#### **DOE Advanced Scientific Computing Research (ASCR)** Emerging Computing Technologies

Dr. Robinson Pino Program Manager, Advanced Computing Technologies September 26, 2024



#### **DOE Missions**

#### Energy

Catalyze the timely, material, and efficient transformation of the nation's energy system and secure U.S. leadership in energy technologies.

**VIEW MORE** 



#### Science and Innovation

Maintain a vibrant U.S. effort in science and engineering as a cornerstone of our economic prosperity with clear leadership in strategic areas.

S VIEW MORE



#### Nuclear Safety and Security

Enhance nuclear security through defense, nonproliferation, and environmental efforts.

S VIEW MORE





#### DOE's Office of Science: Meeting the Nation's Challenges Today and into the Future

The DOE Office of Science (SC) mission is to deliver the scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic, and national security of the United States.

#### Advancing the frontiers of science

Largest Federal supporter of basic research in the physical sciences

Lead for the Nation in Exascale Computing

Research activities support nearly 29,000 PhDs, scientific and engineering professionals, support staff, and graduate/undergraduate students at more than 300 universities and at all 17 DOE laboratories

#### Accelerating discovery with cutting-edge research tools

- Operate 28 scientific user facilities for nearly 34,000 users per year
  - X-ray and neutron sources
  - Physics facilities
  - Nanoscience centers
  - Biocharacterization facilities
- Design and construction of nextgeneration facilities to support the scientific community



# OFFICE OF SCIENCE BY THE NUMBERS

Delivering scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic, and national security of the United States

FY21



#### Office of Science at a Glance FY 2023 Request: \$7.799B



Largest Supporter of Physical Sciences in the U.S.



Funding at >300 Institutions, including 17 DOE Labs



Nearly 29,000 Researchers Supported



Nearly 34,000 Users of 28 SC Scientific Facilities



~35% of Research to Universities



Research: 42.8%, \$3.334B



Facility Operations: 34.5%, \$2.689B



Projects/Other: 22.7%, \$1.776B



Energy.gov/science

# **DOE National Laboratories**

The 17 DOE National Laboratories comprise a preeminent federal research system, providing the Nation with strategic scientific and technological capabilities

SC stewards 10 DOE laboratories that provide essential support to the missions of the SC science programs

U.S. DEPARTMENT OF

Office of

Science



# **Office of Science User Facilities**

- ▲ Open to all interested potential users without regard to nationality or institutional affiliation
- Each facility manages the allocation of facility resources through merit-based peer review of research proposals
- ▲ User fees are not charged for non-proprietary work if the user intends to publish the research results in the open literature
- ▲ Full cost recovery is required for proprietary work









https://science.osti.gov/User-Facilities/User-Resources/Getting-Started









#### U.S. Department of Energy **Office of Science User Facilities, FY 2021**



#### Advanced Scientific Computing Research (ASCR)

- Argonne Leadership Computing Facility (ALCF) Argonne National Laboratory
- Energy Sciences Network (ESnet) 2 Lawrence Berkeley National Laboratory
- National Energy Research Scientific Computing 3 Center (NERSC) Lawrence Berkeley National Laboratory
  - Oak Ridge Leadership Computing Facility (OLCF) Oak Ridge National Laboratory

#### **Basic Energy Sciences (BES)**

#### LIGHT SOURCES

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- Advanced Light Source (ALS) Lawrence Berkeley National Laboratory
- Advanced Photon Source (APS) Argonne National Laboratory
- Linac Coherent Light Source (LCLS) SLAC National Accelerator Laboratory
- National Synchrotron Light Source II (NSLS-II) Brookhaven National Laboratory
- Stanford Synchrotron Radiation Lightsource (SSRL) SLAC National Accelerator Laboratory

#### **NEUTRON SOURCES**

- High Flux Isotope Reactor (HFIR) Oak Ridge National Laboratory
- Spallation Neutron Source (SNS) m Oak Ridge National Laboratory

#### NANOSCALE SCIENCE RESEARCH CENTERS

- Center for Functional Nanomaterials (CFN) Brookhaven National Laboratory
- Center for Integrated Nanotechnologies (CINT) B Sandia National Laboratories and Los Alamos National Laboratory
- Center for Nanophase Materials Sciences (CNMS) 14 Oak Ridge National Laboratory
  - Center for Nanoscale Materials (CNM) Argonne National Laboratory
  - The Molecular Foundry (TMF)
  - Lawrence Berkeley National Laboratory

#### **Biological and Environmental Research (BER)**

- Atmospheric Radiation Measurement (ARM) **User Facility**
- Multi-Site Global Network
- Environmental Molecular Sciences Laboratory (EMSL) Pacific Northwest National Laboratory
  - Joint Genome Institute (JGI) Lawrence Berkeley National Laboratory

#### Fusion Energy Sciences (FES)

- **DIII-D National Fusion Facility General Atomics**
- National Spherical Torus Experiment Upgrade 20 (NSTX-U) Princeton Plasma Physics Laboratory

#### **High Energy Physics (HEP)**

- Accelerator Test Facility (ATF) 21 Brookhaven National Laboratory
  - Facility for Advanced Accelerator Experimental Tests (FACET) SLAC National Accelerator Laboratory
- Fermilab Accelerator Complex 23 Fermi National Accelerator Laboratory

#### Nuclear Physics (NP)

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- Argonne Tandem Linac Accelerator System 24 (ATLAS)
  - Argonne National Laboratory
- **Continuous Electron Beam Accelerator Facility** 25 (CEBAF) Thomas Jefferson National Accelerator Facility
- Facility for Rare Isotope Beams (FRIB) 26 Michigan State University
- Relativistic Heavy Ion Collider (RHIC) 27 Brookhaven National Laboratory

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### The Office of Science Research Portfolio

Advanced Scientific Computing Research	<ul> <li>Delivering world leading computational and networking capabilities to extend the frontiers of science and technology</li> </ul>	
Basic Energy Sciences	<ul> <li>Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels</li> </ul>	
Biological and Environmental Research	<ul> <li>Understanding complex biological, earth, and environmental systems</li> </ul>	
Fusion Energy Sciences	<ul> <li>Building the scientific foundations for a fusion energy source</li> </ul>	
High Energy Physics	<ul> <li>Understanding how the universe works at its most fundamental level</li> </ul>	
Nuclear Physics	<ul> <li>Discovering, exploring, and understanding all forms of nuclear matter</li> </ul>	
Isotope R&D and Production	<ul> <li>Supporting National Preparedness for isotope production and distribution during national crisis</li> </ul>	
Accelerator R&D and Production	<ul> <li>Supporting new technologies for use in SC's scientific facilities and in commercial products</li> </ul>	



# **Advanced Scientific Computing Research (ASCR)**

- ▲ ASCR research lays the groundwork for scientific discoveries
  - Applied Mathematics and Computer Science foundations to advance the understanding of natural and engineered systems and to reveal scientific insight from high end simulations, models, and data.
  - **Advanced Computing** to prepare for the future of science based on emerging advanced computing technologies and microelectronics.
- ASCR facilities drive American global leadership in computing, data and networking
  - As we deploy the world's first **exascale supercomputers** and the Nation's most **advanced scientific network**, we continue to build a more integrated and open national research infrastructure for all.
- ASCR's investments and strategic partnerships enable scientific breakthroughs and advance America's economic competitiveness
  - ASCR's world-leading programs in interdisciplinary research enable scientific applications take full advantage of computing and networking capabilities that push the frontiers.
  - Unique models of partnerships accelerate the competitiveness of American computing technologies, advanced manufacturing, and high-tech companies - large and small.
- ASCR invests in people
  - Computational Science Graduate Fellowship producing computational leaders since 1991.





Quantum Testbeds



Gordon Bell Prize researchers leverage modeling and AI to understand COVID mutations



# **HPC Cybersecurity**

- ▲ DOE Report: Cybersecurity for Scientific Computing Integrity
  - Research and develop means to collect extreme-scale data and knowledge, and develop and apply analytics in order to understand and improve scientific computing integrity and computer security
  - Develop means to learning and maintaining interdependent causal models of the scientific computation, exascale system, and computer security in real-time to enable better, faster recovery to reduce disruptions to scientists' efforts
  - Metrics for quantifying the trustworthiness of scientific data, capturing the likelihood and potential magnitude of errors due to uncertain inputs, incomplete models, incorrect implementations, silent hardware errors, and malicious tampering



### What is scientific computing integrity?

#### Scientific Computing Integrity:

The ability to have high confidence that the scientific data that is generated, computed, processed, stored, or transmitted by computers and computer-connected devices has a process, provenance, and correctness that is understood



# Why DOE Scientific Integrity?

- DOE has the responsibility to address the energy, environmental, and nuclear security challenges that face our nation
- Much of DOE's enterprise involves distributed, collaborative teams
  - A significant fraction involve "open science"
  - Depends on multi-institutional, often international collaborations that must access or share information between sites around the world
- Office of Science mission is the delivery of scientific discoveries and major scientific tools to transform our understanding of nature and to advance the energy, economic, and national security of the United States.
  - To execute its responsibilities, DOE must be able to assure the integrity and availability of scientific facilities and computer systems, and of the scientific, engineering, and operational software and data that support its mission



# **Requirements for Open Science Cybersecurity**

- Office of Science labs function in completely open environments
  - Availability and data sharing are of great importance
  - Are often accessed by authorized users around the world
  - Multiple projects from multiple countries run on the same machine
- ▲ DOE HPC and large-scale science workflows differ from general-purpose computing
  - DOE machines might run one program for weeks on tens of thousands of processors
  - Even other distributed, high-bandwidth services like Netflix or YouTube are smaller



# **HPC Cybersecurity: Basic Research Areas**

- Trustworthy Supercomputing:
  - Research within extreme high-performance computing that can be influenced to incorporate a cybersecurity mindset during R&D
- ▲ Trust within Open, High-End Networking and Data Centers:
  - Research ideas that enable trust within an open shared environment among communications and data at rest or in transit minimizing security overhead
- Extreme Scale Data, Knowledge, and Analytics for Understanding and Improving Cyber Security:
  - Research to correlate, find, or detect patterns from heterogeneous sources of information such as the network, computing nodes, operating system, runtime, applications, etc. for use for cybersecurity, esp. scientific data integrity and provenance



# Emerging applications will require new computing paradigms

Autonomous Vehicles

Smart Grid

Edge Computing









Artificial Intelligence

Machine Learning

Neuromorphic



# Machine Learning Research Goals (2015)

- ▲ Self-aware Runtime and Operating Systems:
  - Explore solutions that are dynamic, adaptive, selfprotective, or self-healing of the applications and services they support.
- ▲ Deep Learning for Big Data:
  - Is it possible to generate knowledge from the data; smart analytics; smart rendering/usability?
- ▲ Resiliency and Trust:
  - Correct computations and results in the presence of faults. Discover new patterns on networks and data, perform anomaly detection, achieve data fusion from multiple sources, analyze social and behavioral networks to identify anomalous behavior, and perhaps fingerprint HPC programs.





# **Neuromorphic computing**

- Neuro-inspired architectures in softwarehardware offer a path for much needed technological evolution
- Success will require multi- and crossdisciplinary effort in materials, physics, chemistry, biology, mathematics, engineering, computer science, neuroscience, etc.
- BES Energy Frontier Research Center: Quantum-Materials for Energy Efficient Neuromorphic-Computing, led by UCSD
- ▲ ASCR Funding Opportunity: Neuromorphic Computing for Accelerating Scientific Discovery (closes on July 1, 2020)





### **5G for Science – Initiative Overview**

Emerging 5G wireless technologies offer new opportunities and capabilities for the advancement of the U.S. Department of Energy and Office of Science mission



### Why DOE Science?

▲ DOE Science since 2019 has been exploring how 5G and advanced wireless networking could impact our mission

▲ Opportunity to modernize existing scientific facilities or to enable and deploy new capabilities for scientific exploration

▲ 5G can enable DOE to continue our tradition of enabling scientific breakthroughs and transformational scientific discoveries



### **5G Unique Features Relevant to DOE Science**

- ▲ Bandwidth: Up to 10Gbps (10 to 100x improvement over 4G and 4.5G)
- ▲ Latency: 1-millisecond (in some circumstances, for control systems, edge)
- ▲ Density: 1M/km2 (100x devices per unit area)
- ▲Volume: 10 TB/s/km2 Small cells, convergence with local WiFi
- ▲ Ultra-Reliable Low-Latency Communications (URLLC): 99.999% availability
- ▲ Designed for control systems and critical monitoring
- ▲90% reduction in network energy usage
- ▲ Up to 10-year battery life for low power Internet of Everything (IoE) devices
- ▲ Network Slices: Provides quality of service (QoS) capabilities
- ▲ Edge computation, running code in 5G infrastructure
- ▲ Ideal for autonomous or remote operation from source to destination



### **AI - 5G Enabled 4th Industrial Revolution**



https://www.salesforce.com/blog/2018/12/what-is-the-fourth-industrial-revolution-4IR.html

https://en.wikipedia.org/wiki/Technological\_revolution



# AI Edge Computing + 5G + SOTA = Digital Continuum



Advanced Microelectronics will enable new embedded devices, sensors, systems on chip for accelerated computing, i.e. Digital, Analog, Neuromorphic, Quantum, ...



### **DOE 5G for Science Initiative - Priority Research Directions**



www.orau.gov/5gscience

- Revolutionize wireless communication in extreme environments through advances in materials science and physics
- Reinvent scientific instrumentation and critical national infrastructure with wireless technology to provide rapid, Al-driven adaptation
- Reinvent the digital continuum linking the wireless edge to advanced scientific user facilities, data centers, and high-performance computing
- Revolutionize Al-enabled edge computing for advanced wireless
- Accelerate innovation: Use community testbeds to explore advanced wireless for science



### **Microelectronics R&D**

- The primary goal of this initiative is to enhance and expand DOE-SC leadership and investments in all aspects of fundamental R&D relevant to future electronics, computing, and power technologies.
- This includes materials, chemistries, synthesis, fabrication, devices, systems, architectures, algorithms, and software.

### Basic Research Needs for **Microelectronics**



Report of the Office of Science Workshop on Basic Research Needs for Microelectronics October 23 – 25, 2018



### **Basic Research Needs for Microelectronics**

- ▲ Priority Research Directions:
  - Flip the current paradigm: Define innovative materials, device, and architecture requirements driven by applications, algorithms, and software
  - Revolutionize memory and data storage
  - Reimagine information flow unconstrained by interconnects
  - Redefine computing by leveraging unexploited physical phenomena
  - Reinvent the electricity grid through new materials, devices, and architectures









100 lbs



#### **ASCR Research Develops With Critical Technology Trends**



Accelerating Science from Exascale to the Edge

#### Energy.gov/science

**Enhancing Scientific Programming** 

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#### Accelerated Research in Quantum Computing

- 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





### 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





Advancements in Artificial Intelligence for Science

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









### 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



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.





#### 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.



# **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
- 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.





• Extreme environments



### **Workshop Reports Published**



REPORT FOR THE ASCR WORKSHOP ON

Basic Research Needs in Quantum Computing and Networking

Office of

Science

JULY 11-13, 2023

DEPARTMENT OF



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

Our thanks to the workshop cochairs, members of the organizing committees, and the many contributing workshop participants!

VISUALIZATION

for Scientific Discovery, Decision-Making, & Communication

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





ASCR Workshop 2023

# Future of Computing for Science – Motivations





# 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

A pre-workshop document prepared by the organizing committee is available on	Computing Research September 9-12, 2	(ASCR) Workshop started with an industry leaders' panel:
the home page.	Bethesda, MD	Industry Panel
	Regency Ballroom Moderator: Tanya Das Bipartisan Policy Center	
Home Agenda Lodging Positio	Panelists:	
Slides from the plenary presentations are linked from the agenda.	om 47 accepted position papers available on the website.	Tamar Eilam, IBM
		Dan Ernst, NVIDIA
		Chris George, Intel
	Mark Helm, Micron	
Workshop featured over 70 in	Andy Hock, Cerebras	
virtual attendees		Andrew Wheeler, Hewlett Packard Labs
		Thomas Zacharia, AMD

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

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2024 Ana	log Computing for Science	Workshop
Sponsored by the l A pre-workshop document	J.S. Department of Energy, Office of Computing Research (ASCR)	f Advanced Scientific
prepared by the organizing committee is available on the home page.	September 11-13, 2024 Bethesda, MD	<ul> <li>Discussions covered:</li> <li>Biological / Chemical</li> <li>Hybrid Systems /</li> </ul>
Home Agenda Lodging Position Papers 🗸 Contacts		<ul> <li>Sensor+Compute Integration</li> <li>Devices/Photonics</li> <li>Analog Electrical and</li> </ul>
Slides from the plenar presentations are linked f the agenda.	y 29 accepted position papers available on the website.	<ul> <li>Computational Memory</li> <li>Probabilistic / Ising</li> <li>Co-design / Software+Hardware+Physics</li> </ul>
<ul> <li>Workshop featured over 50 in-person participants from industry, academic institutions, and national laboratories; a handful of federal observers; and over 130 virtual attendees.</li> </ul>		<ul> <li>Mathematical and Theoretical Foundations</li> <li>Benchmarking</li> </ul>

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

U.S. DEPARTMENT OF

, Office of Science

### 2024 Neuromorphic Computing for Science Workshop

#### Sponsored by the U.S. Department of Energy, Office of Advanced Scientific

A pre-workshop document prepared by the organizing committee is available on the home page.	Computing Research (ASCR) September 12-13, 2024 Bethesda, MD	Discussions covered:
Home Agenda Lodging Position	<ul> <li>Neuroscience-derived computing principles</li> <li>Translation to analog microelectronic circuits</li> </ul>	
Slides from the plenary presentations are linked fro	m 59 accepted position papers available on the website.	<ul> <li>Modeling and simulation approaches</li> </ul>

 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



# Thank you!

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