Advanced Scientific Computing Research Update

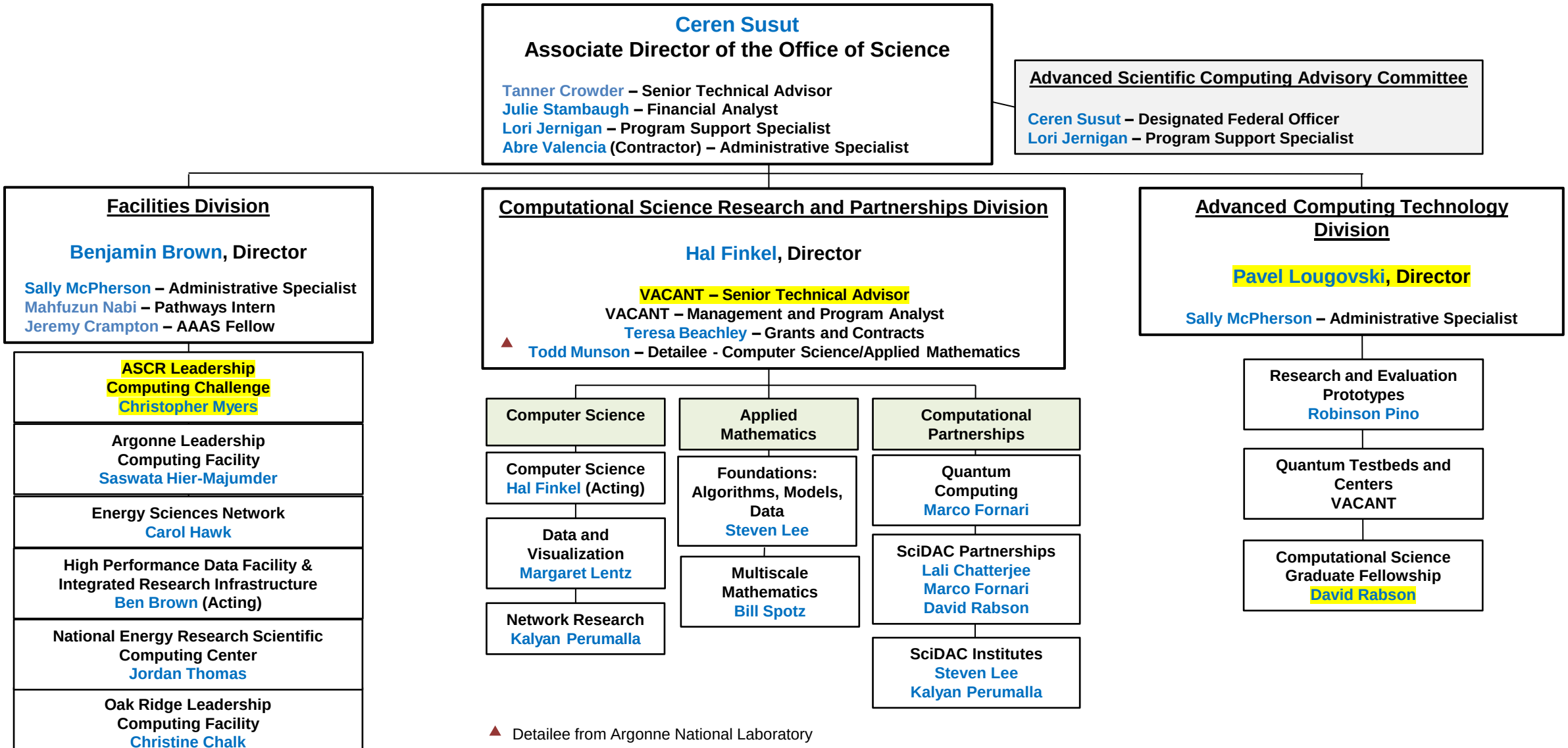
Ceren Susut, PhD
Associate Director of Science
for Advanced Scientific Computing Research

U.S. DEPARTMENT OF ENERGY | Office of Science

U.S. Department of Energy Office of Science
Office of

ADVANCED SCIENTIFIC COMPUTING RESEARCH

Functional Organization Chart



▲ Detailee from Argonne National Laboratory

Dr. Pavel Lougovski

Advanced Computing Technology Division Director

Pavel joined ASCR in January 2025 as the Director of the ACT Division.

Pavel is joining ASCR from Amazon Web Services (AWS) where he spent five years as a principal quantum research scientist and solutions architect. At AWS, Pavel has led R&D activities in quantum computing and networking. He helped launching Amazon Braket (AWS quantum computing service), AWS Center for Quantum Networking, and led the launch of AWS Quantum Embark program. Prior to AWS, Pavel spent seven years as a research scientist at Oak Ridge National Lab (ORNL). At ORNL, Pavel was a principal investigator for several quantum computing projects sponsored by ASCR. His team has done the first quantum computation of nuclear structure and quantum field theory using cloud-based quantum computers and developed QCOR – a C++ language extension for heterogeneous quantum-classical computing.

Pavel holds a Ph.D. in Physics from Ludwig Maximilian University of Munich, where he studied quantum information processing with atomic systems.

Dr. Chris Myers
ASCR Leadership Computing Challenge Program Manager

Dr. Christopher (Chris) Myers is the new ASCR Leadership Computing Challenge (ALCC) Program Manger in the Facilities Division effective January 13.

Chris comes to ASCR from a postdoctoral research position at University of California Merced, where he developed quantum chemistry models for mixed QM/MM and nonadiabatic simulations of condensed-phase chromophore systems. He holds doctoral and bachelor's degrees in physics from the University at Albany (SUNY).

Chris's research career has focused on working in multidisciplinary teams to develop scientific software for HPC. He has experience developing tools and models to tackle a variety of scientific challenges, including optical spectroscopy, structural biology, and solid-state materials research.

Departing ASCR
Best Wishes To: Ashley Predith

Dr. Ashley Predith has left ASCR to pursue other opportunities. Ashley served as Senior Technical Advisor in the Computational Science Research and Partnerships Division in ASCR until December 2024. Ashley has a strong interest in developing teams and organizations to achieve science and technology goals and brought that interest to ASCR in a zealous fashion. Ashley continued within ASCR not only helping with our internal organization but also helping to tackle larger problems including roadblocks preventing interagency collaborative activities.

Ashley previously advanced efforts in biosecurity and other crosscutting and special initiatives within SC. Before coming to SC, Ashley served as Assistant Director and then Executive Director of the President's Council of Advisors on Science and Technology in the White House Office of Science and Technology Policy. Ashley holds PhD in Materials Science from the Massachusetts Institute of Technology and a BS in Materials Science & Engineering from the University of Illinois at Urbana-Champaign.

Best wishes to Ashley on her future endeavors.

ASCR FY 2025 Request

(dollars in thousands)

	FY 2023 Enacted	FY 2024 Enacted	FY 2025 Request	FY 2025 Request vs FY 2024 Enacted		FY 2025 Request vs FY 2023 Enacted	
Advanced Scientific Computing Research							
Applied Mathematics Research	61,035	52,182	77,565	+25,383	+48.64%	+16,530	+27.08%
Computer Sciences Research	60,667	66,718	86,736	+20,018	+30.00%	+26,069	+42.97%
Computational Partnerships	95,875	75,182	93,449	+18,267	+24.30%	-2,426	-2.53%
Advanced Computing Research	108,920	108,918	148,197	+39,279	+36.06%	+39,277	+36.06%
Energy Earthshot Research Centers	12,500	5,000	12,500	+7,500	+150.00%	–	–
Total, Mathematical, Computational, and Computer Sciences Research	**338,997**	**308,000**	**418,447**	**+110,447**	**+35.86%**	**+79,450**	**+23.44%**
High Performance Production Computing	132,003	142,000	146,500	+4,500	+3.17%	+14,497	+10.98%
Leadership Computing Facilities	430,000	474,000	475,195	+1,195	+0.25%	+45,195	+10.51%
High Performance Network Facilities and Testbeds	90,000	91,000	93,540	+2,540	+2.79%	+3,540	+3.93%
Integrated Research Infrastructure	–	–	3,000	+3,000	–	+3,000	–
Total, High Performance Computing and Network Facilities	**652,003**	**707,000**	**718,235**	**+11,235**	**+1.59%**	**+66,232**	**+10.16%**
17-SC-20, SC Exascale Computing Project	**77,000**	**–**	**–**	**–**	**–**	**-77,000**	**-100.00%**
Subtotal, Advanced Scientific Computing Research	**1,068,000**	**1,015,000**	**1,136,682**	**+121,682**	**+11.99%**	**+68,682**	**+6.43%**
24-SC-20 High Performance Data Facility	–	1,000	16,000	+15,000	+1,500.00 %	+16,000	–
Subtotal, Construction	**–**	**1,000**	**16,000**	**+15,000**	**+1,500.00 %**	**+16,000**	**–**
Total, Advanced Scientific Computing Research	**1,068,000**	**1,016,000**	**1,152,682**	**+136,682**	**+13.45%**	**+84,682**	**+7.93%**

DOE Exascale Supercomputers Lead in Performance and Efficiency

TOP500 #1

El Capitain @ Livermore in California

1.74 EF HPE/AMD

Frontier @ Oak Ridge in Tennessee

1.35 EF HPE/AMD

TOP500 #2

HPL-MxP AI #2

GREEN 500 **Honorable Mention**

Aurora @ Argonne in Illinois

1.01 EF Intel/HPE

TOP500 #3

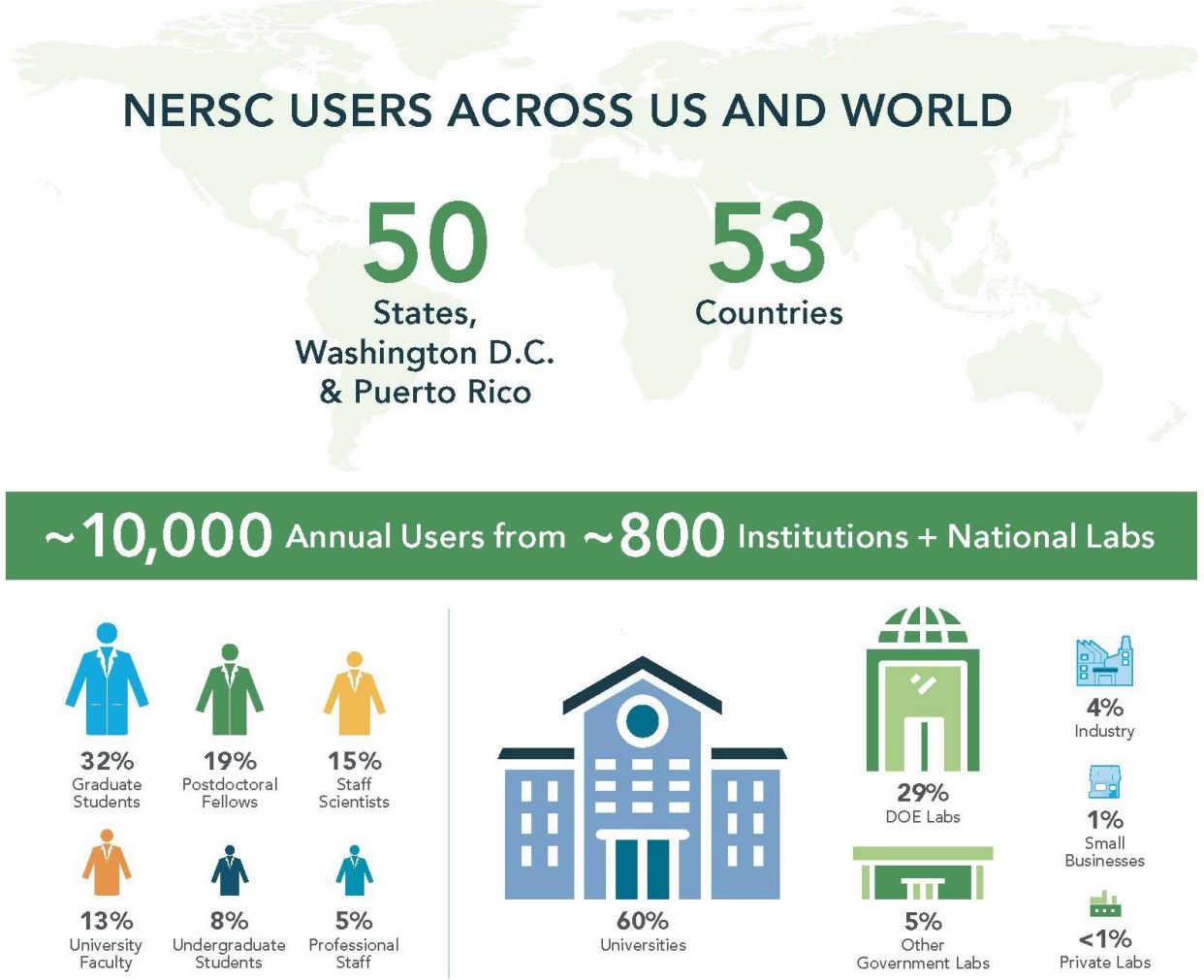
HPL-MxP AI #1

Farewell to Summit

Summit's Gordon Bell Prizes

- 2018 Prize:
  - 5 finalists for the prize used Summit
  - Joint winners: Jacobson (ORNL) and Prabhat (LBNL)
- 2019 Prize:
  - 2 finalists for the prized used Summit
  - Winner: Hoefler (ETH Zurich)
- 2020 Prize:
  - 4 finalists for the prize used Summit
  - Winner: Prabhat (LBNL)
- 2020 Special Prize for Covid:
  - 2 finalists for the prize used Summit
  - Winner: Amaro (UCSD)
- 2021 Prize:
  - 1 finalist for the prize used Summit
- 2021 Special Prize for Covid:
  - 2 finalists for the special prize used Summit
  - Winner: Amaro (UCSD)
- 2022 Prize:
  - 2 finalists for the prize used Summit
- 2022 Special Prize for Covid:
  - 1 finalist for the special prize used Summit

NERSC Turned 50!



Please see Sudip's talk tomorrow morning!

CDC 6600 at LLNL 1974

Record-Breaking Run on Frontier Sets New Bar for Simulating the Universe in the Exascale Era

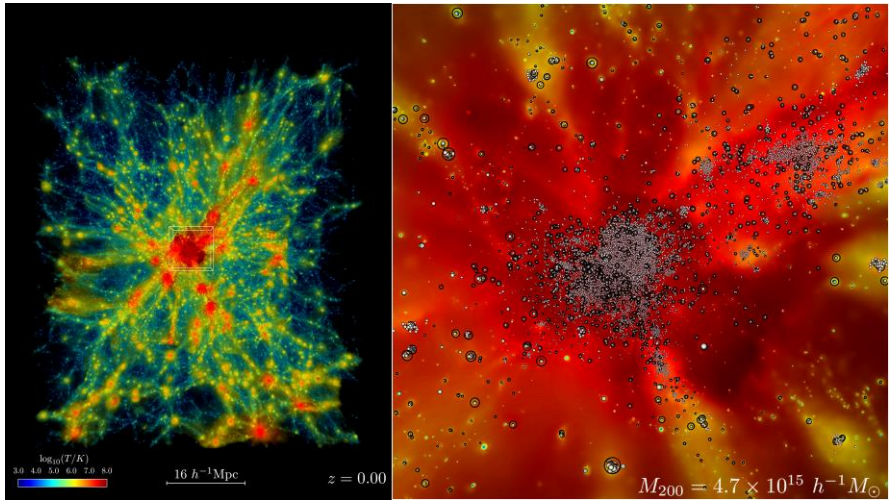
World's largest simulation of the cosmos lays new computational foundation for simultaneous extreme-scale dark matter and astrophysical investigations

The Science

In November 2024, researchers used the fastest supercomputer on the planet to run the largest astrophysical simulation of the universe ever conducted. A true understanding of structure formation in the Universe requires cosmological hydrodynamics simulations. That is, simulations of both dark matter — which only interacts through gravity — and atomic matter that involves complex physics like hot gas dynamics, star formation, and black holes. Until now, simulating a universe-scale volume with that level of detail was unthinkable.

The Impact

A research team from the Department of Energy's Argonne National Laboratory used the Frontier supercomputer at Oak Ridge National Laboratory to set a new benchmark for cosmological hydrodynamics simulations and provide a new foundation for simulating the physics of atomic matter and dark matter simultaneously. The simulation size corresponds to surveys undertaken by modern, large synoptic telescope surveys, a feat that until now has not been possible at this scale. In addition, cosmological hydrodynamics simulations are vastly more computationally demanding than those focusing solely on gravity. The supercomputer code used in the simulation is called HACC (Hardware/Hybrid Accelerated Cosmology Code). HACC was significantly upgraded through ExaSky, part of DOE's Exascale Computing Project (ECP).

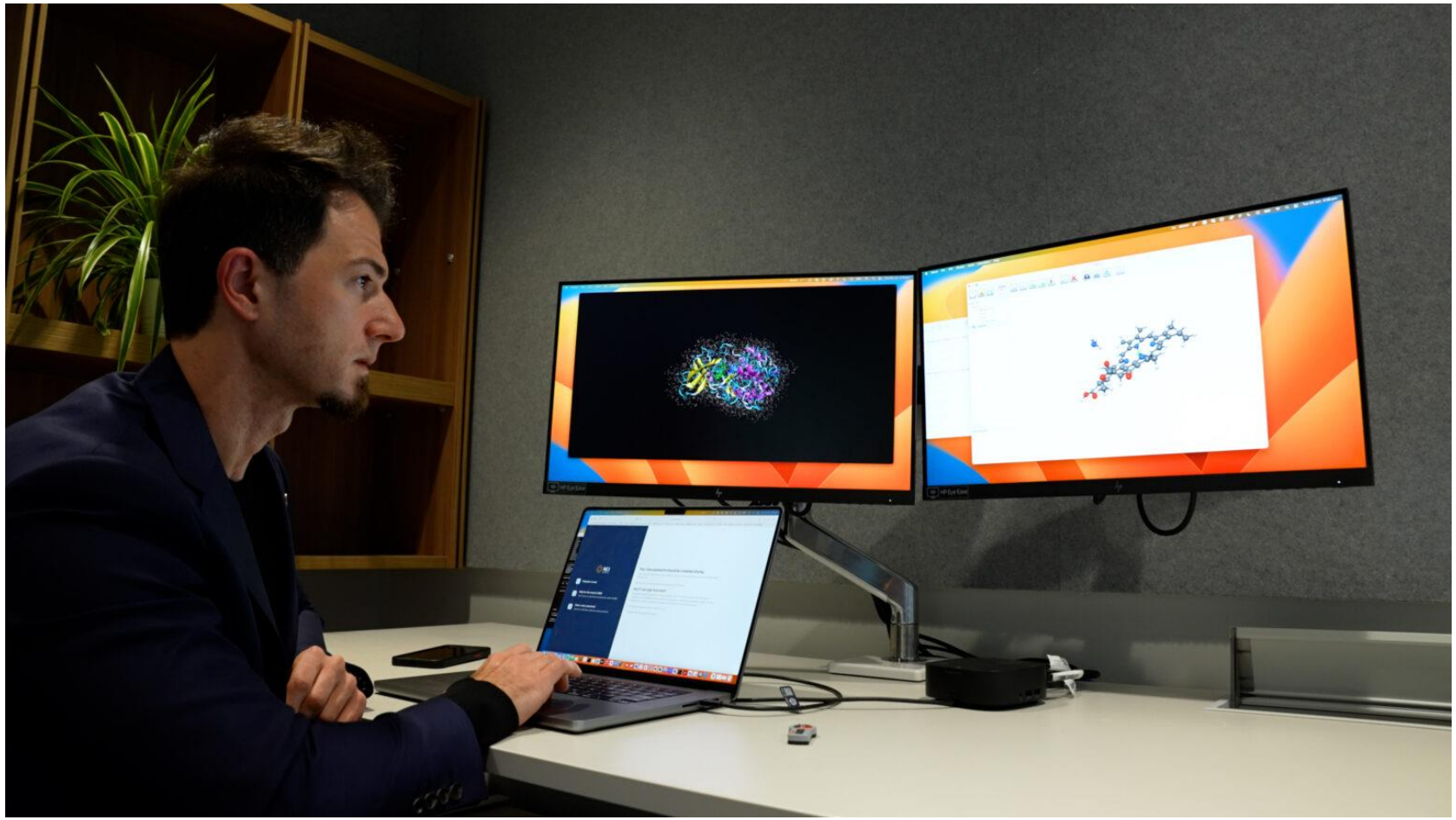


A small sample from the Frontier simulations reveals the evolution of the expanding universe in a region containing a massive cluster of galaxies from billions of years ago to present day (left). Red areas show hotter gasses, with temperatures reaching 100 million Kelvin or more. Zooming in (right), star tracer particles track the formation of galaxies and their movement over time. Credit: Argonne National Laboratory, U.S Dept of Energy

PI/Facility Lead(s): Salman Habib/ANL
ASCR Program/Facility: OLCF/Frontier
ASCR PM: Christine Chalk
Funding: OLCF ECP
Publication(s) for this work: *pending*

Game-Changing Quantum Chemistry Calculations on Frontier Earn Gordon Bell Prize

Researchers conduct largest and most accurate molecular dynamics simulations to date of 2 million correlated electrons by using the world's fastest supercomputer



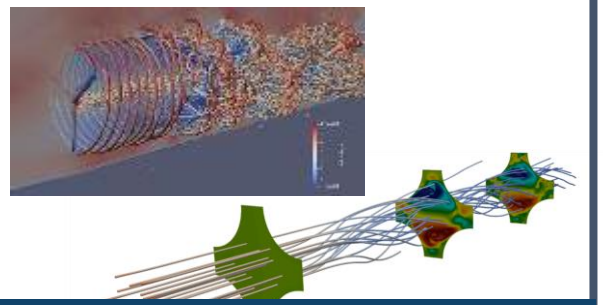
Please see Giuseppe's talk this afternoon!

PI/Facility Lead(s): Giuseppe Barca, Univ. Melbourne
ASCR Program/Facility: OLCF/Summit and Frontier
ASCR PM: Christine Chalk
Funding: SummitPLUS, DD
Publication(s) for this work: R. Stocks, et al., *SC '24: Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis.* November 2024, Article No. 9, 1-12.

University of Melbourne's Giuseppe Barca and his team were awarded the 2024 Gordon Bell Prize after using the Frontier supercomputer to perform the first quantum chemistry calculations to exceed an exaflop. Credit: University of Melbourne

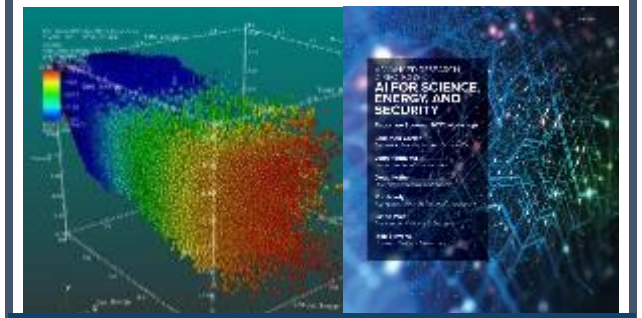
Reinvigorating ASCR Research To Respond to Critical Technology Trends

Advanced Modeling, Simulation, and Visualization



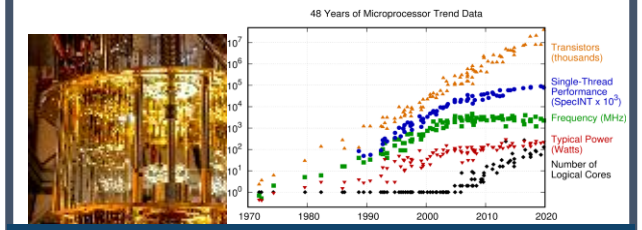
Empowering Science Through Fundamental Research

Frontier AI & Data



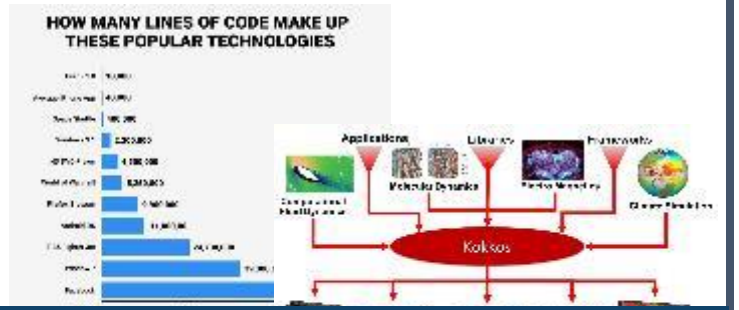
Creating Responsible and Energy Efficient Frontier AI

Heterogeneous, Distributed, Co-Designed, Energy-Efficient Computing and Algorithms



Transforming Fundamentals of Computing

Software Complexity for Increased Versatility



Enhancing Scientific Programming

High-Performance Computing and Networking across Experiments, Exascale and the Edge

Accelerating Science from Exascale to the Edge

Department of Energy Announces $179 Million for Microelectronics Science Research Centers

- Centers focus on basic research to transform the energy efficiency of microelectronics and create microelectronics for extreme environments.
- The centers are formed as networks of projects, 16 in total led out of 10 national laboratories:
  - *The Microelectronics Energy Efficiency Research Center for Advanced Technologies* (MEERCAT) is committed to revolutionizing energy-efficient microelectronics by advancing integrated innovations across materials, devices, information-carrying modalities, and systems' architectures.
    - Focuses on intelligent sensing, data bandwidth, multiplexing, and advanced computing. The center will explore transformative solutions that seamlessly bridge sensing, edge processing, artificial intelligence, and HPC.
  - *The Co-design and Heterogeneous Integration in Microelectronics for Extreme Environments* (CHIME) Center aims to drive transformative advancements in extreme environment electronics through heterogeneous integration and a seamless fusion of diverse materials, processes, and technologies to enable next-generation systems.
    - Will create robust, high-performance solutions capable of excelling in the most challenging conditions, including extreme thermal and radiation environments.
  - *The Extreme Lithography & Materials Innovation Center* (ELMIC) aims to advance the fundamental science driving the integration of new materials and processes into future microelectronic systems.
    - Focuses on key areas such as plasma-based nanofabrication, extreme ultraviolet (EUV) photon sources, 2D-material systems, and extreme-scale memory.

https://www.energy.gov/science/articles/department-energy-announces-179-million-microelectronics-science-research-centers

FY 2025 Solicitations (Released to Date)

- **Scientific Discovery through Advanced Computing (SciDAC) Institutes [LAB 25-3510]**
  - Pre-Proposal is required; due Date: January 23, 2025, at 5:00 PM Eastern.
  - Proposal Due Date: April 10, 2025, at 5:00 PM Eastern.

- **Competitive Portfolios for Advanced Scientific Computing Research: Data Management and Visualization [LAB 25-3520]**
  - Letter of Intent (LOI) is Required; due March 11, 2025, at 5:00 PM Eastern.
  - Proposal Due Date: May 13, 2025, at 5:00 PM Eastern.

- **National Quantum Information Science Research Centers [LAB 25-3530]**
  - Pre-Proposal is required; due Date: March 12, 2025, at 5:00 PM Eastern.
  - Proposal Due Date: June 4, 2025, at 5:00 PM Eastern.

For more information, see https://science.osti.gov/ascr/Funding-Opportunities.

ChatBLAS: The First AI-Generated and Portable BLAS Library

Scientific Achievement

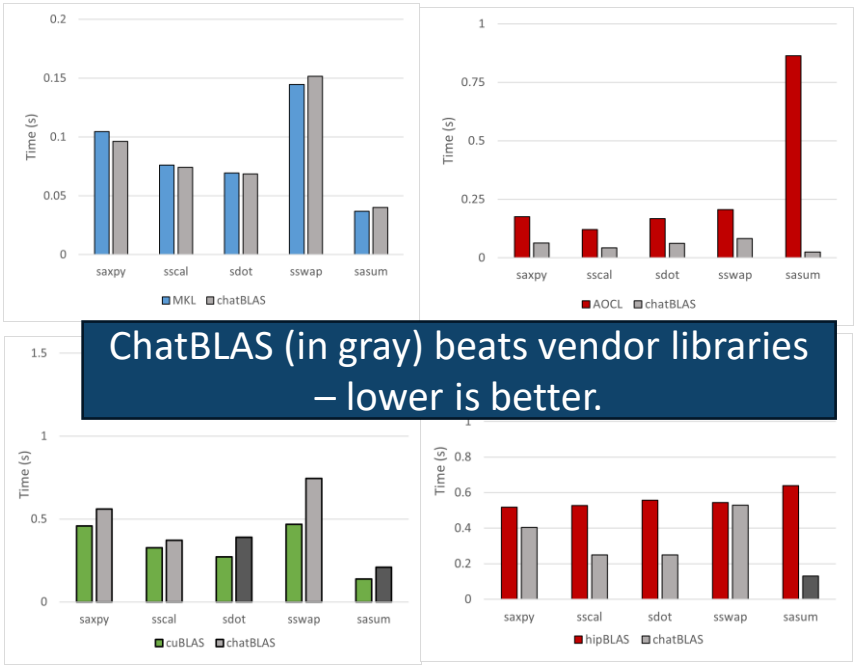
- A team of researchers introduced ChatBLAS, **the first AI-generated and multi-vendor portable basic linear algebra subroutines**, or BLAS, library.
- The work proved that **large language model, or LLM, code generation combined with human fine-tuning efforts provides either competitive or better performance than the highly optimized vendor-specific BLAS libraries**.
- This work was presented at the SC24 AI4S workshop.

Significance and Impact

- ChatBLAS demonstrates how LLMs, a revolutionary AI technology, can elevate productivity in the development, management, and optimization of the complex, highly specialized, and demanding HPC software ecosystem.
- The research team continues leveraging the large industry investment while identifying performance and trustworthiness gaps.

Technical Approach

1. The study used the state-of-the-art foundational ChatGPT LLMs 3.5-Turbo and 4o to generate ChatBLAS as a portable HPC library for BLAS level-1 operations.
2. The team compared the performance of ChatBLAS, fine-tuned when needed, against vendor BLAS implementations of: a) CPUS: Intel's MKL and AMD's AOCL; and b) GPUs: NVIDIA's cuBLAS and AMD's hipBLAS.



ChatBLAS performance versus four vendor-specific BLAS libraries: Intel's CPU MKL, AMD's CPU AOCL, NVIDIA's GPU cuBLAS, and AMD's GPU hipBLAS for BLAS level-1 subroutines.
Credit: ORNL

PI: Rob Ross, Keita Teranishi
ASCR Programs: RAPIDS2 SciDAC Institute for Computer Science, Data, and Artificial Intelligence, ASCR X-Stack, Next Generation of Scientific Software Technologies (NGSST) S4PST
ASCR PMs: Kalyan Perumalla, Hal Finkel
Publication for this work: Valero-Lara et al., "ChatBLAS: The First AI-Generated and Portable BLAS Library," *Proceedings of the SC'24 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*
DOI: 10.1109/SCW63240.2024.00010

∂FEM: Differentiating Large-Scale Finite Element Applications

Scientific Achievement

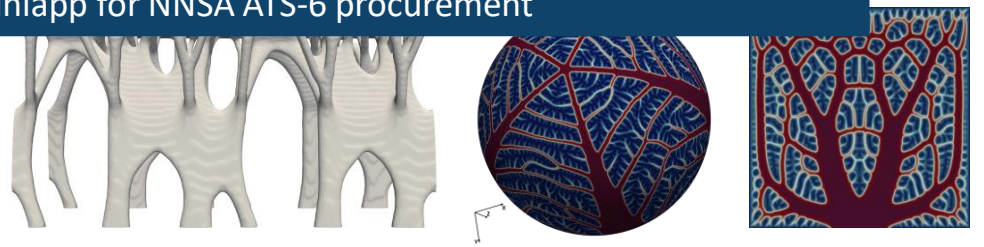
- Researched and developed an algebraic formulation for efficient solution and parameter derivatives of decomposed finite element operators
- Developed user-friendly C++ interface that allows flexible description and derivative evaluation of general FEM kernels
- Further developed and improved the Enzyme AD tool (e.g. C++ interface)

Significance and Impact

- New ∂FEM algorithms enable efficient gradient and sensitivity computation in fields like Optimization, Uncertainty Quantification and Machine Learning.
- The continued development and improvements of Enzyme benefit broader scientific computing community.
- Development of analysis tools for floating point exception detection allow for additional insight and more robust algorithms.

Successful EXPRESS collaboration:

- 15+ papers and 2024 SIGHPC Outstanding Doctoral Dissertation Award!
- Follow-on work in AMMTO (Scalable and Differentiable Multiphysics Solvers for Design and Optimization) and ASCR Competitive Portfolios (Foundations for Decision Support Through Cognitive Simulation).
- Application miniapp for NNSA ATS-6 procurement

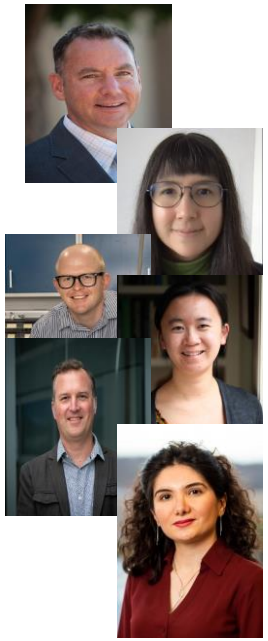


One of the target applications in topology optimization under uncertainty: Finite elements for Matern-type random fields: Uncertainty in computational mechanics and design optimization, arXiv:2403.03658.

PI: Tzanio Kolev, LLNL • Collaborating Institutions: University of Illinois Urbana-Champaign
ASCR Program: EXPRESS • ASCR PM: Hal Finkel
Publications: [1] *Retargeting and Respecializing GPU Workloads for Performance Portability, I. Ivanov, O. Zinenko, J. Domke, T. Endo and W. Moses, 2024 IEEE/ACM Int. Symposium on Code Generation and Optimization* • [2] *Understanding Automatic Differentiation Pitfalls, J. Hückelheim, H. Menon, W. Moses, B. Christianson, P. Hovland, L. Hascoet; ICML Workshop 2023*
Code Developed or Datasets: https://mfem.org, https://enzyme.mit.edu

ASCR PECASE Awardees

Congratulations to the ASCR-funded recipients of the Presidential Early Career Award for Scientists and Engineers (PECASE), the highest honor bestowed by the U.S. government on outstanding scientists and engineers early in their careers!



- **Peter Bosler**, Sandia National Laboratories, "High performance adaptive multiscale simulation with data-driven scale selective subgrid parameterizations"
- **Katherine Isaacs**, University of Utah, "Node-to-Code Comparison-Centered Interactive Performance Visualization"
- **Joseph Michael Lukens**, Purdue University, "Scalable Architectures for Hybrid Quantum/Classical Networking"
- **Bei Wang Phillips**, University of Utah, "Topology-Preserving Data Sketching for Scientific Visualization"
- **Stefan Wild**, Lawrence Berkeley National Laboratory, "Structure Exploiting, Adaptive, Zero-Order Optimization to Improve Efficiency"
- **Zohreh Davoudi**, University of Maryland, "Analog and Digital Quantum Simulations of Strongly Interacting Theories for Applications in Nuclear Physics".

For more information, see https://www.whitehouse.gov/ostp/news-updates/2025/01/14/president-biden-honors-nearly-400-federally-funded-early-career-scientists/.

Community News

- DOE QIS Applications Roadmap Published: https://science.osti.gov/Initiatives/QIS/Community-Resources/SC-Sponsored-Reports
  - **Please see Susan's talk!**

- DOE-SC Roundtables: Transformational Science Enabled by Artificial Intelligence – Held on October 28-31 & November 7 – 8, 2024

- Workshops:
  - DOE BER/ASCR Workshop on Envisioning Frontiers in AI and Computing for Biological Research. To be held on February 4 – 6, 2025. Workshop website: https://www.orau.gov/BER-ASCR-Workshop:

ASCR and SC Office Hours

- Researchers, educators, and leaders within research administration from all institutional types are encouraged to join
- A primary goal of the virtual office hours is to broaden awareness of our programs; no prior history of funding from DOE is required to join
- Program managers are available to answer questions

See the ASCR website (https://science.osti.gov/ascr/officehours) for more information, including slides and recordings of past ASCR office hours. See the SC office hours website (https://science.osti.gov/officehours) for more information, including slides and recordings of past SC office hours.