U.S. DEPARTMENT OF ENERGY | Office of Science

View from Germantown

Advanced Scientific Computing Research Update

Barbara Helland, Associate Director

July 21, 2022

New ASCAC Members

Professor Tina Brower-Thomas, Executive Director of Center Integrated Quantum Materials, Howard University

Emeritus Professor Mark Dean, Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville

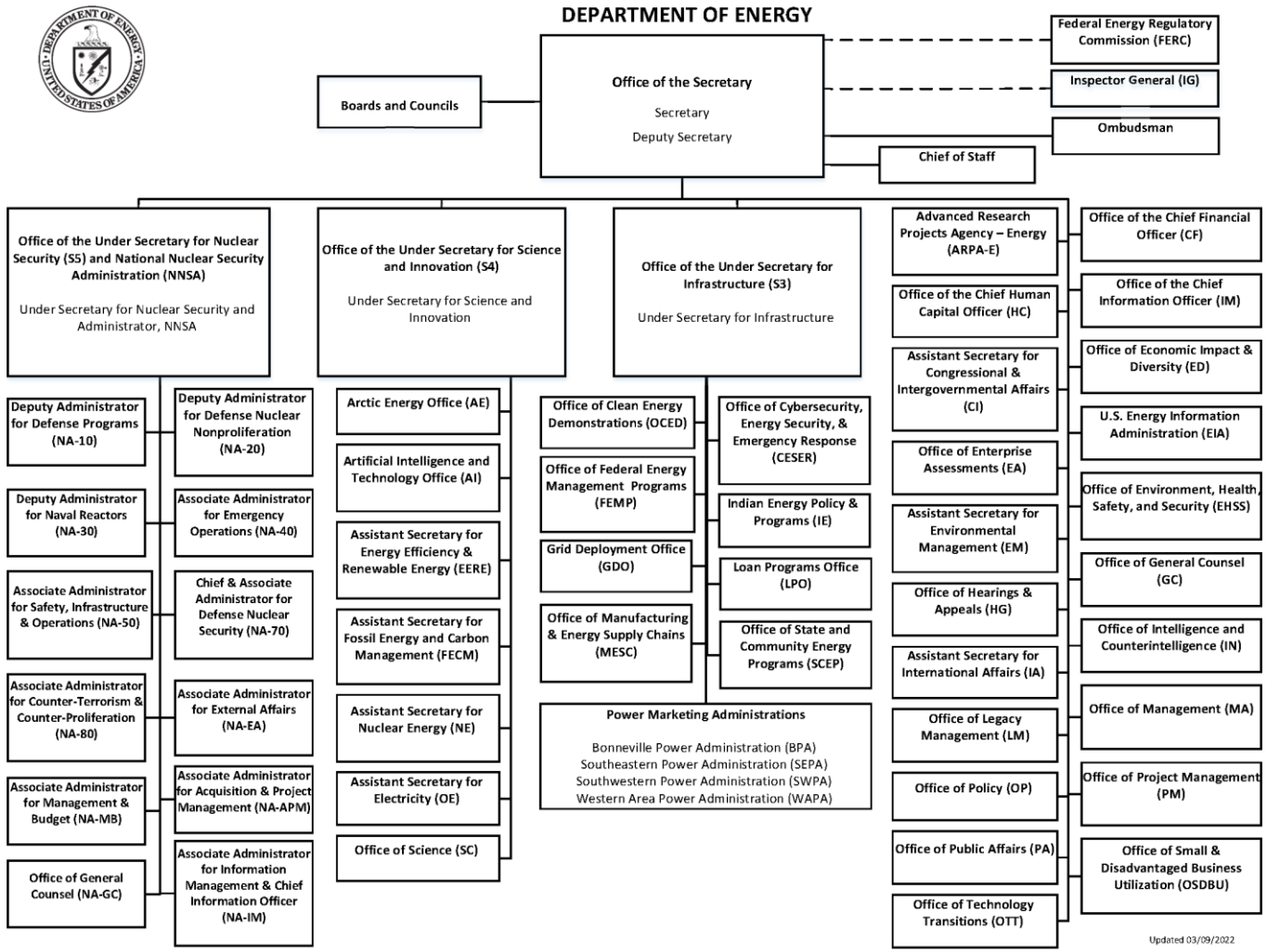
Dr. Gil Hererra, Director of Research, National Security Agency

Dr. Mary Ann Leung, Founder and President of Sustainable Horizons Institute

Professor Edward Seidel, President of the University of Wyoming

Dr. Valerie Taylor, Director of the Mathematics and Computer Science Division, Argonne National Laboratory

DOE Organization



DOE: From the Secretary to Office of Science

Jennifer Granholm
Secretary

Dr. Geri Richmond,
Under Secretary of
Science and Innovation

Dr. Asmeret
Asefaw Berhe
Director, Office of
Science

ASCR BUDGET UPDATES

- FY2023 President's Budget Request (PBR)
- FY2023 House Marks

ASCR - FY 2023 President's Request

(Dollars in thousands)

	FY 2021 Enacted	FY 2022 Enacted	FY 2023 Request	FY 2023 Request vs FY 2022 Enacted		FY 2023 Request vs FY 2021 Enacted	
Advanced Scientific Computing Research							
Applied Mathematics Research	48,570	51,048	71,938	20,890	40.92%	23,368	48.11%
Computer Sciences Research	46,827	49,773	70,326	20,553	41.29%	23,499	50.18%
Computational Partnerships	76,194	79,456	97,861	18,405	23.16%	21,667	28.44%
Advanced Computing Research	88,274	105,723	113,598	7,875	7.45%	25,324	28.69%
Energy Earthshot Research Centers	...	...	25,000	25,000	...	25,000	...
Mathematical, Computational, and Computer Sciences Research	**259,865**	**286,000**	**378,723**	**92,723**	**32.42%**	**118,858**	**45.74%**
High Performance Production Computing	113,786	120,000	115,033	-4,967	-4.14%	1,247	1.10%
Leadership Computing Facilities	381,075	410,000	407,772	-2,228	-0.54%	26,697	7.01%
High Performance Network Facilities and Testbeds	91,329	90,000	90,213	213	0.24%	-1,116	-1.22%
High Performance Computing and Network Facilities	**586,190**	**620,000**	**613,018**	**-6,982**	**-1.13%**	**26,828**	**4.58%**
17-SC-20 SC Exascale Computing Project	**168,945**	**129,000**	**77,000**	**-52,000**	**-40.31%**	**-91,945**	**-54.42%**
Total Advanced Scientific Computing Research	**1,015,000**	**1,035,000**	**1,068,741**	**33,741**	**3.26%**	**53,741**	**5.29%**

ASCR's FY2023: House Markup

- The Advanced Scientific Computing Research (ASCR) program develops and hosts some of the world's fastest computing and network capabilities to enable science and energy modeling, simulation, and research.
- **High Performance Computing and Network Facilities.— not less than**
  - $170,000,000 for the Argonne Leadership Computing Facility,
  - $250,000,000 for the Oak Ridge Leadership Computing Facility
  - $120,000,000 for the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory.
  - $90,000,000 to support necessary infrastructure up-grades and operations for ESnet.
- The Department is directed to support continued planning and design for the **High-Performance Data Facility**.
- **Mathematical, Computational, and Computer Sciences Research.—**
  - Not less than $300,000,000 for Mathematical, Computational, and Computer Sciences Research.

ASCR's FY2023 House Markup (cont.)

- Not less than $15,000,000 and up to $45,000,000 for the development of **advanced memory technologies** to advance artificial intelligence and analytics for science applications by a **U.S.-based manufacturer of memory systems and memory semantic storage**.
- The Committee supports the **Center for Advanced Mathematics for Energy Research Applications (CAMERA)** encourages the Department to support the creation of a crosscutting research program that leverages applied math, computer science and computational science to deliver artificial intelligence research, development, and deployment to increase the scientific productivity of the user facilities.
- The Department is encouraged to **explore the viability of photonic quantum computing,** in coordination with other federal agencies. The Department is encouraged to **consider mechanisms to provide access to ion trap quantum computing resources**, particularly with the ability to integrate with existing high-performance computing resources. The Department is **directed to provide to the Committee not later than 120 days after enactment of this Act a briefing on the Department's recent actions and future plans related to photonic quantum computing and ion trap quantum computing**.

FY2023 House Markup –Other Guidance

- **HBCU/MSI Engagement.—**The recommendation provides not less than $60,000,000, including through the Reaching a New Energy Sciences Workforce (RENEW) and Funding for Accelerated, Inclusive Research (FAIR) programs,
- **Energy Earthshots.—**provides up to $100,000,000 for Energy Earthshots, **including up to $25,000,000 from Advanced Scientific Computing Research,** up to $50,000,000 from Basic Energy Sciences, and up to $25,000,000 from Biological and Environmental Research.
- **Facility Operations.—**The Committee is disappointed with the Department's lack of support for robust user facility operations in the budget request. …The Department is directed to prioritize the stewardship of the user facilities in fiscal year 2023 and in future budget requests.
- **Established Program to Stimulate Competitive Research**.—The recommendation provides not less than $35,000,000 across the Office of Science programs for the Established Program to Stimulate Competitive Research.

FY 2022 Congressional Action: A closer look at the House Mark

($ in thousands)

	FY2022 Enacted	FY2023 Request	House Mark Language (not less than)	Difference FY2023 Request and House Mark
ASCR	**1,035,000**	**1,068,730**	**1,050,000**	**-18,730**
ALCF	152,955	159,047	170,000	+10,953
OLCF	228,120	249,066	250,000	+934
NERSC	120,000	115,033	120,000	+4,967
Esnet*	90,000	90,213	90,000	-213
Exascale	129,000	77,000	77,000	-52,000
Total Research	286,000	378.723	>340,000	~-38.723

ASCR FY2022 Actions

- Funding Opportunities
- Planning for the Future

FY2022 ASCR Solicitations

Title	Max DOE Funding	Announcement Release	Proposals Due
Randomized Algorithms for Combinatorial Scientific Computing	$10,000,000	04/14/2022	06/30/2022
2022 Mathematical Multifaceted Integrated Capability Centers (MMICCs)	$40,000,000	04/14/2022	06/28/2022
Data Visualization for Scientific Discovery, Decision-Making, and Communication	$13,000,000	04/14/2022	06/21/2022
Management and Storage of Scientific Data	$13,000,000	04/14/2022	06/13/2022
Reaching a New Energy Science Workforce (RENEW)	$5,000,000	05/25/2022	09/16/2022
Advancing Computer Modeling and Epidemiology for Biopreparedness and Response	$5,000,000	6/10/2022	07/29/2022
SciDAC-5 Partnership in Nuclear Energy* (NE)	$9,250,000	12/14/2021	04/19/2022
SciDAC-5 Partnership in Earth System Science (BER)*	$70,000,000	11/22/2021	04/11/2022
SciDAC-5 Partnership in High Energy Physics (HEP)*	$30,000,000	11/03/2021	02/09/2022
SciDAC-5 Partnership in Nuclear Physics (NP)*	$40,000,000	12/22/2021	04/26/2022
***Total funds for SciDAC-5 includes Partner and ASCR funding for 5 years**			

FY2022 Solicitations (cont.)

Title	Max DOE Funding	Announcement Release	Proposals Due
EXPRESS	$20,000,000	04/14/2022	06/23/2022
Federated Scientific Machine Learning			
Differentiable Programming			
Explainable Artificial Intelligence			
Parallel Discreet Event Simulation			
Quantum Algorithms and Mathematical Methods			
Quantum Computing at the Edge			

"Driving U.S. Competitiveness and Innovation: A New Era of Science for Transformative Industry"

The DOE Office of Science— through its basic research funding, user facilities, and National Laboratories—accelerates U.S. innovation and industrial competitiveness in key emergent technologies.

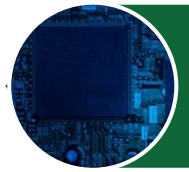
- Between March 18 and May 20, SC hosted a series of briefings for the members of Congress. ASCR community members took on leadership roles to make the sessions a success.

Artificial Intelligence

Quantum Information Science

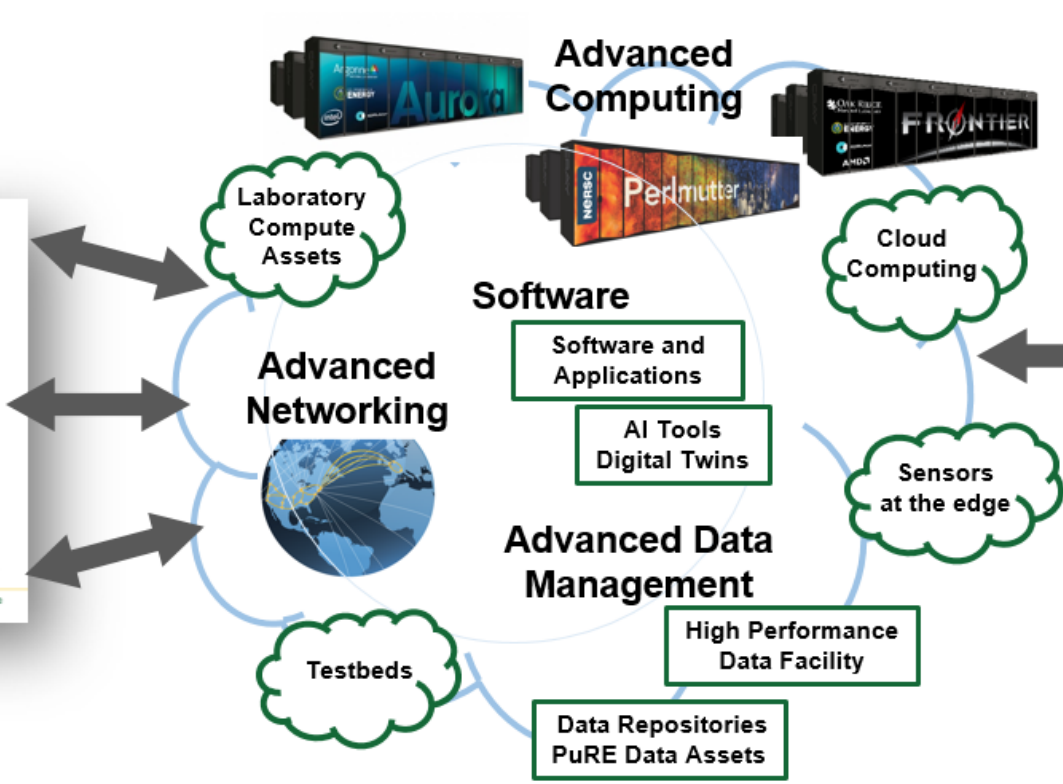
Materials and Chemistry for Clean Energy

Bioeconomy

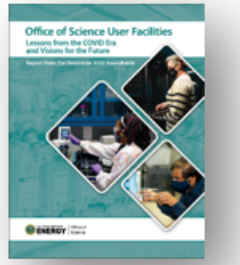


Microelectronics

A DOE/SC integrated research ecosystem that transforms science via seamless interoperability



Strategic goal: Broadening participation



New modes of integrated science

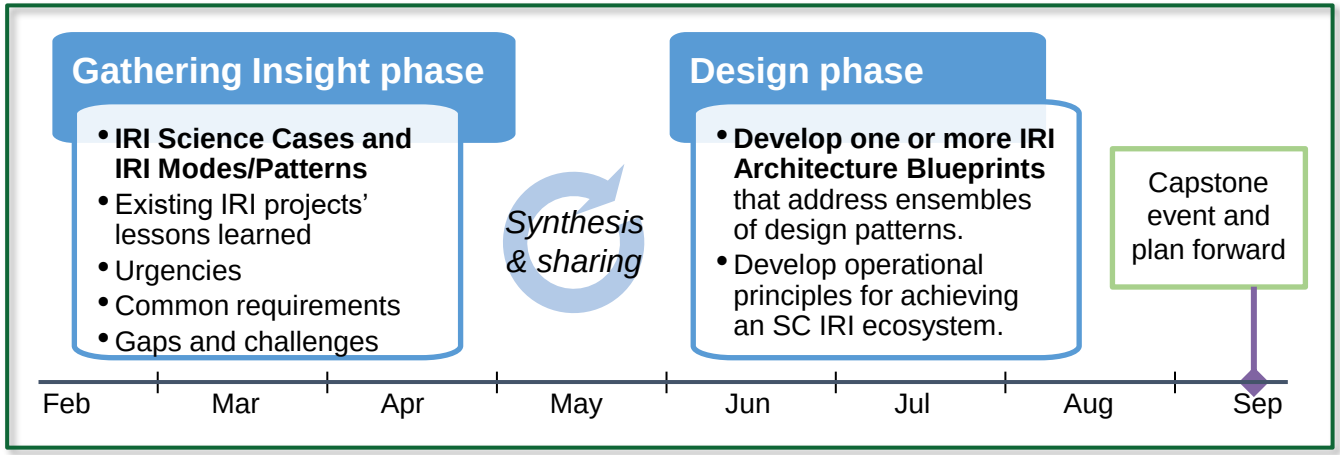
- Rapid data analysis and steering of experiments
- Novel models for multi-facility allocation/utilization
- AI-enabled insight from dynamic, vast multi-modal data
- Seamless user interconnectivity via federated IDs

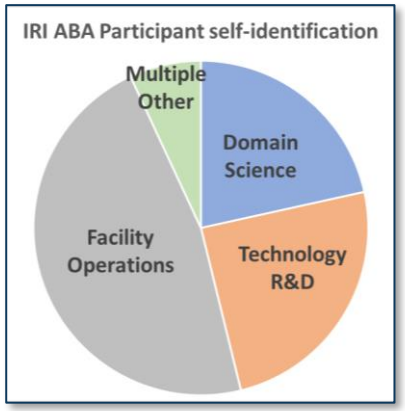
SC Integrated Research Infrastructure Architecture Blueprint Activity (IRI ABA)

An Office of Science strategic effort led by ASCR Facilities Division (Leads: Ben Brown and Bill Miller)

Aim: *Produce the* ***reference conceptual foundations*** *to inform a coordinated "whole-of-SC" strategy for an integrative research ecosystem.*

- Greenlighted by SC leadership in Nov. 2021 and formally launched in Feb. 2022
- HQ level org: IRI ABA Coordination Group representing all SC program offices
- Lab level org: IRI ABA Leadership Group representing IRI science and technology space
- Participants: 130+ DOE experts across science, User Facilities, Nat. Labs, & enterprise stakeholders





ASCR Facilities
Vendor Request for Information (RFI)

- **DOE Agency Priority Goal:** Sustain U.S. leadership in Advanced Computing technologies and enable continued progress in science and engineering applications
- FY2023 APG Milestone: DOE Laboratories issues a joint RFI to computing technology vendors to solicit input concerning future technologies, Advanced Computing Ecosystem components, non-recurring engineering (NRE) and other factors that will help inform how DOE and the labs approach the next generation of supercomputing systems in the 2025 to 2030 timeframe
- RFI released on June 28, 2022 with responses are due July 31, 2022

ASCAC Discussion of Future of Advance Computing

ASCR Software-Stewardship: Next Steps

1. Finalize the targeted scope of potential software-stewardship activities for FY23.

2. Define the relationship between those software-stewardship activities and synergistic activities in the Facilities, Research, and Advanced Computing Technologies (ACT) Divisions.

3. Develop a funding opportunity targeting participation from national laboratories, universities, nonprofit organizations, and the private sector.

4. In the case of a Continuing Resolution or other delay of the release of the funding opportunity announcement, prepare a Dear Colleague letter to outline ASCR's software-stewardship strategy.

5. Work with ECP, ASCR facilities, and other stakeholders to enable a common understanding of how all stakeholders will contribute to the overall process.

New ASCR Program Manager Position Now Open

GS-15 Interdisciplinary Physical Scientist/Computer Scientist Position in the Research Division, Computer Science Group

- Manage the computer science and networking research portfolios that include quantum communications and advanced wireless communications such as 6G and related Artificial Intelligence (AI) technologies, workflows, and cybersecurity systems

- Open between July 19 and August 1

- Two parallel announcements in USAJobs.gov
  - To be considered as a computer scientist, the applicants should apply to: https://www.usajobs.gov/job/664848100
  - To be considered as a physical scientist, the applicants should apply to the Open Continuous Direct Hire Announcement CY-22-OCDH-1301-11434839-DH posted in: https://www.usajobs.gov/job/646322700

Awards and Highlights

ORNL has delivered exascale for the nation

TOP500 The List.

TOP500 list
#1 Frontier
1.1 EF of performance on the May 2022 Top500 list

GREEN500 list
#1 Frontier
52.23 GF/watt power efficiency

HPL-AI list
#1 Frontier
6.88 EFs on the HPL-AI benchmark

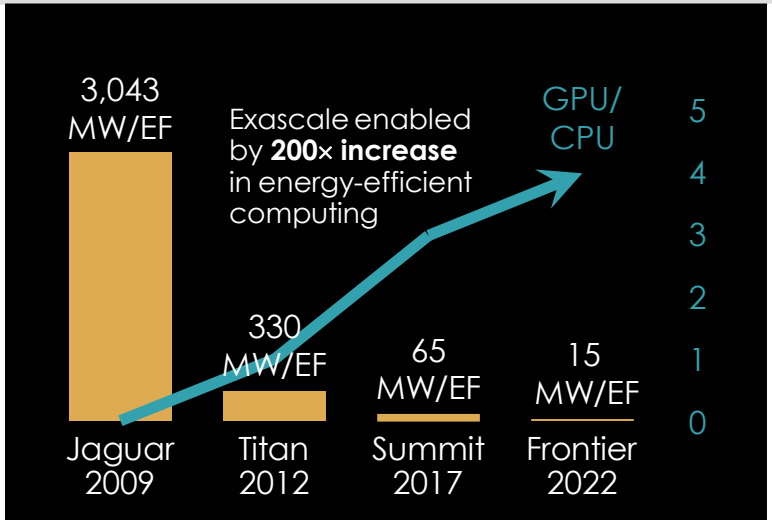
9,408 nodes, each with 1 CPU and 4 GPUs and coherent memory

74 HPE Cray EX cabinets

700 petabytes of storage capacity, peak write speeds of 5 terabytes per second using Cray Clusterstor Storage System

90 miles of HPE Slingshot networking cables

Frontier continues ORNL's reputation for delivering history-making computing systems, joining Eagle, Phoenix, Jaguar, Titan, and Summit



See Justin Whitt's presentation on Frontier for more information

Society for Industrial and Applied Mathematics - SIAM Fellows

2022 SIAM Fellow – Raymond Tuminaro, Sandia National Labs

For contributions in iterative linear solver algorithms and software to address scientific computing applications on large-scale parallel systems.

2021 SIAM Fellow – Robert D. Falgout, Lawrence Livermore National Lab

For contributions to the theory, practice, and large-scale applications of multilevel solvers and for widely used parallel software.

2021 SIAM Fellow – Habib N. Najm, Sandia National Labs

For pioneering contributions to uncertainty quantification and the use of Bayesian methods in physical modeling, with applications to combustion and far beyond.

ERNEST ORLANDO LAWRENCE AWARDEES

Luis Chacón, LANL

Fusion and Plasma Science: For his seminal contributions in multiscale algorithms for fluid, kinetic, and hybrid simulation of plasmas, enabling scientific breakthroughs in fast magnetic reconnection and self-organization in magnetic fusion systems, and in reactivity degradation in inertial fusion systems."

Andrew Landahl, SNL

Computer, Information and Knowledge Science: For his groundbreaking contributions to quantum computing, including the invention of transformational quantum error correction protocols and decoding algorithms, for scientific leadership in the development of quantum computing technology and quantum programming languages, and for professional service to the quantum information science community

DOE will host a hybrid award ceremony in Washington, DC, on September 22, 2022. Proceedings will be broadcast live online, and a recording will be available following the event. For more information, and to RSVP for the Lawrence Awards ceremony, go to https://science.osti.gov/lawrence/Ceremony. Please RSVP by September 15, 2022.

Jeff Nichols

Jeff Nichols, theoretical chemist and software developer, recently retired after serving over 13 years as the Associate Laboratory Director for Computing and Computational Science at Oak Ridge National Laboratory. In that position, he oversees the Department of Energy's (DOE) National Center for Computational Sciences (NCCS), the site of the Oak Ridge Leadership Computing Facility (OLCF), which delivers state-of-the-art scientific research and technological innovations. The OLCF is home to Frontier, the nation's most powerful computing resource. Jeff also led ORNL's agenda in advanced high-performance computing in priority areas such as materials science, fusion energy, and health data, as well as the laboratory's quantum computing and artificial intelligence initiatives.

Before coming to ORNL in 2022, he was the deputy director of the Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory, where high priority was given to the development, deployment, and use of scalable computational science community codes to solve grand-challenge problems crucial to the nation.

Jeff received his B.A. degrees in chemistry and mathematics from Malone College (Canton, Ohio) and a Ph.D. in physical chemistry from Texas A&M University.

David Brown

David Brown, an applied mathematician, recently retired after 10 years at Lawrence Berkeley National Laboratory as the Director of the Applied Mathematics and Computational Research Division at. His 38-year career with DOE National Laboratories included 14 years at Los Alamos National Laboratory and 13 years at Lawrence Livermore National Laboratory, where he was technical lead of several major research projects and held several line and program management positions.

Brown's research expertise and interests lie in the development and analysis of algorithms for the solution of partial differential equations. He is also particularly enthusiastic about promoting opportunities in computational science for young scientists from diverse backgrounds and is a founding member of the DOE Computational Science Graduate Fellowship program. More recently, he helped create the Sustainable Research Pathways program to bring faculty and students from diverse backgrounds for summer research experiences at Berkeley Lab.

David earned his PhD in Applied Mathematics from the California Institute of Technology in 1982. He also a B.S. in Physics and an M.S. in Geophysics from Stanford University.

Ewing ("Rusty") Lusk (1943 – 2022)

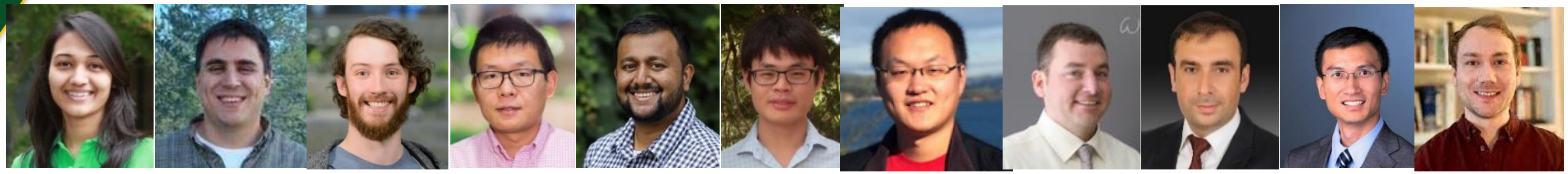
Ewing Lusk, known as “Rusty” for his red hair, received his B.A. in mathematics from the University of Notre Dame in 1965 and his Ph.D. in mathematics from the University of Maryland in 1970, after which he joined the Mathematics Department of Northern Illinois University. He joined the Mathematics and Computer Science Division at Argonne National Laboratory in 1980, was instrumental in founding the Advanced Computing Research Facility in 1983, and retired in 2012 as an Argonne Distinguished Fellow and a senior fellow of the Computation Institute of the University of Chicago.

Rusty was a leading member of the team responsible for the MPICH implementation of the MPI message-passing-interface standard, a founder of the MPI Forum, and worked on parallel performance-analysis tools and system software for clusters.

Rusty was the author of six books and more than a hundred research articles in mathematics, automated reasoning, and parallel computing. He won an R&D 100 award for his work in parallel computing and received the University of Chicago’s medal for distinguished performance.

The ANL CELS directorate will be holding a Research symposia in his honor this fall

FY22 ASCR Early Career Research Program



Name	Institution	Title	Research Area
Tanzima Islam	Texas State University	INTELYTICS: An Efficient Data-Driven Decision-Making Engine for Performance In the Era of Heterogeneity	Computer Sci
Brian Summa	Tulane University	Efficient and Accessible Interactive Visual Analytics of Exascale Scientific Data	Computer Sci
Johannes Doerfert	Argonne National Laboratory	HPC-OMP-CAR: HPC OpenMP Compiler and Runtimes	Computer Sci
Hanqi Guo	Ohio State University	Multidimensional Parameter-Space Feature Tracking, Analysis, and Visualization	Computer Sci
Aditya Nair	Florida State University	Network-based Modeling And Simulation Of Coupled Multi-physics Systems	Applied Math
Lu Lu	University of Pennsylvania	Physics-informed Neural Operators for Fast Prediction of Multiscale Systems	Applied Math
Guannan Zhang	Oak Ridge National Laboratory	Advanced Uncertainty Quantification Methods for Scientific Inverse Problems	Applied Math
Peter Bosler	Sandia National Laboratory (NM)	High Performance Adaptive Multiscale Simulations With Data-driven Scale Selective Subgrid Parameterizations	Applied Math
Sabit Ekin	Oklahoma State University	CommAwareNet: Towards Communication-Aware Smart Facilities: Designing an Energy-efficient High-data-rate and Reliable Hybrid THz/VLC Comm. Arch. Reinforced with Intelligent Surfaces for Future Network	Networking
Chenyun Pan	The University of Texas at Arlington	Scalable Reconfigurable Computing Circuit Using Emerging Device Technologies	Microelectronics
Tim Proctor	Sandia National Laboratory (CA)	Quantum Capability Learning	Quantum

Application-Oriented Performance Benchmarks for Quantum Computing

Scientific Achievement

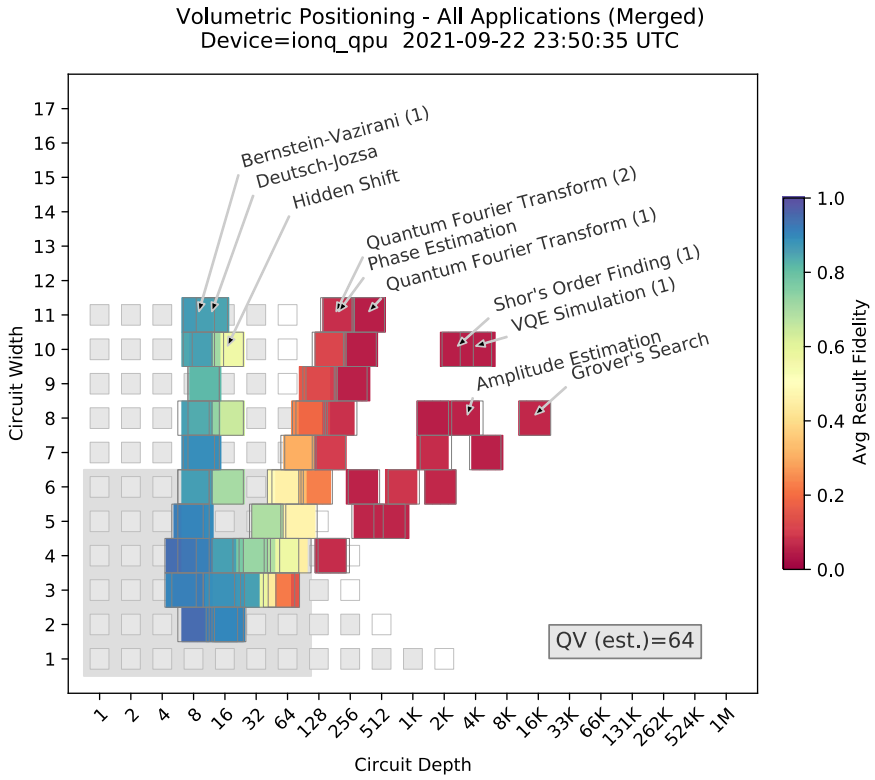
In collaboration with a team from the Quantum Economic Development Consortium (QEC-C), we created and one of the first application-oriented benchmarking suites for quantum computers, and used it to explore the performance of current hardware.

Significance and Impact

This is one of the first benchmarking suites that measures performance on tasks that are similar to future real-world quantum computing applications.

Research Details

- Our QED-C collaborators selected important algorithms and subroutines.
- We collaborated with them to turn them into benchmarks using our volumetric benchmarking framework.
- These benchmarks enable transparent comparisons between devices on application-like tasks.
- Our experimental results show that the predictive power of single number performance metrics like quantum volume is limited.



An example of the results obtained by running our benchmarking suite (this device is one of IonQ's 11-qubit ion trap quantum computers).

QED-C Sandia National Laboratories QPL

Thomas Lubinski, Sonika Johri, Paul Varosy, Jeremiah Coleman, Luning Zhao, Jason Necaise, Charles Baldwin, Karl Mayer, **Timothy Proctor arXiv:2110.03137**

Design of Many-Core Big Little µBrains for Energy-Efficient Embedded Neuromorphic Computing

The Challenge

- Increase Energy efficiency of artificial intelligence to sustain advancement and new applications.
- State-of-the-art digital hardware use crossbar-connected cores, but a significant fraction of the resources in each crossbar remains underutilized.
- The on-chip network becomes the primary energy and performance bottleneck as these systems scale up.

New Approach

- Hardware-software co-design, combining *µ*Brain cores using a novel segmented bus (SB) interconnect and system software called SentryOS (compared to Intel's Loihi):
  - Reduces energy between 37% and 98%
  - Reduces latency between 9% and 25%
  - Increases throughput between 20% and 36%

Impact

- Better scaling than previous digital neuromorphic designs, promising to enable large-scale applications.
- The segmented bus (SB) interconnect can enable virtualization of neuromorphic systems, enabling hardware sharable by many users.
- SentryOS can be used for faster application development and deployment on neuromorphic hardware.

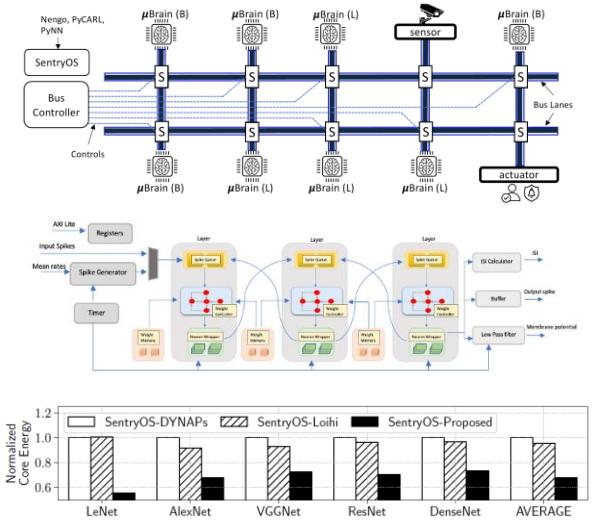


Fig: (a) Design of a many-core neuromorphic hardware with big-little µBrain cores and segmented bus (SB) interconnect. (b) A µ Brain design implemented on FPGA. (c) µBrain-based many-core hardware with SB is better than DYNAPs and Intel's Loihi.

PI(s)/Facility Lead(s): **Anup Das, ASCR Early Career awardee, 2021**
Collaborating Institutions: Drexel University, Imec (Netherlands and Belgium)
Publication(s) for this work: L. M. Varshika, et al., "Design Of Many-core Big Little µBrains For Energy-efficient Embedded Neuromorphic Computing," *Design Automation and Test in Europe (DATE) Conference* (2022).

APPFL: The Argonne Privacy-Preserving Federated Learning Framework

Scientific Achievement

Privacy-preserving federated learning framework APPFL enables supervised learning of a model on distributed sensitive datasets while preserving the data privacy

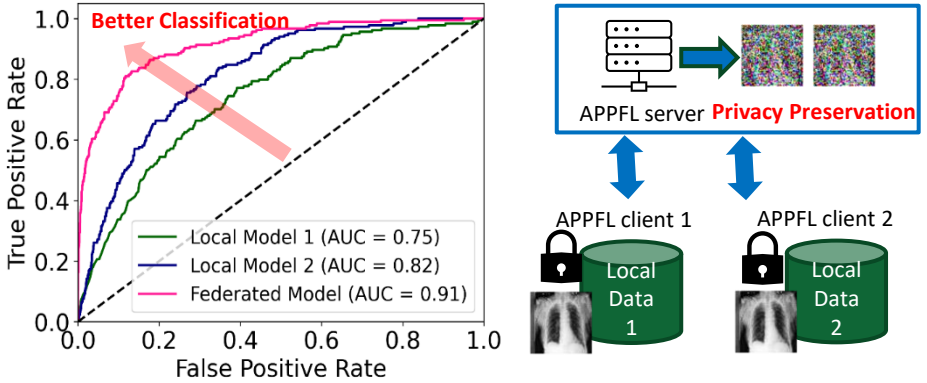
Significance and Impact

APPFL will enable research collaborations across countries and institutions while addressing the privacy and data shift challenges in many DOE applications (e.g., scientific machine learning, critical infrastructure)

Research Details

- Novel distributed optimization algorithms with differential privacy result in better convergence and learning performance
- In collaboration with medical institutions, APPFL is used to train image classification models on private chest x-ray data
- APPFL used for federated control of power system operations maintaining data privacy against an adversary

Privacy Preservation: *With stronger privacy, APPFL can prevent reconstruction of chest X-ray images from model weights by leveraging the gradient transfer during federated learning*



Data Shift Challenge: *Federated learning produces more accurate models in classifying chest X-ray image for COVID-19 compared to the models trained on local datasets*

Ryu, Kim, Kim, Madduri. "APPFL: Open-Source Software Framework for Privacy-Preserving Federated Learning" *2022 IEEE IPDPS Workshop (accepted);* https://github.com/APPFL/APPFL

Ryu, Kim. "Differentially Private Federated Learning via Inexact ADMM with Multiple Local Updates" *arXiv:2022.09409*, 2022

Ryu, Kim. "A Privacy-Preserving Distributed Control of Optimal Power Flow" *IEEE Transactions on Power Systems*, 2021

Some ASCAC Agenda Details

- HOWES SCHOLAR PRESENTATIONS
  - OPTIMIZING THE PERFORMANCE OF FUSION REACTORS AT EXASCALE, *Noah Mandell, Massachusetts Institute of Technology and DOE CSGF Alumnus*
  - DYNAMIC MODELING AND OPTIMAL SCHEDULING OF CHEMICAL PROCESSES PARTICIPATING IN FAST-CHANGING ELECTRICITY MARKETS, *Morgan Kelley, Dell Technologies and DOE CSGF Alumnus*
- BESAC ASSESSMENT ON INTERNATIONAL STANDING, *Cynthia M. Friend, President of the Kavli Foundation*
- EXASCALE UPDATE – *Lori Diachin, Lawrence Livermore National Laboratory*
- ARTIFICIAL INTELLIGENCE TESTBEDS AT ARGONNE, *Venkat Vishwanath, Argonne National Laboratory*
- PROGRAM RESPONSE TO THE COV REPORT – *Ceren Susut, ASCR*
- ASCR LEADERSHIP COMPUTING CHALLENGE PORTFOLIO FOR 22-23 ALLOCATION YEAR – *Jordan Thomas, ASCR*
- UPDATE ON EXASCALE SYSTEMS - FRONTIER*, Justin Whitt, Oak Ridge National Laboratory*
- GENERAL ELECTRIC (GE) COLLABORATIONS WITH DOE AT THE EXASCALE - *Rick Arthur, GE Research and ASCAC*