, TN  
**Smoky Mountains Computational Sciences & Engineering Conference**



**SEP 11-15** BRISTOL, UK  
**EuroMPI 2023 / MPI Forum**



**SEP 24-29** HEIDELBERG, GERMANY  
**Heidelberg Laureate Forum**



**SEP 25-29** VIRTUAL  
**IEEE High Performance Extreme Computing Virtual Conference (HPEC)**



**OCT 9-11** BUENOS AIRES, ARGENTINA  
**Enhancing Transdisciplinary Networks through Strategic Partnerships between the University of Tennessee and Argentina**



**OCT 16-17** DOHA, QATAR  
**ICSEC23**  
 International Computational Science and Engineering Conference



**OCT 18-19** CHICAGO, IL  
**Workshop on Sparse Tensor Computations**



**OCT 26-27** NEW YORK, NY  
**EPEXA Project Meeting**



**OCT 29 - NOV 3** WEST PALM BEACH, FL  
**Radiobioassay and Radiochemical Measurements Conference**



**OCT 31 - NOV 1** SANTA FE, NM  
**IEEE Cluster 2023**



**OCT 31 - NOV 1** ATLANTA, GA  
**ORNL Core Universities AI Workshop 2023**



**NOV 11-17** DENVER, CO  
**SC23**



**NOV 20-28** KARLSRUHE, GERMANY  
**WarmWorld Workshop Karlsruhe**



**DEC 4-7** VIRTUAL  
**MPI Forum**



**DEC 12-15** ALBUQUERQUE, NM  
**Kokkos User Group Meeting**

## 2023 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 2023 papers, including journal articles, book chapters, and conference proceedings. Many of these are available for download from our website.

Abdelfattah, A., S. Tomov, P. Luszczek, H. Anzt, and J. Dongarra  
**GPU-based LU Factorization and Solve on Batches of Matrices with Band Structure**  
*SC-W 2023: Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*, Denver, CO, ACM, November 2023

Barry, D., H. Jagode, A. Danalis, and J. Dongarra  
**Memory Traffic and Complete Application Profiling with PAPI Multi-Component Measurements**  
*2023 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*, St. Petersburg, Florida, IEEE, August 2023

Deshmukh, S., R. Yokota, G. Bosilca, and Q. Ma  
**O(N) distributed direct factorization of structured dense matrices using runtime systems**  
*52nd International Conference on Parallel Processing (ICPP 2023)*, Salt Lake City, Utah, ACM, August 2023



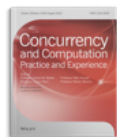
Aggarwal, I., P. Nayak, A. Kashi, and H. Anzt  
**Preconditioners for Batched Iterative Linear Solvers on GPUs**  
*SMC 2022: Accelerating Science and Engineering Discoveries Through Integrated Research Infrastructure for Experiment, Big Data, Modeling and Simulation*, January 2023



Benoit, A., T. Herault, L. Perotin, Y. Robert, and F. Vivien  
**Revisiting I/O bandwidth-sharing strategies for HPC applications**  
*INRIA Research Report*, no. RR-9502: INRIA, March 2023



Grützmacher, T., H. Anzt, and E. S. Quintana-Ortí  
**Using Ginkgo's memory accessor for improving the accuracy of memory-bound low precision BLAS**  
*Software: Practice and Experience*, vol. 532, issue 1, January 2023



Aliaga, J. I., H. Anzt, E. S. Quintana-Ortí, and A. E. Thomas  
**Sparse matrix-vector and matrix-multivector products for the truncated SVD on graphics processors**  
*Concurrency and Computation: Practice and Experience*, August 2023

Cao, Q., S. Abdulah, H. Ltaief, M. G. Genton, D. Keyes, and G. Bosilca  
**Reducing Data Motion and Energy Consumption of Geospatial Modeling Applications Using Automated Precision Conversion**  
*2023 IEEE International Conference on Cluster Computing (CLUSTER)*, Santa Fe, NM, USA, IEEE, November 2023



Hoefler, T., et al.  
**Earth Virtualization Engines - A Technical Perspective**  
*Computing in Science & Engineering*, vol. 25, no. 03, May-June 2023

Barbut, Q., A. Benoit, T. Herault, Y. Robert, and F. Vivien  
**When to checkpoint at the end of a fixed-length reservation?**  
*Fault Tolerance for HPC at eXtreme Scales (FTXS) Workshop*, Denver, United States, August 2023



Deshmukh, S., R. Yokota, and G. Bosilca  
**Cache Optimization and Performance Modeling of Batched, Small, and Rectangular Matrix Multiplication on Intel, AMD, and Fujitsu Processors**  
*ACM Transactions on Mathematical Software*, vol. 49, issue 3, September 2023

Li, J., G. Bosilca, A. Bouteiller, and B. Nicolae  
**Elastic deep learning through resilient collective operations**  
*SC-W 2023: Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*, Denver, CO, ACM, November 2023

**BEST PAPER FINALIST**

Lindquist, N., P. Luszczek, and J. Dongarra  
**Using Additive Modifications in LU Factorization Instead of Pivoting**  
*37th ACM International Conference on Supercomputing (ICS23)*, Orlando, FL, ACM, June 2023



Luszczek, P., W. M. Sid-Lakhdar, and J. Dongarra  
**Combining multitask and transfer learning with deep Gaussian processes for autotuning-based performance engineering**  
*The International Journal of High Performance Computing Applications*, March 2023

Mishler, D., J. Ciesko, S. Olivier, and G. Bosilca  
**Performance Insights into Device-initiated RMA Using Kokkos Remote Spaces**  
*2023 IEEE International Conference on Cluster Computing Workshops (CLUSTER Workshops)*, Santa Fe, NM, USA, IEEE, November 2023

Ribizel, T., and H. Anzt  
**Parallel Symbolic Cholesky Factorization**  
*SC-W 2023: Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*, Denver, CO, ACM, November 2023

**BEST PAPER FINALIST**

Sid-Lakhdar, W., S. Cayrols, D. Bielich, A. Abdelfattah, P. Luszczek, M. Gates, S. Tomov, H. Johansen, D. Williams-Young, T. Davis, et al.  
**PAQR: Pivoting Avoiding QR factorization**  
*2023 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*, St. Petersburg, FL, USA, IEEE, 2023



Schuchart, J., S. Hunold, and G. Bosilca  
**Synchronizing MPI Processes in Space and Time**  
*EUROMPI '23: 30th European MPI Users' Group Meeting*, Bristol, United Kingdom, ACM, September 2023

Sukkari, D., M. Gates, M. Al Farhan, H. Anzt, and J. Dongarra  
**Task-Based Polar Decomposition Using SLATE on Massively Parallel Systems with Hardware Accelerators**  
*SC-W '23: Proceedings of the SC '23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*, Denver, CO, ACM, November 2023



Thiyagalingam, J., G. von Laszewski, J. Yin, M. Emani, J. Papay, G. Barrett, P. Luszczek, A. Tsaris, C. Kirkpatrick, F. Wang, et al.  
**AI Benchmarking for Science: Efforts from the MLCommons Science Working Group**  
*Lecture Notes in Computer Science*, vol. 13387: Springer International Publishing, January 2023

Mor, O., G. Bosilca, and M. Snir  
**Improving the Scaling of an Asynchronous Many-Task Runtime with a Lightweight Communication Engine**  
*ICPP '23: Proceedings of the 52nd International Conference on Parallel Processing*, Salt Lake City, Utah, ACM, September 2023



Schuchart, J., and G. Bosilca  
**MPI Continuations And How To Invoke Them**  
*Sustained Simulation Performance 2021*, Cham, Springer International Publishing, February 2023



Tsai, Y.-H. Mike, N. Beams, and H. Anzt  
**Mixed Precision Algebraic Multigrid on GPUs**  
*Parallel Processing and Applied Mathematics (PPAM 2022)*, vol. 13826, Cham, Springer International Publishing, April 2023



Tsai, Y.-H. Mike, N. Beams, and H. Anzt  
**Three-precision algebraic multigrid on GPUs**  
*Future Generation Computer Systems*, July 2023



Reed, D., D. Gannon, and J. Dongarra  
**HPC Forecast: Cloudy and Uncertain**  
*Communications of the ACM*, vol. 66, issue 2, January 2023



S. Slattery, K. A. Surjuse, C. Peterson, D. Penchoff, and E. Valeev  
**Economical Quasi-Newton Unitary Optimization of Electronic Orbitals**  
*Physical Chemistry Chemical Physics*, December 2023



Valeev, E., R. J. Harrison, A. Holmes, C. Peterson, and D. Penchoff  
**Direct determination of optimal real-space orbitals for correlated electronic structure of molecules**  
*Journal of Chemical Theory and Computation*, October 2023

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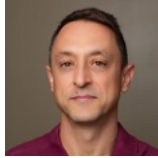
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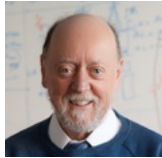
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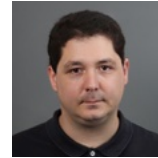
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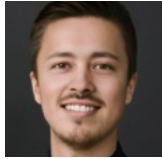
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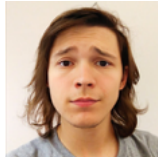
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SINCE ITS INCEPTION in 1989, ICL has fostered relationships with many academic institutions and research centers, and proactively built enduring collaborative partnerships with HPC vendors and industry leaders, in the US and abroad. In this section, we recognize many of those partners and collaborators.

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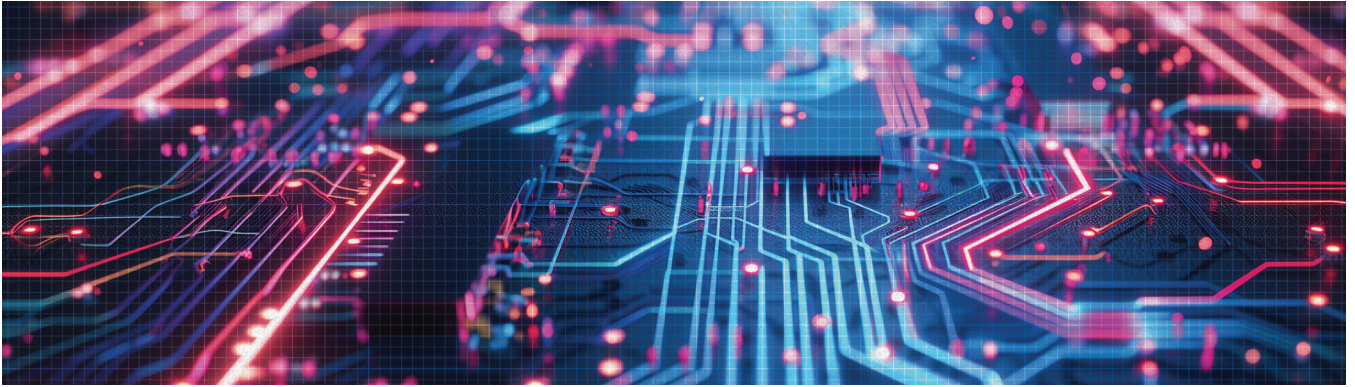
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## ACKNOWLEDGMENTS



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