Update from ASCR Research: Fiscal Year 2024

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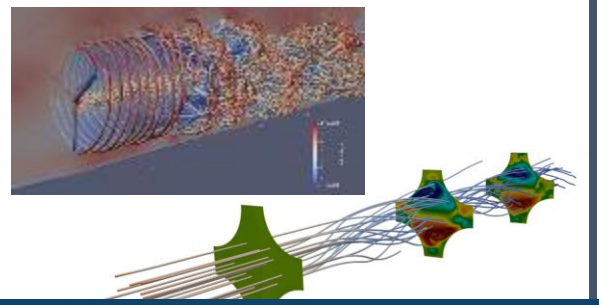
U.S. DEPARTMENT OF ENERGY | Office of Science

Energy.gov/science

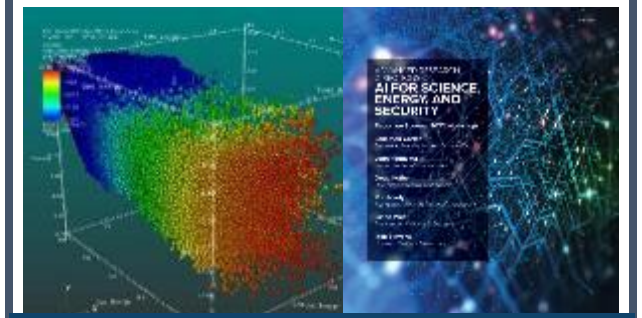
ASCR Research Develops With Critical Technology Trends

Advanced Modeling, Simulation, and Visualization



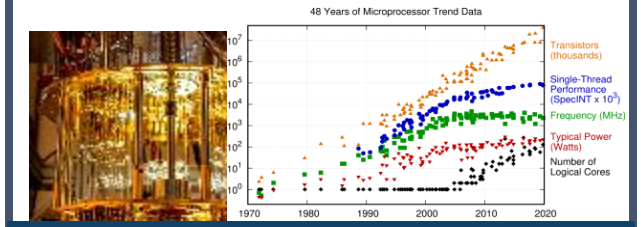
Empowering Science Through Fundamental Research

Frontier AI & Data



Creating Trustworthy and Energy Efficient Frontier AI

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



Transforming Fundamentals of Computing

Software Complexity for Increased Versatility

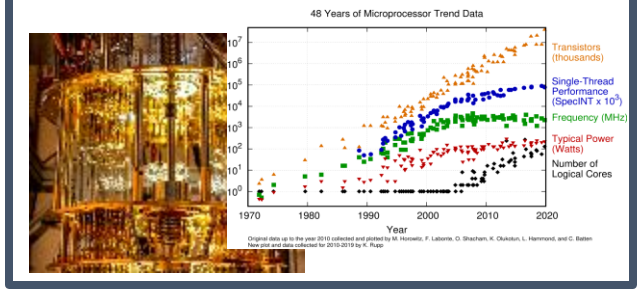
Enhancing Scientific Programming

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

Accelerating Science from Exascale to the Edge

Targeted Funding Solicitations

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



Accelerated Research in Quantum Computing

$65M planned in total for the portfolio of 5-year projects.

- Modular Software Stack
  - Addresses practical and fundamental bottlenecks that hinder modularity and potential synergy among selected hardware technologies;
  - Pursues general approaches to integration that may remain relevant for future technologies;
  - Devises ways to embed quantum processors in parallel and distributed computing models; and
  - Integrates error management across the software stack
- Quantum Utility
  - Choose generalizable application-inspired target problems;
  - Develop algorithms for optimized math kernels and math primitives for selected current
  - (NISQ) and future quantum systems that significantly advance state-of-the-art performance for the selected target problems;
  - Adapt, if needed, any level of the software stack for the specific target problems; and
  - Estimate quantum resources by employing important complementary metrics, including energy-to-solution

Topic	PI	Lead Institution	Collaborative Awards	Title
Modular Software Stack	De Jong, Wibe	Lawrence Berkeley National Laboratory	Argonne National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, Sandia National Laboratories, The University of Chicago	MACH-Q: Modular and Error-Aware Software Stack for Heterogeneous Quantum Computing Ecosystems
Modular Software Stack	Quiroz, Gregory	The Johns Hopkins University	Lawrence Livermore National Laboratory; University of Michigan; The University of Chicago; Unitary Fund, ColdQuanta, Inc.	SMART Stack (Scalable, Modular, Adaptable, Reconfigurable, error-Targeted approaches to quantum stack design)

Targeted Funding Solicitations

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

Accelerated Research in Quantum Computing (Continued)

Topic	PI	Lead Institution	Collaborative Awards	Title
Quantum Utility	Bennink, Ryan	Oak Ridge National Laboratory	NASA, Georgetown University, North Carolina State University	Algorithms for Quantum Utility: Intelligent, Robust, and Efficiently Distributed (AQUIRED)
Quantum Utility	Liu, Yuan	North Carolina State University	NASA; Lawrence Berkeley National Laboratory; Pacific Northwest National Laboratory; University of Massachusetts Amherst; Rutgers, The State University of New Jersey	Achieving Quantum Utility with Hybrid Discrete Continuous Variable Quantum Processors
Quantum Utility	Whaley, Birgitta	University of California, Berkeley		Quantum Computing for Partial Differential Equations
Quantum Utility	Perciano Costa Leite, Talita	Lawrence Berkeley National Laboratory	Argonne National Laboratory, San Francisco State University	AQuA-DATA: Advanced Quantum Algorithms for Diverse Applications and Theoretical Advancements in Science
Quantum Utility	Aaronson, Scott	The University of Texas at Austin		Accelerated Research In Quantum Computing
Quantum Utility	Barnes, Edwin	Virginia Polytechnic Institute		Quantum Utility with hardware- and application- Informed Near-Term Algorithms (QUINTA)
Quantum Utility	Chan, Garnet	California Institute of Technology	Lawrence Berkeley National Laboratory	Quantum Utility Through Advanced Computational Quantum Algorithm (QUACQ)
Quantum Utility	Parekh, Ojas	Sandia National Laboratories	Argonne National Laboratory , Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, University of Maryland, University of New Mexico, California Institute of Technology	FAR-Qu: Fundamental Algorithmic Research toward Quantum Utility

A First-of-its-kind Exponential Quantum Space Advantage

Scientific Achievement

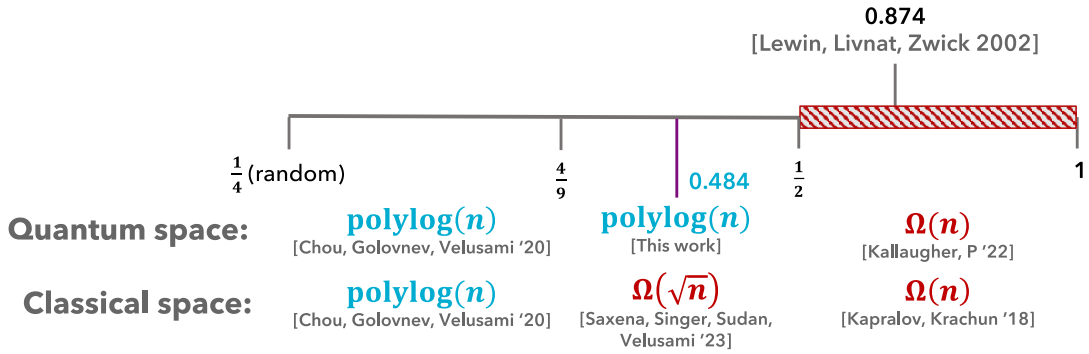
We obtained the first exponential quantum advantage for approximating a natural discrete optimization problem in a realistic model of computing. We discovered that, while *no* quantum space advantage is possible for the well-known Max-Cut problem in the streaming model of computing, considering Max-Cut on directed graphs allows for an exponential *space* advantage.

Significance and Impact

The Quantum Approximation Optimization Algorithm has inspired a decade of work seeking quantum advantages for discrete optimization, without clear success. For unconventional but practically relevant models of computing, we demonstrate that exponential quantum advantages are possible. Another critical message is that problem-specific details can significantly impact the potential for quantum advantages. We resolved a 15-year-old open problem.

Technical Approach

- Our quantum streaming algorithm approximates the Max Directed Cut value to within 0.484 of optimal using logarithmic space in the size of the graph.
- A new quantum implementation of a graph data structure enables the result.



Space requirements for approximating streaming Max Directed Cut. Space is a critical resource for quantum computing since robust and scalable qubits are scarce. The number of vertices in the input graph is *n.* The approximation guarantees above indicate the fraction of an optimal solution value guaranteed by various algorithms; larger is better, with 1 being optimal. While classical algorithms need square root of *n* space to get a 0.484 approximation guarantee, our quantum algorithm can achieve this using only logarithmic space – an exponential improvement. Approximations beyond 0.5 require linear space for both classical and quantum algorithms.

PI(s)/Facility Lead(s): Ojas Parekh
Collaborating Institutions: Sandia National Laboratories, Boston University
ASCR Program: Accelerated Research in Quantum Computing
ASCR PM: Marco Fornari
Publication(s) for this work: Kallaugher, Parekh, Voronova, Exponential Quantum Space Advantage for Approximating Maximum Directed Cut in the Streaming Model, arXiv:2311.14123. To appear in Proc of 56th ACM Symposium on Theory of Computing (STOC), 2024. Presented at QIP, 2024.

Targeted Funding Solicitations

Frontier AI & Data

$5.5M planned in total for the portfolio of 3-year projects.

Data Reduction for Science

- Effective algorithms and tools that can be trusted by scientists for accuracy and efficiency
- Progressive reduction algorithms that enable data to be prioritized for efficient streaming
- Algorithms which can preserve information in features and quantities of interest with quantified uncertainty
- Mapping techniques to new architectures and use cases

PI	Lead Institution	Collaborative Awards	Title
Kilmer, Misha	Tufts University	Argonne National Laboratory; Wake Forest University; North Carolina State University	Tensor-based Streaming Algorithms for Scientific Data Compression
Garcia Cardona, Cristina	Los Alamos National Laboratory	University of California, Los Angeles	Principled, Structure-Preserving, and Uncertainty-Quantified Machine Learning for Scientific Data
Kileel, Joseph	The University of Texas at Austin		Adaptive, Efficient, and Safe: General Tools for Streaming Large-Scale Tensors
Cappello, Franck	Argonne National Laboratory	Virginia Polytechnic Institute	ZF: A novel framework to design trustworthy lossy compressors for scientific data approaching lossy compressibility limits
Archibald, Richard	Oak Ridge National Laboratory	New York University; Dartmouth College; Clemson University	Infrastructure and Application Aware Reduction Methods for Scientific Data

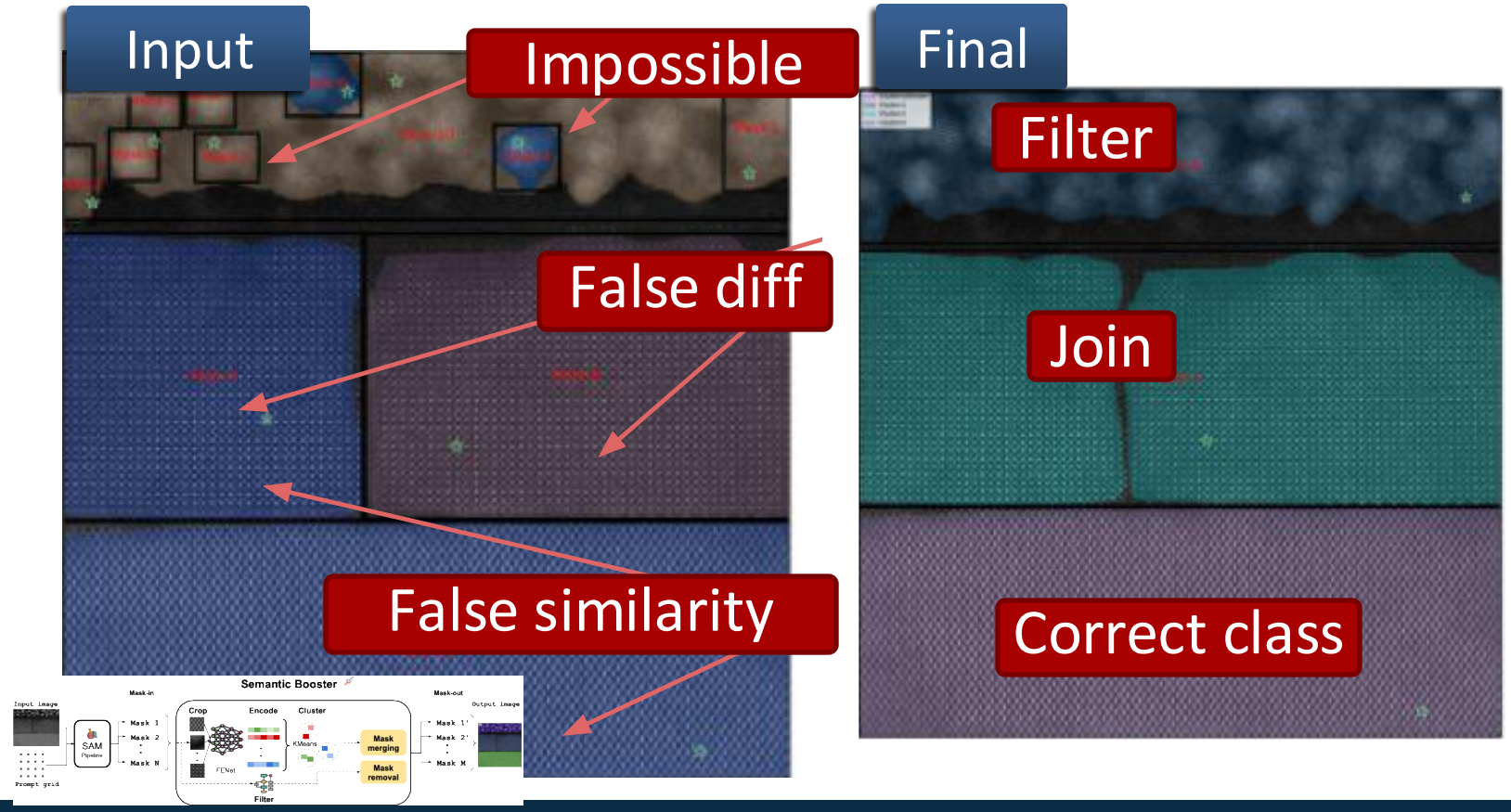
Accelerating Investment in AI for Science

Note that the October 2023 “Executive Order on the Safe, Secure, and Trustworthy Development and Use of Artificial Intelligence” directed activities directly relevant to ASCR, including:

- “support the development of safe, secure, and trustworthy AI technologies, as well as to support the design, development, and deployment of associated PETs [Privacy Enhancing Technologies]”
- “develop tools that facilitate building foundation models useful for basic and applied science”

Why do we need specific work on foundation models for science? A visual example from work by Nathan Tallent at Pacific Northwest National Laboratory under his Early Career Research project and collaborators at Iowa State University (Abebe et al., Comp. Mat. Sci (to appear)):

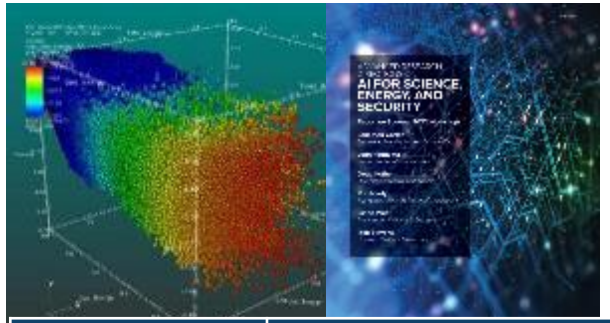
- Using a best-in-class image segmentation foundation model (left) does not produce a scientifically-relevant result.
- A workflow, including generative AI / LLMs, has been constructed to correct the deficiencies.



Targeted Funding Solicitations

Over 500 pre-proposals received!

Frontier AI & Data



Advancements in Artificial Intelligence for Science

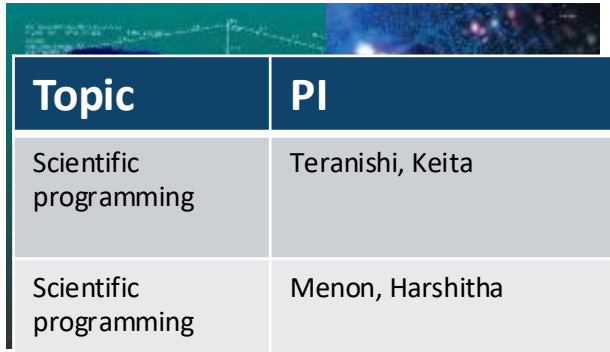
- Foundation models for computational science
- Automated scientific workflows and laboratories
- Scientific programming and scientific-knowledge-management systems
- Federated and privacy-preserving training for foundation and other AI models for science
- Energy-efficient AI algorithms and hardware for science.

$67M planned in total for the portfolio of 3-year projects.

Topic	PI	Lead Institution	Collaborative Awards	Title
Foundation models	Mahoney, Michael	Lawrence Berkeley National Laboratory	Oak Ridge National Laboratory, Dartmouth College	SciGPT: Scalable Foundational Model for Scientific Machine Learning
Foundation models	Zhang, Zheng	University of California, Santa Barbara	Argonne National Laboratory	Tensor-Compressed Sustainable Pre-Training of Extreme-Scale Foundation Models
Foundation models	Emami, Patrick	National Renewable Energy Laboratory	Pacific Northwest National Laboratory, Johns Hopkins University, Rensselaer Polytechnic Institute	Theseus: A Computational Science Foundation Model
Automated workflows	Zhang, Guannan	Oak Ridge National Laboratory	Sandia National Laboratories, Florida State University, Auburn University, Columbia University, University of South Carolina	DyGenAI: Dynamic Generative Artificial Intelligence for Prediction and Control of High-Dimensional Nonlinear Complex Systems
Automated workflows	Mueller, Juliane	National Renewable Energy Laboratory	Lawrence Livermore National Laboratory; University of Colorado, Boulder	DS4MEAMS: Decision support for machine learning enabled autonomous multi-scale simulations

Targeted Funding Solicitations

Frontier AI & Data

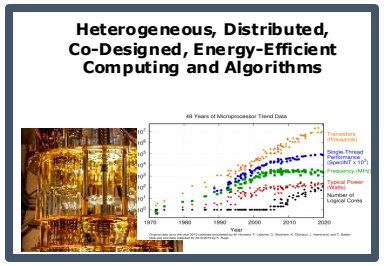


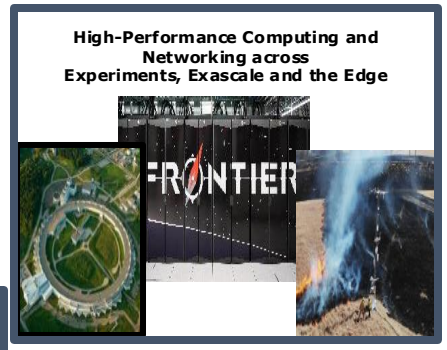
Advancements in Artificial Intelligence for Science (Continued)

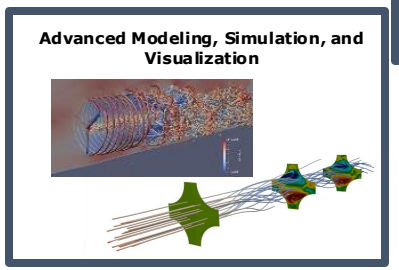
Topic	PI	Lead Institution	Collaborative Awards	Title
Scientific programming	Teranishi, Keita	Oak Ridge National Laboratory	Lawrence Berkeley National Laboratory, Carnegie Mellon University	Durban: Enhancing Performance Portability in HPC Software with Artificial Intelligence
Scientific programming	Menon, Harshitha	Lawrence Livermore National Laboratory	Oak Ridge National Laboratory, University of Maryland, Northeastern University	Productive AI-Assisted HPC Software Ecosystem
Federated and privacy-preserving	Lu, Lu	Yale University	Lawrence Berkeley National Laboratory; Los Alamos National Laboratory; University of North Carolina at Chapel Hill; University of California, San Diego; Florida State University	FedNeMO: Physics-Informed and Energy-Aware Federated Learning of Neural Multi-Operator Learners as Scientific Foundation Models
Federated and privacy-preserving	Kim, Kibaek	Argonne National Laboratory	Brookhaven National Laboratory; Oak Ridge National Laboratory; Arizona State University; Rutgers, The State University of New Jersey	Privacy-Preserving Federated Learning for Science: Building Sustainable and Trustworthy Foundation Models
Energy-efficient AI	Kirst, Christoph	University of California, San Francisco	Lawrence Berkeley National Laboratory; University of Southern California	Flexible brain inspired hybrid analog-spiking neuronal network computation in energy-efficient neuromorphic hardware
Energy-efficient AI	Potok, Thomas	Oak Ridge National Laboratory	George Washington University, George Mason University, University of Tennessee	ENGAGE: (E)nergy-efficient (N)ovel Al(g)orithms and (A)rchitectures for (G)raph L(e)arningres

Targeted Funding Solicitations

$10.8M planned in total for the portfolio of 2-year projects.





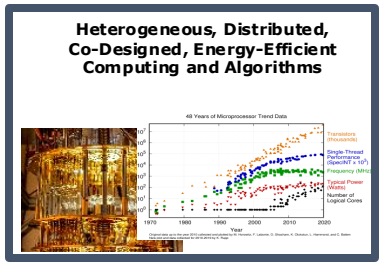


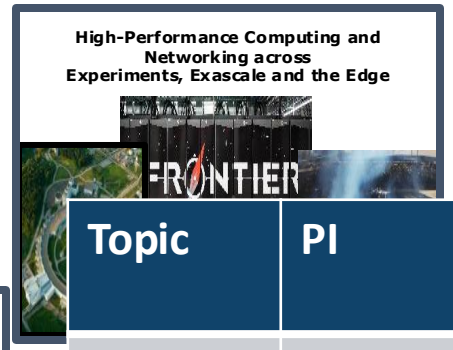
EXPRESS: 2024 Exploratory Research for Extreme-Scale Science

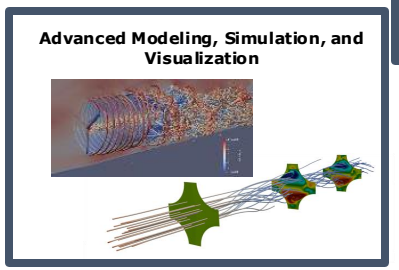
- Harnessing Technology Innovations to Accelerate Science through Visualization
- Scalable Space-Time Memories for Large Discrete/Agent-Based Models
- Neuromorphic Computing
- Advanced Wireless
- Quantum Hardware Emulation

Topic	PI	Lead Institution	Collaborative Awards	Title
Quantum	Proctor, Timothy	Sandia National Laboratories		Emulating quantum computers with physics-aware neural networks
Quantum	Iancu, Costin	Lawrence Berkeley National Laboratory		FLEQ*: Functional Level Qualitative Emulation of Quantum Programs
Quantum	Petersson, Anders	Lawrence Livermore National Laboratory		Pulse-level Emulation Of A Multi-qubit Quantum Computing Device
Quantum	Appelo, Daniel	Virginia Polytechnic Institute	University of New Mexico	Quantum Digital Twins
Visualization	Ushizima, Daniela	Lawrence Berkeley National Laboratory		Autonomous Solutions for Computational Research with Immersive Browsing & Exploration
Visualization	Ferrier, Nicola	Argonne National Laboratory		Digital twins and AI-enabled & IMmmersive Environments for Automated Scientific Laboratories (DAIMSL)

Targeted Funding Solicitations







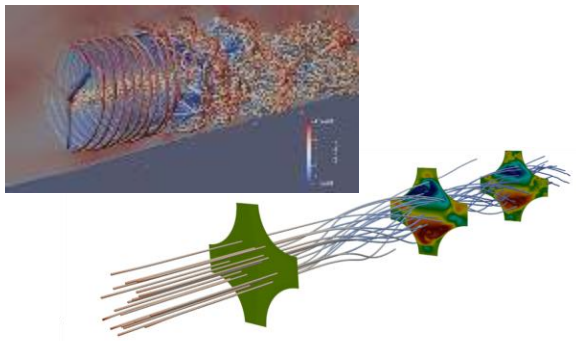
EXPRESS: 2024 Exploratory Research for Extreme-Scale Science (Continued)

Topic	PI	Lead Institution	Collaborative Awards	Title
Space-Time	Zaman, Luis	University of Michigan, Ann Arbor	Michigan State University	Dynamic Space-Time Memory Curation for Traceable Wafer-Scale Agent-Based Models
Space-Time	Santhi, Nandakishore	Los Alamos National Laboratory	Florida International University	Scalable Space-Time Memory Coupled AI-Agent Simulators for Emergent Controlled Divergence
Space-Time	Brown, Kevin	Argonne National Laboratory		TimeWeave: Towards a Unified Infrastructure for PDES and Distributed ABMS
Neuromorphic	Merkel, Cory	Rochester Institute of Technology		Design and Fabrication of Analog Neuromorphic Systems based on Active Dendrites with non-linear Synaptic Devices for Energy-Efficient Scientific Discovery
Neuromorphic	Zeng, Yuping	University Of Delaware		Neuron blocks using HfZrO/GaN field effect transistors for energy efficiency computing
Wireless	Kilic, Ozgur [Jha, Shantenu]	Brookhaven National Laboratory	University of California, Santa Barbara; University of Notre Dame; University of Nebraska-Lincoln	Coupling Sensor Networks and HPC Facilities with Advanced Wireless Networks for Near-Real-Time Simulation of Digital Agriculture
Wireless	Butko, Anastasiia	Lawrence Berkeley National Laboratory		INDIE: Intelligent Distribution for Advanced Wireless Networks with Scientific Data

Targeted Funding Solicitations

$6M planned in total for the portfolio of 3-year projects.

Advanced Modeling, Simulation, and Visualization



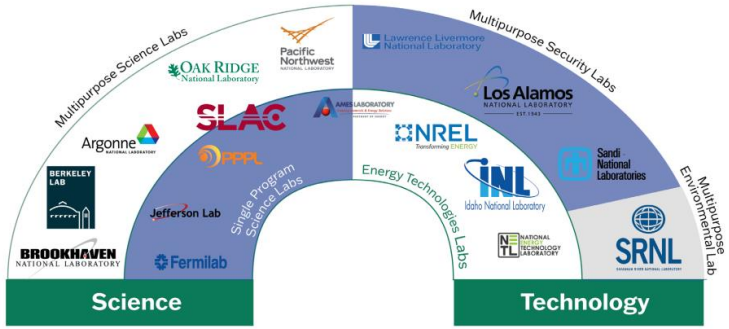
Scientific Discovery through Advanced Computing (SciDAC): Partnership in Electricity [with DOE Office of Electricity]

- Areas of fundamental computational research may include artificial intelligence/machine learning, federated learning with data privacy, dynamical systems, rare-events modeling, uncertainty quantification, real-time data processing and cyber-physical control, and classical and quantum optimization.
- Application-research areas may be drawn from transformer resilience and components, microgrids, grid-enhancing technologies, transmission reliability, advanced grid modeling, resilient distribution systems, grid operations, secure grid communications, and energy-storage R&D.

PI	Lead Institution	Collaborators	Title
Peles, Slaven	Oak Ridge National Laboratory	Lawrence Livermore National Laboratory, National Renewable Energy Laboratory, Texas A&M University, Virginia Polytechnic Institute	Next Generation Dynamic Simulations for Reliable, Resilient and Decarbonized Grid
Petra, Cosmin	Lawrence Livermore National Laboratory	Argonne National Laboratory, University of Connecticut	Scalable Learning and Optimization for Secure and Economic Grid Operations

Targeted Funding Solicitations

$87M planned in total for the portfolio of 4-year projects.



Competitive Portfolios for Advanced Scientific Computing Research

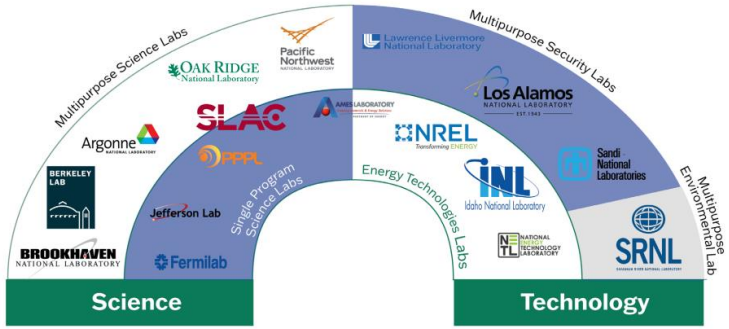
To ensure continued leadership in delivering on the promise of computational science, and drive innovation in energy-efficient and versatile high-performance computing for science, ASCR seeks to invest in DOE National Laboratory-led portfolios that:

- Support long-term, high-impact research,
- Aggressively respond to, and take advantage of, emerging science and technology trends, and
- Collaborate with a diverse community of the most-promising academic and industry partners.

- This solicitation, open to all DOE National Laboratories, served as a full recompetition of ASCR's "base program", expanded to include applied mathematics, computer science, and advanced computing technologies / testbeds.
- 15 of the 17 DOE laboratories proposed over 60 distinct research thrusts plus integration activities.

PI	Lead Institution	Collaborators	Title	Topics
Borders, Tammie	National Energy Technology Laboratory	Cerebras Systems Inc.	SCI-NE3WS - Scientific Computing Interface for Novel Energy-Efficient, Extreme-Speed Wafer-Scale Engine	Basic research on Wafer Scale Engine Architecture and Integration, understanding how the next-generation AI architecture can be leveraged for physical modeling and simulation workloads and hybrid AI workloads.
Hagberg, Aric	Los Alamos National Laboratory	University of Arizona; Virginia Polytechnic Institute; Texas A&M University	Foundations for High Productivity, High-Confidence, High-Fidelity Simulations	Basic research topics including: Data-driven reduced order modeling; Multiphysics model- and scale bridging; and Multiscale and Multiphysics mathematical methods.

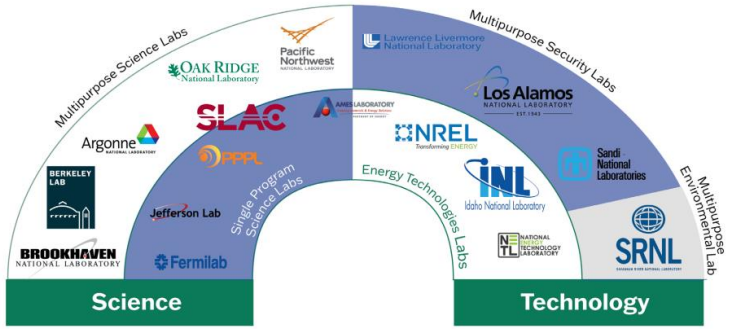
Targeted Funding Solicitations



Competitive Portfolios for Advanced Scientific Computing Research (Continued)

PI	Lead Institution	Collaborators	Title	Topics
Hittinger, Jeffrey	Lawrence Livermore National Laboratory	Lawrence Berkeley National Laboratory, Portland State University, University of Illinois Urbana-Champaign, Dihedral LLC	Foundations for Decision Support Through Cognitive Simulation	Basic research topics including: Next-Generation Methods for PDEs; and Foundations for Next Generation Decision Support.
Parks, Michael	Oak Ridge National Laboratory	Sandia National Laboratories, Carnegie Mellon University	MAGNET: MAthematics, ComputinG, and NETworking for Resource-Efficient Computational Science	Basic research topics including: Foundations of Learning: Graphs, Linear Algebra, Stats; Performance Portability on Extremely Heterogeneous Architectures (PPEHA); and AI GREEC: Artificial Intelligence and Knowledge Graphs to Accelerate Energy- Efficient Computing.
Rallo, Robert	Pacific Northwest National Laboratory	Arizona State University; Zero ASIC Corporation	End-to-end co-design for performance, energy efficiency, and security in AI-enabled computational science (ENCODE)	Basic research topics including: Intelligent and Scalable Hardware Design Automation; and Advanced Architecture Testbeds.

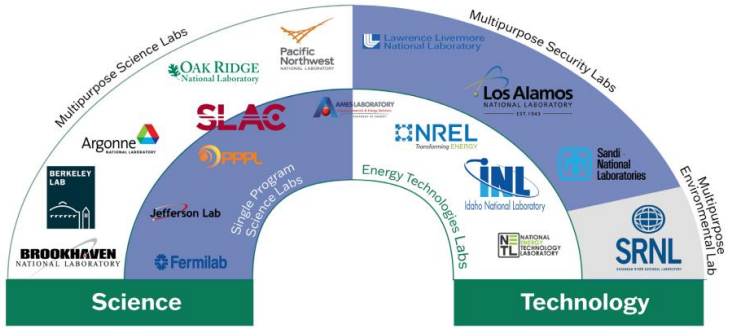
Targeted Funding Solicitations



Competitive Portfolios for Advanced Scientific Computing Research (Continued)

PI	Lead Institution	Collaborators	Title	Topics
Stewart, James	Sandia National Laboratories	Los Alamos National Laboratory, University of New Mexico	ASCEND: Applied mathematics and Scientific Computing Ecosystem for the New Digital era	Basic research topics including: Advanced Discretizations and Linear Solvers; Multiscale and Multiphysics mathematical methods; Optimization; Randomized Algorithms and Tensors; Uncertainty Quantification; and AIGREEC: Artificial Intelligence and Knowledge Graphs to Accelerate Energy-Efficient Computing.
Taylor, Valerie	Argonne National Laboratory	Lawrence Berkeley National Laboratory; University of Colorado, Boulder; University of Buffalo; University of Texas at Austin; The Pennsylvania State University; University of California, Merced	Energy Efficient Computing: A Holistic Methodology	Basic research topics including: Automatic Differentiation; Efficient Data-Driven HPC Modeling and Simulation for Energy; Energy-Efficient Composable Solvers; Energy Efficient Optimization under Uncertainty for Multicomponent, Multiscale, Multiphysics Systems; Foundations of Surrogate Models and UQ; and Algorithm-Driven Codesign of Specialized Architectures for Energy-Efficient HPC.

Targeted Funding Solicitations



Competitive Portfolios for Advanced Scientific Computing Research (Continued)

PI	Lead Institution	Collaborators	Title	Topics
Wild, Stefan	Lawrence Berkeley National Laboratory	Oak Ridge National Laboratory; University of Michigan; University of Kentucky; Dartmouth College; Portland State University; University of Wisconsin–Madison; University of California, Berkeley; University of Massachusetts Lowell	Advancing the Foundations of Scientific Computing Research	Basic research topics including: Energy-Efficient Composable Solvers; Foundations of Learning: Graphs, Linear Algebra, Stats; Frontiers in Computational Physics: New Mathematics for Fluids, Interfaces, and Materials; Next-Generation Methods for PDEs; and Algorithm-Driven Codesign of Specialized Architectures for Energy-Efficient HPC.

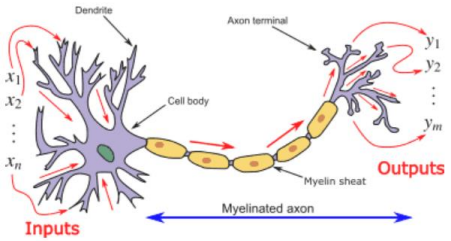
Many projects, in this and essentially all other portfolios, are building on ECP investments!

Abisko Microelectronics Codesign Overview

OAK RIDGE National Laboratory · Sandia National Laboratories · ASU Arizona State University · Georgia Tech · HARVARD UNIVERSITY

Collaborator: Fermilab

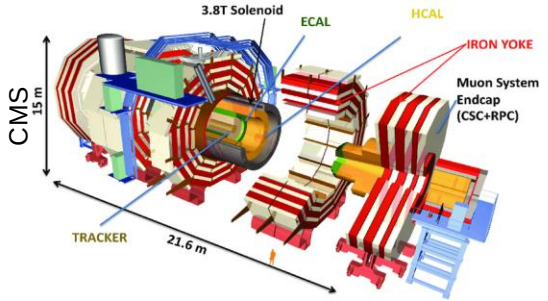
1. Develop better techniques for codesign from algorithms to devices and materials
2. Design Spiking Neural Network chiplet that can be integrated with contemporary computer architectures
3. Explore new devices and materials for the SNN chiplet (neuron, synapse, plasticity, etc.)
4. Design language abstractions and runtime support for SNN chiplet



Source: Wikipedia

Applications

Motivation
- Transportation
- CMS Sensors



Motifs, Composition

Algorithms

Algorithms
- ML: SLAYER, Whetstone, EONS, eProp, STDP
- Non-ML: Graph algorithms, CSP
- Simulators: NEST, Brian2

nest :: · BRIAN

API, Motifs

J.S. Vetter *et al.*, *"Abisko: Deep codesign of an architecture for spiking neural networks using novel neuromorphic materials,"* International Journal of High Performance Computing Applications, 37(3-4):351-79, 2023, https://doi.org/10.1177/10943420231178537

Software

Software
- DSL and API for neuromorphic co-processing
- Built on LLVM and MLIR
- Portable across Abisko chiplet, GPUs, etc.

LLVM COMPILER INFRASTRUCTURE · MLIR · XACC

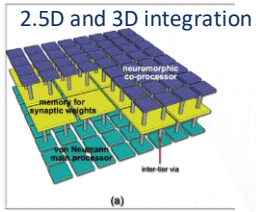
ISA, IR

Architecture

Architecture
- Design neuromorphic chiplet
- RISC-V neuromorphic extensions
- Heterogeneous integration with contemporary technologies

RISC-V

2.5D and 3D integration



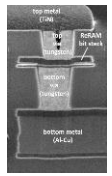
Simulation/Emulation: ALADDIN · gem5

Circuit scale up, Interconnects, PDK

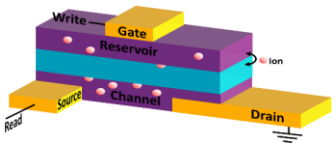
Devices and Circuits

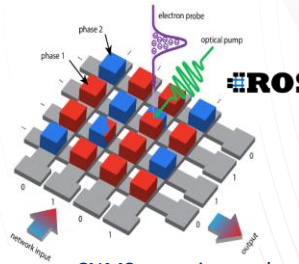
Devices and Circuits
- ion insertion (reversible doping) sets analog states
- mRaman captures transition linear, non-linear switching
- Will extend to 36x36 x-bar array
- Electronic and other optical spectroscopies

TaOx ReRAM



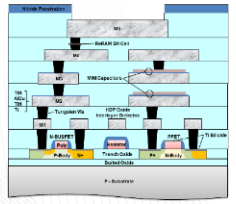
ECRAM



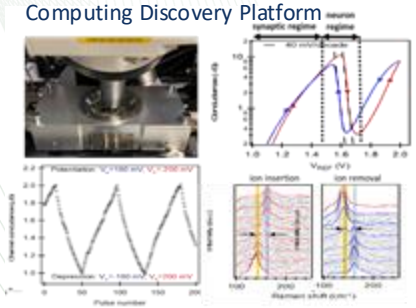


CROSS SIM

MesaFAB ReRAM

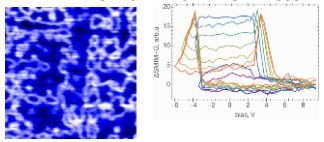


Computing Discovery Platform

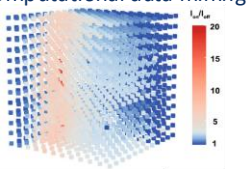


Compact models

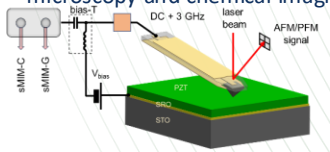
Domain wall memristor



Computational data mining



CNMS scanning probe microscopy and chemical imaging



Materials

Materials
- Non-equilibrium probes to few nm
- Data-driven modeling
- On-demand neuromorphism

J.S. Vetter *et al.*, *"Abisko: Deep codesign of an architecture for spiking neural networks using novel neuromorphic materials,"* International Journal of High Performance Computing Applications, 37(3-4):351-79, 2023, https://doi.org/10.1177/10943420231178537.

DOE Microelectronics Research Centers

- As authorized by the CHIPS and Science Act (Section 10731, Micro Act) the DOE FY 2024 President's Budget request includes $60M/year to establish **Microelectronics Science Research Centers.**
- Centers will perform mission-driven research to address foundational challenges in the design, development, characterization, prototyping, demonstration, and fabrication of microelectronics.
- **Centers will focus on fundamental science and early-stage research, complementing the investments already made through the CHIPS Act, such as:**
  - ❖ DOC National Semiconductor Technology Center (NSTC) and National Advanced Packaging Manufacturing Program (NAPMP)
  - ❖ DOD Microelectronics Commons

Two FY 2024 focus areas:
- Energy efficiency
- Extreme environments

- **Centers will leverage infrastructure and expertise at the DOE National Labs. Initial laboratory solicitation for center projects closed in July 2024, with selections to be announced in the near future.**

Growing and Diversifying Our Research Community

Solicitations (FY 2024):

▲Early Career Research Program, 2024.

- Eight ASCR awards, five of which to university faculty.

For more information on the ECRP program, including abstracts for all awards, visit: https://science.osti.gov/early-career

PI Name	Institution	Proposal Title
Gina Adam	George Washington University	Energy-efficient Neuromorphic Technologies for Scientific Computing
Carlee Joe-Wong	Carnegie Mellon University	Learning to Adaptively Manage Heterogeneous Scientific Workloads on Heterogeneous Clusters
Anil Damle	Cornell University	Fine-grained Theory and Robust Algorithms for Randomized Numerical Linear Algebra
Scott Dawson	Illinois Institute of Technology	Adaptive Multiscale Modeling using Pseudospectral Wavepackets
Su Yan	Howard University	Randomized Algorithms for Multiscale Electromagnetics and Multiphysics Problems
Shusen Liu	Lawrence Livermore National Laboratory	Narrowing the Human-AI Knowledge Gap through Audience-Aware Visualization
Jeffrey Donatelli	Lawrence Berkeley National Laboratory	Multi-Tiered Algorithms for Solving Extreme-Scale Inverse Problems Emerging from New Experiments
Gianluca Geraci	Sandia National Laboratories	Enabling Scientific Data-Driven Modeling from Heterogeneous, Multi-Model, Massive, and Distributed Datasets

Growing and Diversifying Our Research Community

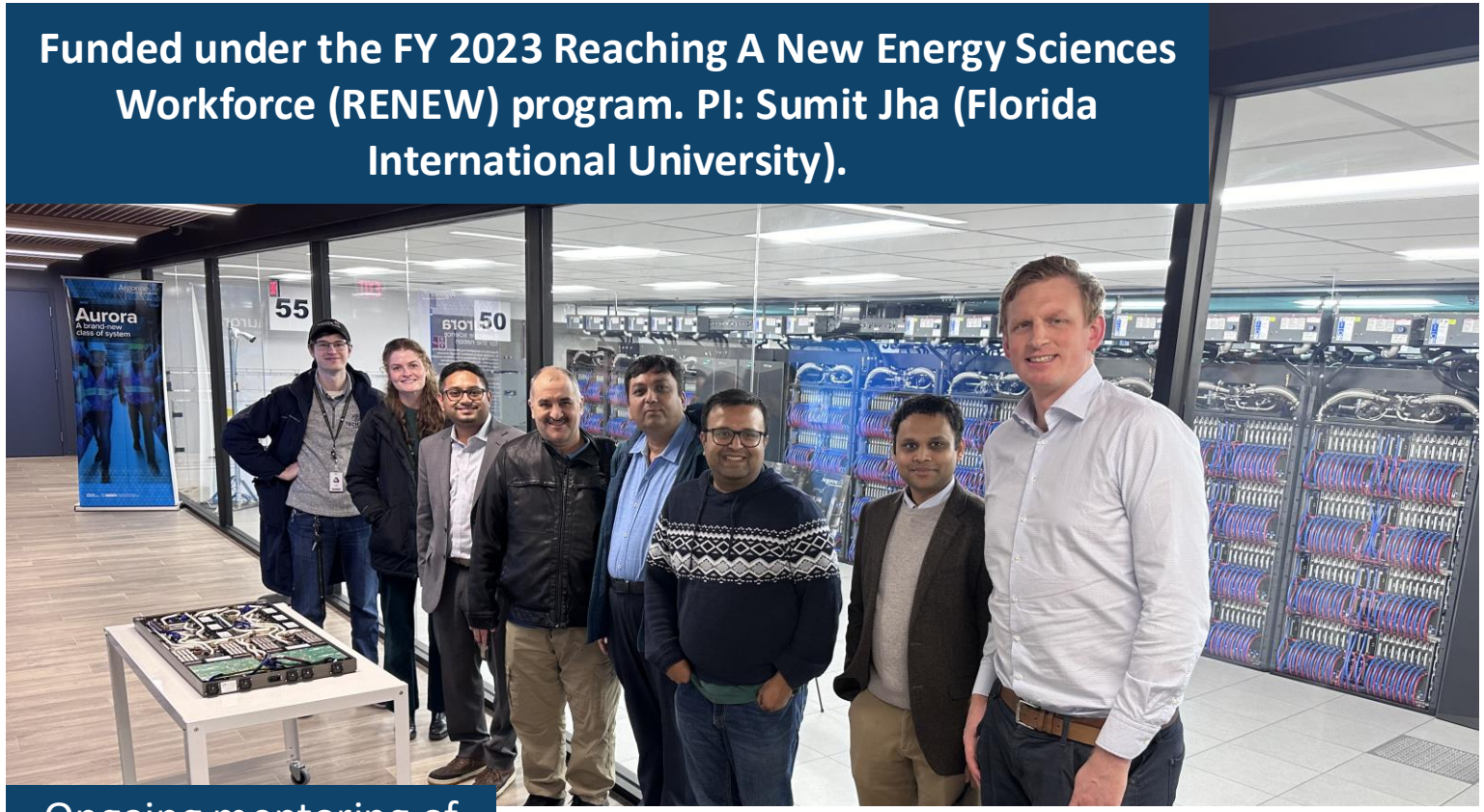
Solicitations (FY 2024):

- Building EPSCoR-State/National Laboratory Partnerships, 2024.

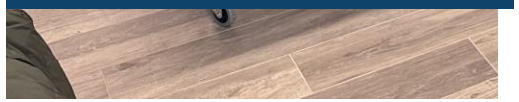
PI Name	Institution	Proposal Title
Kung, Patrick	The University of Alabama	Enhancing Quantum Networking Research Capabilities in Alabama: Integrating RF Photonic Controls for High-Frequency Cryogenic Links in GHz-THz Bands
Wang, Jinhui	University of South Alabama	Memristor Enabled Neuromorphic System with Robust Immunity to Non-ideal Property

Mobilizing the Emerging Diverse AI Talent (MEDAL) through Design and Automated Control of Autonomous Scientific Laboratories

Funded under the FY 2023 Reaching A New Energy Sciences Workforce (RENEW) program. PI: Sumit Jha (Florida International University).



Ongoing mentoring of over 30 Students from five institutions:



Bowie State University 1865 — 2 Graduate, 4 Undergraduate Students

Oakland University 1957 — 1 Graduate, 3 Undergraduate, 2 High-school students

University of Central Florida 1963 — 1 Graduate, 11 Undergraduate Students

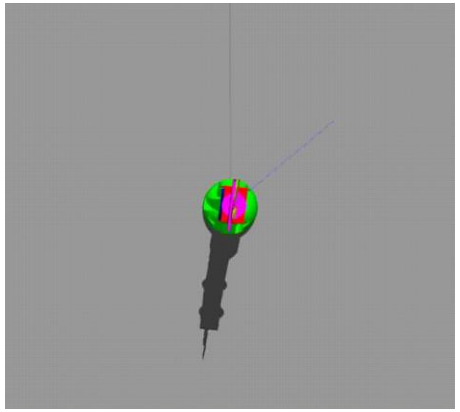
Cleveland State University 1964 — 4 Graduate Students

Florida International University 1965 — 1 Graduate, 3 Undergraduate Students

Undergraduate Research Exemplar:

- New academic surrogate for Argonne National Laboratory (ANL)'s Rapid Prototyping Lab.
  - Braccio robot with 6 degrees of freedom.
  - Test-bed to demonstrate foundation-model-based (LLM) control.
  - Leveraging ANL's Workflow Execution Interface (WEI) library.

Braccio robot.



Simulation environment controlled by LLM-generated code.

Growing and Diversifying Our Research Community

Solicitations (FY 2024):

- FY 2024 Funding for Accelerated, Inclusive Research (FAIR), 2024.
  - ASCR topics in:
    - Extreme-Scale Algorithms for Scientific Computing
    - Scalable Scientific Data Analysis and Reduction
    - Systems (Programming Models, Runtime Systems, etc.)
    - Data Management, Visualization, and Analytics
    - Quantum Computing and Networking
    - Emerging Computing (Neuromorphic, Advanced Wireless, etc.)
  - Selection announcement forthcoming.
- FY 2024 Reaching A New Energy Sciences Workforce (RENEW), 2024.
  - ASCR topics broadly covering applied mathematics, computer science, and advanced computing technologies.
  - Selection announcement forthcoming.

Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR)

FY 2024 ASCR SBIR/STTR Phase I Awards:

Many projects will build on ECP investments!

Topic	Company	Title	State
Accelerating The Deployment Of Advanced Software Technologies	NexGen Analytics LC	Work Visualizer: a user support tool to facilitate general computing using heterogeneous architectures at scale.	WY
Accelerating The Deployment Of Advanced Software Technologies	Simmetrix Inc	Geometry and Meshing Technologies to Support Fusion Energy System Simulations	NY
Accelerating The Deployment Of Advanced Software Technologies	Veracity Nuclear, LLC	High Fidelity Nuclear Reactor Core Simulation for Efficient Microreactor Design	TN
Accelerating The Deployment Of Advanced Software Technologies	Aperi Computational Mechanics Consulting, Llc	Leveraging Compadre and MFEM in Geometrically Versatile Numerical Methods	NM
Accelerating The Deployment Of Advanced Software Technologies	Coreform LLC	Accurate and performant finite element analysis of giga-cast parts	UT
Accelerating The Deployment Of Advanced Software Technologies	IERUS Technologies, Inc.	Development of an Efficient Metalens Design and Optimization Package	AL
HPC Cybersecurity	Lifeboat LLC	Protecting the confidentiality and integrity of data stored in HDF5	IL
HPC Cybersecurity	X-ScaleSolutions	Secure-MPI: A High-Performance MPI Library with Secured Communication for HPC Applicationspping	OH
Digital-twin Capabilities For Science Network Infrastructures	Kitware Inc.	Composable Digital Twins for Science Network Infrastructures using Parallel Discrete Event Simulation	NY
Artificial Intelligence Tools For Catalyzing Interdisciplinary Science	Aptima, Inc.	FusionSci: Augmented Intelligence to Empower Interdisciplinary Research	MA
Artificial Intelligence Tools For Catalyzing Interdisciplinary Science	Stottler Henke Associates, Inc.	05a Generative Embeddings Network-based Semantic Inference and Search (GENESIS)	CA
Mixed Integer Solver Technology For Accelerated Computing Systems	Optimal Solutions, Inc.	Novel Branch & Bound Tree Management for Fast Convergence of MIPs on Parallel Computers	NJ

Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR)

FY 2024 ASCR SBIR/STTR Phase II Awards:

Topic	Phase	Company	Title	State
HPC Code And Software Tools	IIB	Continuum Dynamics, Inc.	Advanced Methods for Efficient Aeroelastic Analysis of Wind Turbines and Wind Farms	NJ
Technology To Facilitate The Use Of Near-term Quantum Computing Hardware	IIB	ColdQuanta, Inc.	Increased Reliability for Near-Term Quantum Computers via Low-Level Control	CO
Accelerating The Deployment Of Advanced Software Technologies	II	Lifeboat LLC	Supporting Sparse Data in HDF5	IL
Accelerating The Deployment Of Advanced Software Technologies	II	Advanced Cooling Technologies, Inc.	Semiconductor Device Simulation Software with Monte Carlo Based Thermal Transport Modeling	PA
Accelerating The Deployment Of Advanced Software Technologies	II	Coreform LLC	Advanced tire tread simulation through adaptive isogeometric analysis	UT
Accelerating The Deployment Of Advanced Software Technologies	II	Osazda Energy	An Optimization-Based Design Ecosystem Targeting Performance, Reliability, and Stability of Photovoltaic Modules in Solar Energy Market	NM
Technology To Facilitate The Use Of Near-term Quantum Computing Hardware	II	Atlantic Quantum Corp	Software for Automatic Control, Calibration and Validation of Quantum Processors	MA
Technology To Facilitate The Use Of Near-term Quantum Computing Hardware	II	HighRI Optics, Inc	Highly Efficient Low Loss Fiber-Chip Light Coupling for Quantum Networks	CA

ECP EXASCALE COMPUTING PROJECT

Many projects are building on ECP investments!

Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR)

FY 2025 ASCR SBIR/STTR Phase I Topics:

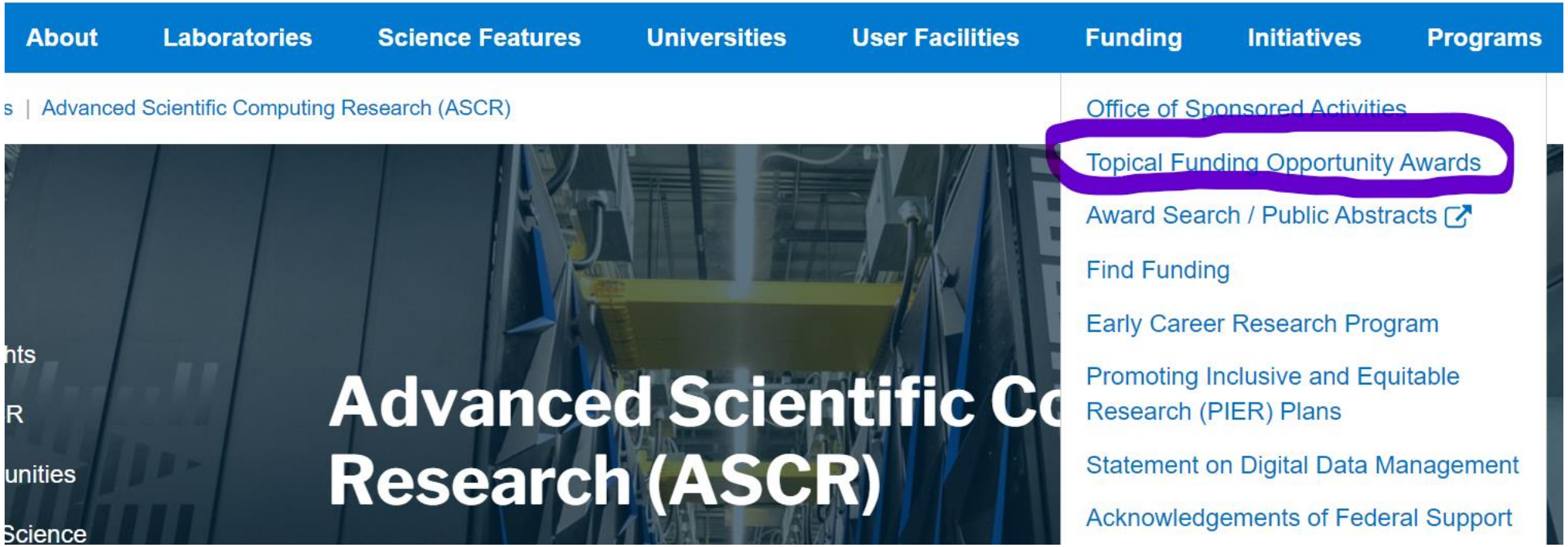
"Grant applications are sought to take one or more ASCR-funded software packages and make them easier to use by a wide variety of industries or in commercial venues by developing commercial offerings based on those ASCR-funded software packages." See the topic description for more information.

"This topic's goal is to strengthen the isolation between HPC users, specifically in the context of either the HPC scheduler or the HPC filesystem." See the topic description for more information.

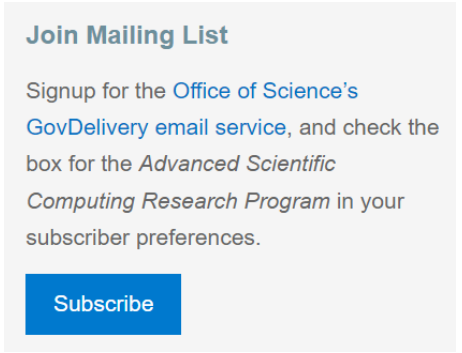
"Grant applications are sought to take one or more ASCR funded libraries and integrate them into new or existing, commercially supported software products to provide unique, transformative capabilities." See the topic description for more information.

For more information, see Phase I Release 1 Topics on https://science.osti.gov/sbir/Funding-Opportunities.

Award Lists – A New Website Location



Award lists are now posted to https://science.osti.gov/Funding-Opportunities/Award along with other awards from the Office of Science. To receive award and solicitation announcements, and other ASCR-related news, signup for the Office of Science's GovDelivery email service, and check the box for the Advanced Scientific Computing Research Program in your subscriber preferences:

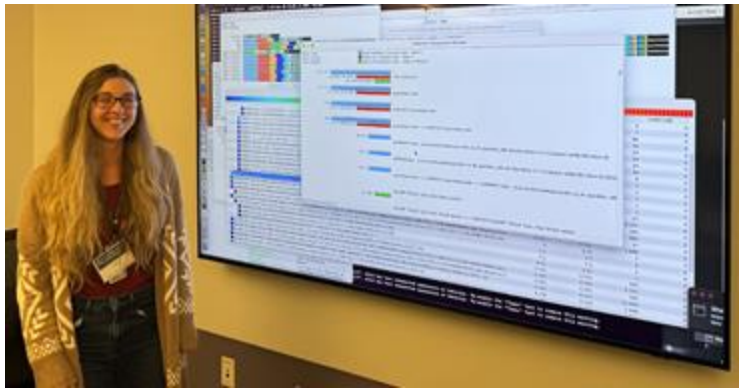


CASS: Consortium for the Advancement of Scientific Software

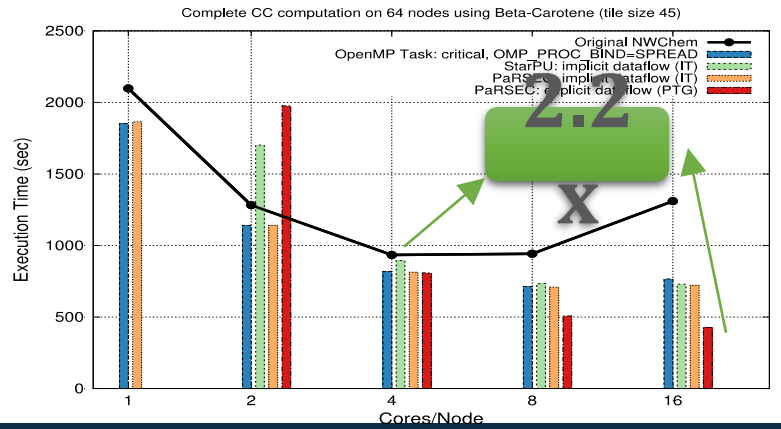
An ASCR investment in our next-generation software stack

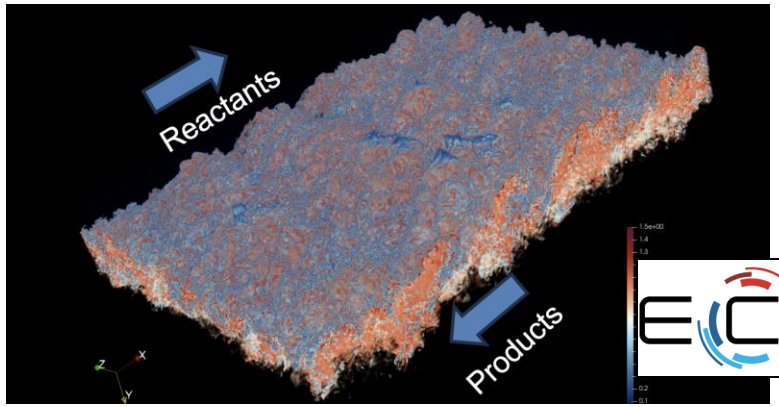
Software tools enabling science at exascale, on heterogeneous hardware

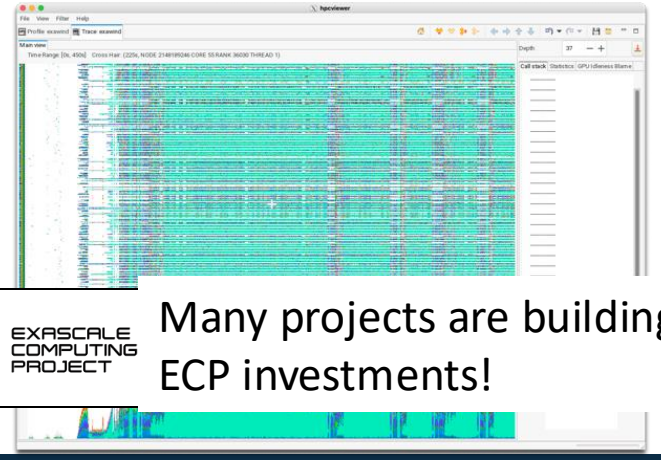
Recent example: 28x speedup of ECP code ExaWind



- Compilers
- Profilers
- Math libraries (SciDAC FASTMath)
- Computer science (SciDAC RAPIDS2)
- Integration (E4S, Spack)
- Collaborations with non-profit foundations and industry



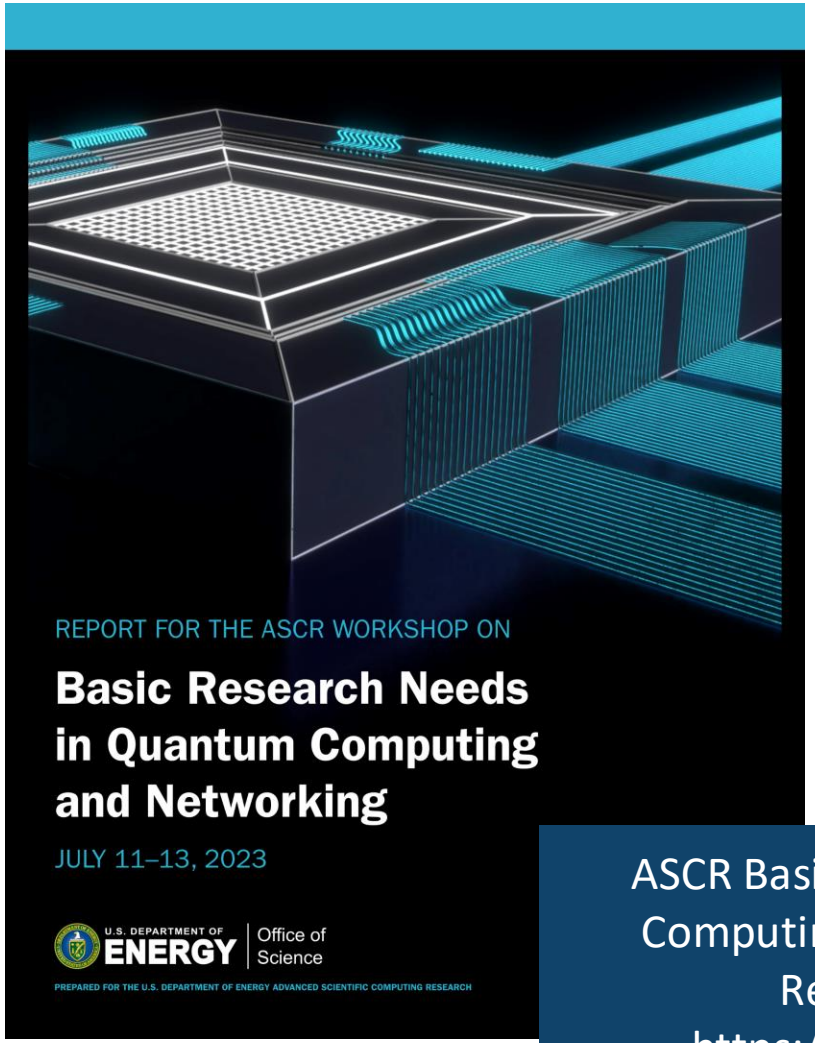




ECP EXASCALE COMPUTING PROJECT

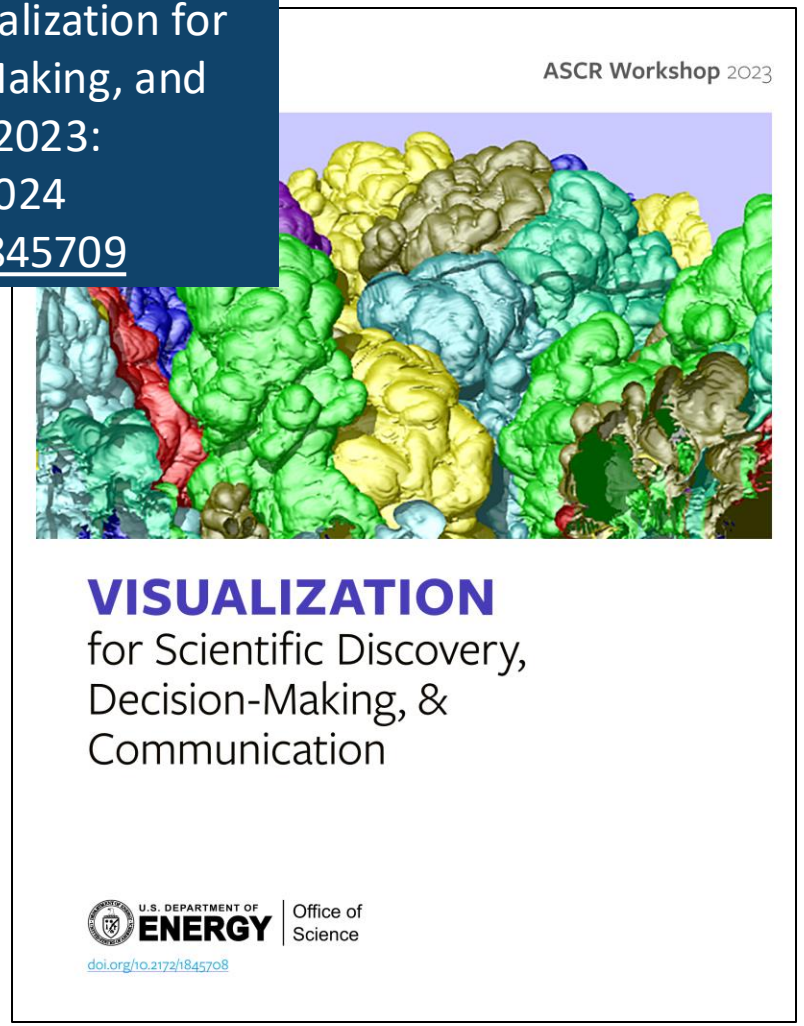
Many projects are building on ECP investments!

Workshop Reports Published



ASCR Basic Research Needs Visualization for Scientific Discovery, Decision-Making, and Communication, January 2023:
Report Posted August 2024
https://doi.org/10.2172/1845709

Our thanks to the workshop co-chairs, members of the organizing committees, and the many contributing workshop participants!

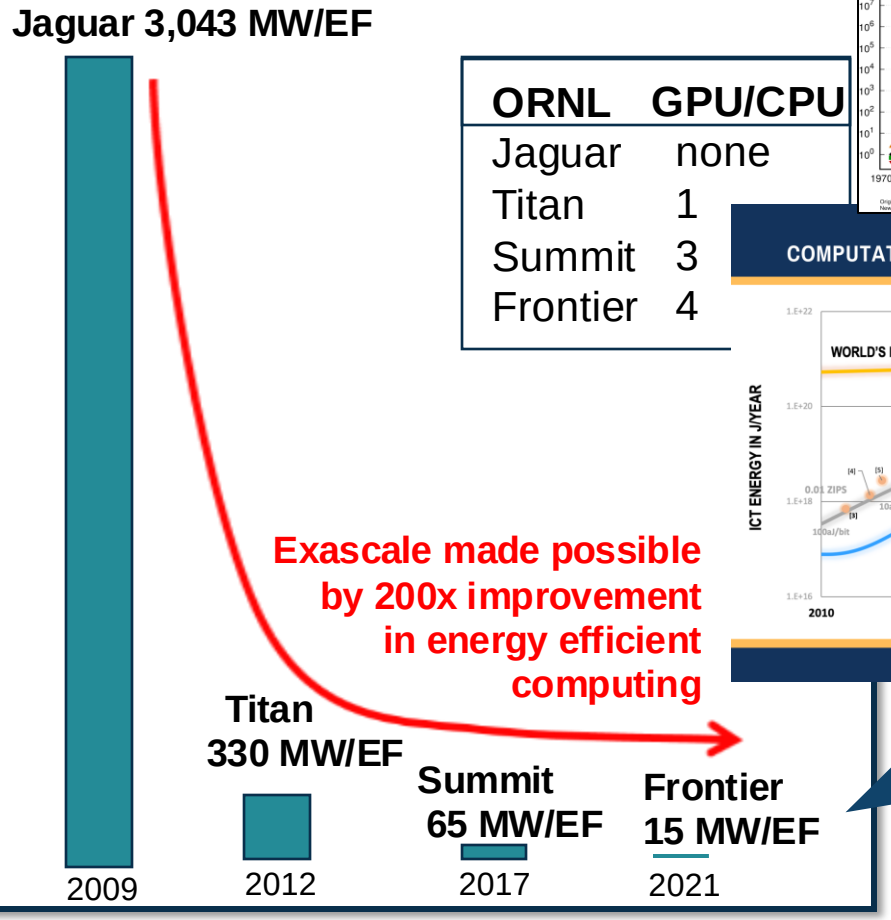


ASCR Basic Research Needs in Quantum Computing and Networking, July 2023:
Report Posted May 2024
https://doi.org/10.2172/2001045

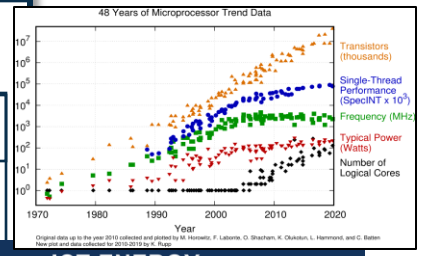
Future of Computing for Science – Motivations

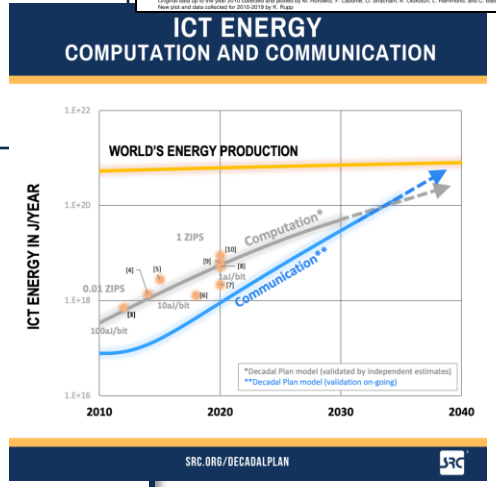
Frontier first US Exascale computer

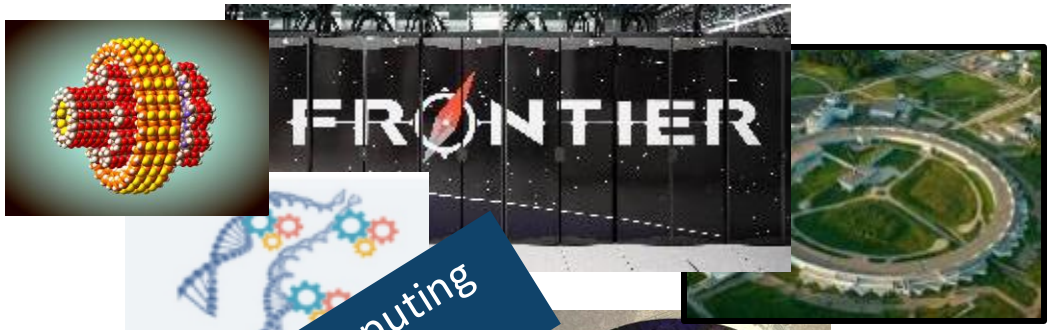
Multiple GPU per CPU drove energy efficiency

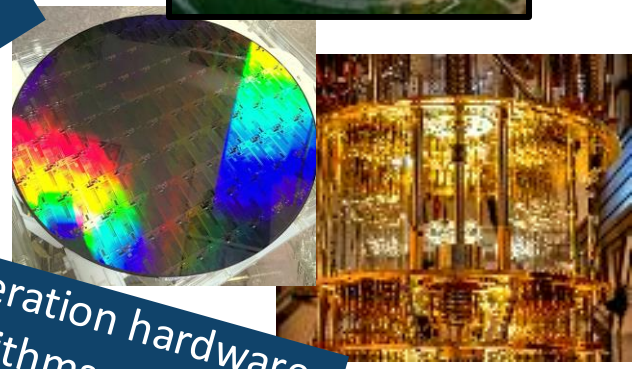


ORNL	GPU/CPU
Jaguar	none
Titan	1
Summit	3
Frontier	4





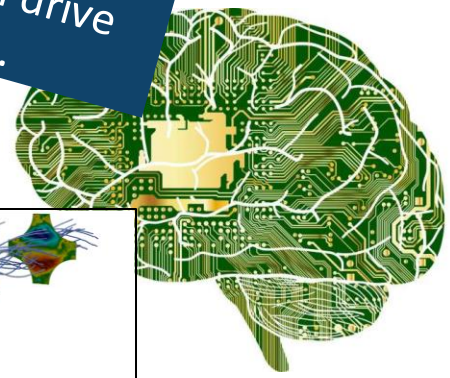


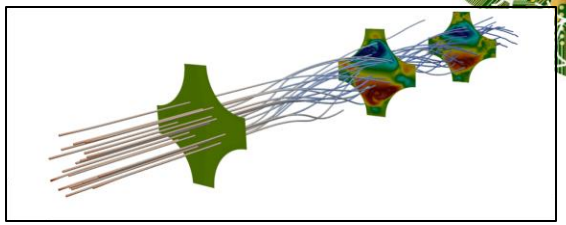


Advanced computing pervades science.

Next-generation hardware and algorithms will drive breakthroughs.

Challenges + Opportunities ► ***Progress***!





We need, and the Nation needs, this trend to continue – but how?

Workshops on the Future of Computing for Science

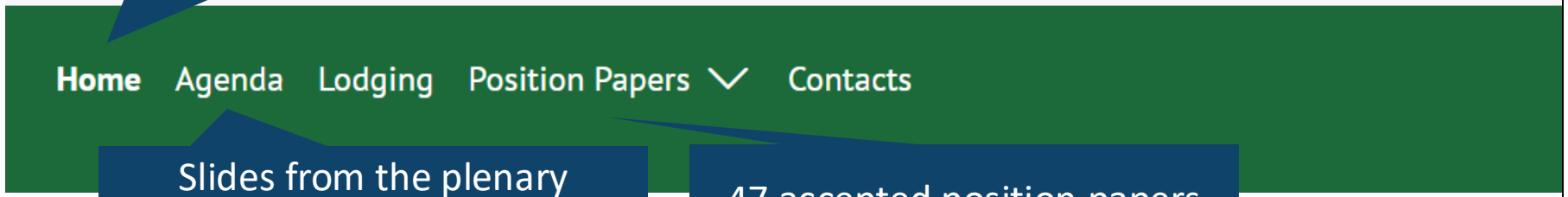
- To help invigorate thinking about post-exascale opportunities, ASCR sponsored three synergistic workshops in September 2024.
- The workshops explored basic research needs in computer science, applied mathematics, and advanced computing technologies.
- Concept papers submitted in response to open calls helped inform workshop organization and attendee invitations.
- Plenary sessions supported open-registration, hybrid attendance.

Date	Event	Website
September 9-12, 2024	ASCR Workshop on Energy-Efficient Computing for Science	https://www.orau.gov/2024EECWorkshop
September 11-13, 2024	ASCR Workshop on Analog Computing for Science	https://www.orau.gov/2024AnalogComputingWorkshop
September 12-13, 2024	ASCR Workshop on Neuromorphic Computing for Science	https://www.orau.gov/2024NeuromorphicComputing

2024 Energy-Efficient Computing for Science Workshop

Sponsored by the U.S. Department of Energy, Office of Advanced Scientific Computing Research (ASCR)
September 9-12, 2024
Bethesda, MD

A pre-workshop document prepared by the organizing committee is available on the home page.



Slides from the plenary presentations are linked from the agenda.

47 accepted position papers available on the website.

Workshop started with an industry leaders' panel:

Industry Panel

Regency Ballroom

Moderator: Tanya Das, Bipartisan Policy Center

Panelists:

Tamar Eilam, IBM

Dan Ernst, NVIDIA

Chris George, Intel

Mark Helm, Micron

Andy Hock, Cerebras

Andrew Wheeler, Hewlett Packard Labs

Thomas Zacharia, AMD

- Workshop featured over 70 in-person participants from industry, academic institutions, and national laboratories; a handful of federal observers; and over 200 virtual attendees.

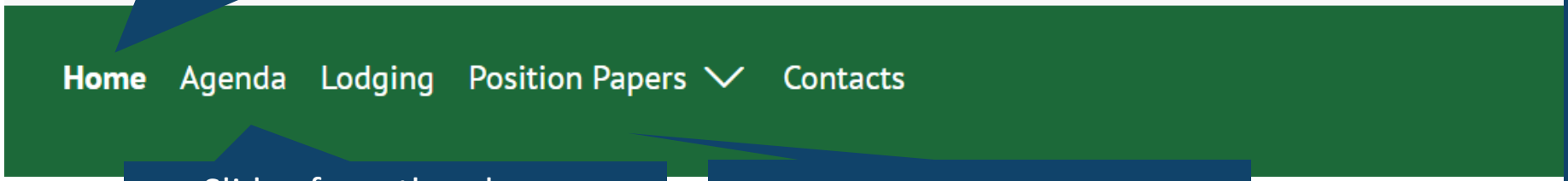
https://www.orau.gov/2024EECWorkshop

2024 Analog Computing for Science Workshop

Sponsored by the U.S. Department of Energy, Office of Advanced Scientific Computing Research (ASCR)

September 11-13, 2024
Bethesda, MD

A pre-workshop document prepared by the organizing committee is available on the home page.



Slides from the plenary presentations are linked from the agenda.

29 accepted position papers available on the website.

Discussions covered:
- Biological / Chemical
- Hybrid Systems / Sensor+Compute Integration
- Devices/Photonics
- Analog Electrical and Computational Memory
- Probabilistic / Ising
- Co-design / Software+Hardware+Physics
- Mathematical and Theoretical Foundations
- Benchmarking

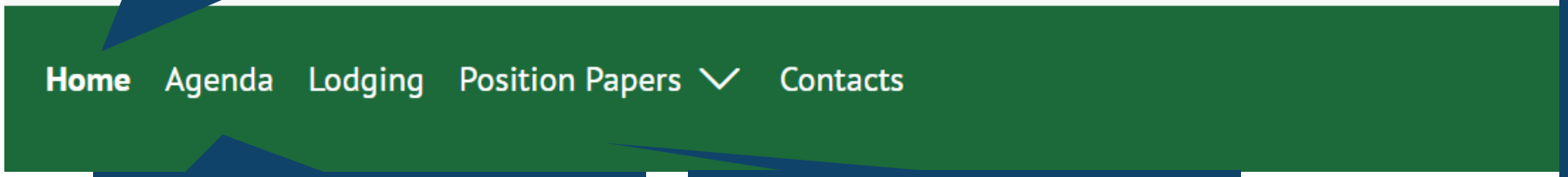
- Workshop featured over 50 in-person participants from industry, academic institutions, and national laboratories; a handful of federal observers; and over 130 virtual attendees.

https://www.orau.gov/2024AnalogComputingWorkshop

2024 Neuromorphic Computing for Science Workshop

Sponsored by the U.S. Department of Energy, Office of Advanced Scientific Computing Research (ASCR)
September 12-13, 2024
Bethesda, MD

A pre-workshop document prepared by the organizing committee is available on the home page.



Slides from the plenary presentations are linked from the agenda.

59 accepted position papers available on the website.

Discussions covered:
- Neuroscience-derived computing principles
- Translation to analog microelectronic circuits
- Modeling and simulation approaches

- Workshop featured over 65 in-person participants from industry, academic institutions, and national laboratories; a handful of federal observers; and over 225 virtual attendees.

https://www.orau.gov/2024NeuromorphicComputing

Finding Out More About ASCR – Program Documents

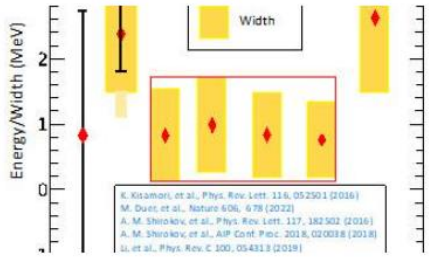
science.osti.gov/ascr/Community-Resources/Program-Documents

The "Program Documents" page has recent reports, with "Priority Research Directions" and "Priority Research Opportunities" in different areas of interest.

- Community Resources
  - ASCR Discovery
  - **ASCR Program Documents**
  - ASCR Workshops and Conferences
  - ASCR Presentations
  - 100Gbps Science Network
  - Related Links

Highlights

View all »



Discovered Tetraneutron Resonance Confirms Theoretical Predictions

DOE APPLICATIONS OF A SCIDAC HPC SOFTWARE

advance industry applica
Outreach and Assistanc
Transfer Programs Office.

Report: June, 2022

Envisioning Science in 2050

To explore future-focused questions that could impact the future of DOE, a Community (COI) on Future Scientific Methodologies, sponsored by the Office of Advanced Scien Computing Research (ASCR), was held over three non-consecutive days in Novembe COI's charge was to create a vision for how future computational fabrics might shape, shaped by, scientific and technological advances over the next 10 to 30 years.

Workshop Report: March 22, 2022

Basic Research Needs for the Science of Scientific-Software Development and Use

In December 2021, ASCR convened a workshop on basic research needs for the Scie Scientific Software Development and Use (SSSDU). Workshop participants identified research directions (PRDs) and three important crosscutting themes that center on the overarching insight: software has become an essential part of modern science that im discovery, policy, and technological development. To have full confidence in science d software, we must improve the processes and tools that help us create and use it, and this enhancement deep understanding of the diverse array of teams and individuals doing the work.

Workshop Brochure: January 1, 2022

Finding Out More About ASCR – GovDelivery

For updates from ASCR (announcements for ASCAC meetings, FOAs, awards, workshops, etc.) signup for the GovDelivery email service.

This link is near the bottom of https://science.osti.gov/ascr