Welcome to the ASCR Workshop on Energy-Efficient Computing for Science

Hal Finkel, PhD

Director, Computational Science Research and Partnerships Division

Advanced Scientific Computing Research

U.S. DEPARTMENT OF ENERGY | Office of Science

Our Mission:

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

More than **34,000 r**esearchers supported at more than **300** institutions and **17** DOE national laboratories

Steward **10** of the 17 DOE national laboratories

More than **37,000** users of **28** Office of Science scientific user facilities

$8.1B
(FY 23 enacted)

The Office of Science Research Portfolio

Advanced Scientific Computing Research
- Delivering world leading computational and networking capabilities to extend the frontiers of science and technology

Basic Energy Sciences
- Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels

Biological and Environmental Research
- Understanding complex biological, earth, and environmental systems

Fusion Energy Sciences
- Supporting the development of a fusion energy source and supporting research in plasma science

High Energy Physics
- Understanding how the universe works at its most fundamental level

Nuclear Physics
- Discovering, exploring, and understanding all forms of nuclear matter

Isotope R&D and Production
- Supporting isotope research, development, production, processing and distribution to meet the needs of the Nation
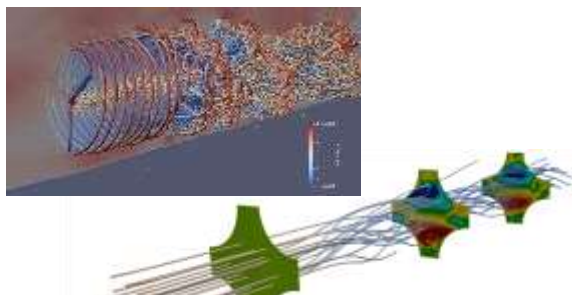
Accelerator R&D and Production
- Supporting new technologies for use in SC's scientific facilities and in commercial products
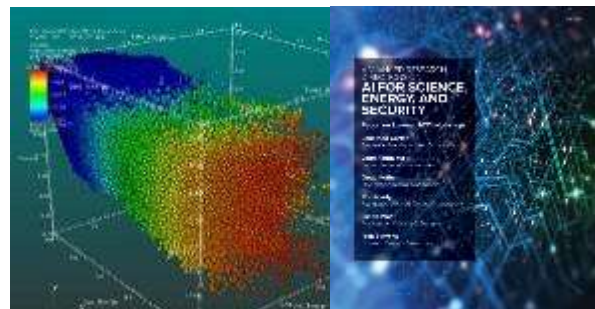
Reinvigorating ASCR Research To Respond to Critical Technology Trends

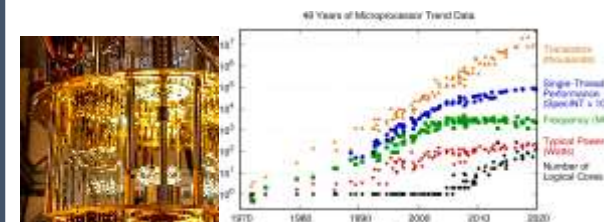**Advanced Modeling, Simulation, and Visualization**

Empowering Science Through Fundamental Research

Frontier AI & Data

Creating Trustworthy and Energy Efficient Frontier AI
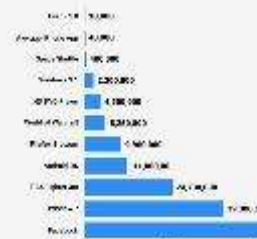
Heterogeneous, Distributed, Co-Designed, Energy-Efficient Computing and Algorithms

Transforming Fundamentals of Computing

Software Complexity for Increased Versatility
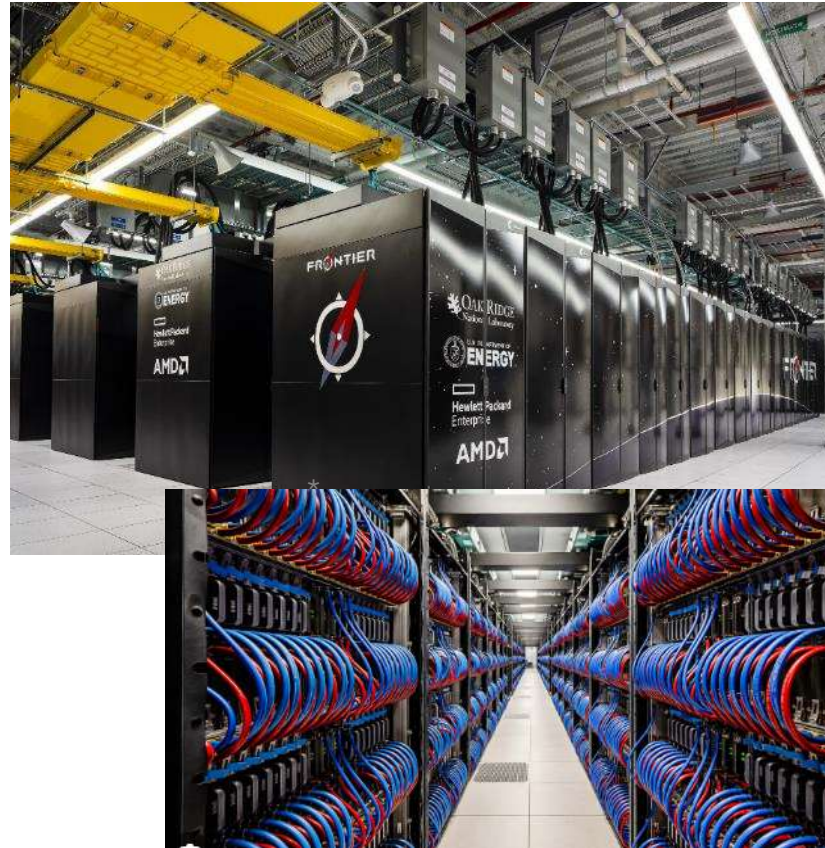

Enhancing Scientific Programming

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

Accelerating Science from Exascale to the Edge

A New Science Era: Exascale Today Enables the AI of Tomorrow

Long-term investments in applied mathematics and computer science enabled exascale.

MPICH2

2005

Frontier and Aurora #1 and #2 on the Top500, **lead the world in computational capability.** Aurora is **#1 in the world for AI capability**, and both systems exceed 10 exaops of mixed precision performance.

The exascale and AI-enabled science era will lead to dramatic capabilities to predict extreme events and their impacts on the electric grid across weather and climate time scales...
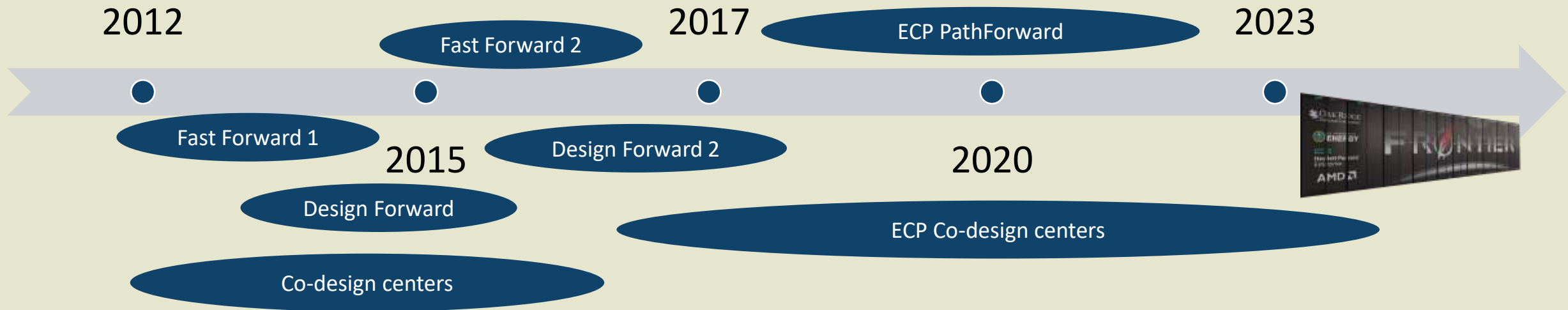

and will accelerate the design and deployment of clean-energy technologies to create a better future.
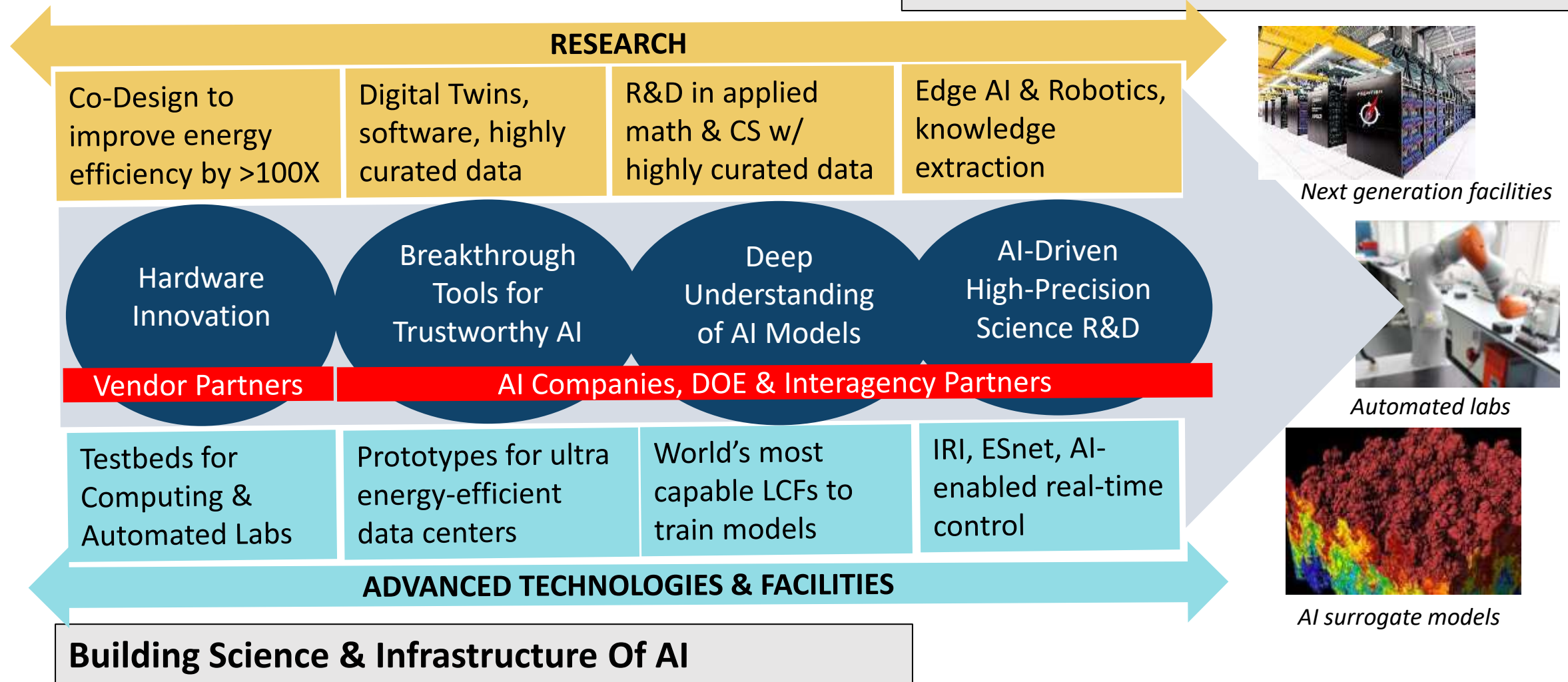
Public/Private Partnerships Lead to Exascale

- **Frontier, DOE's first exascale supercomputer, was also #2 in the world on energy efficiency (on the Green500) in addition to being #1 in the world on performance (on the Top500).**

- **Frontier's performance and efficiency were enabled by the public/private R&D partnerships in the Exascale Computing Program (ECP)'s PathForward Program.**

2012   Fast Forward 2   2017   ECP PathForward   2023

Fast Forward 1   2015   Design Forward 2   2020

Design Forward

ECP Co-design centers

Co-design centers

- **The ECP PathForward program built on a long history of DOE *Forward programs and co-design centers.**

  - **Partnered with AMD, Cray, HPE, IBM, Intel, NVIDIA on technologies related to compute, memory, networking, and storage.**

- **ASCR partnerships continue, for example, the Artificial Intelligence (AI) for Science (AMAIS) project at PNNL, is an ongoing partnership with Micron. With ORNL and PNNL, ASCR has supported the DOE/Micron collaboration since 2017.**

ASCR's End-to-End Approach for Trustworthy and Energy-Efficient Frontier AI

Transforming Discovery Science & Infrastructure by AI

RESEARCH

Co-Design to improve energy efficiency by >100X	Digital Twins, software, highly curated data	R&D in applied math & CS w/ highly curated data	Edge AI & Robotics, knowledge extraction

Next generation facilities

Hardware Innovation	Breakthrough Tools for Trustworthy AI	Deep Understanding of AI Models	AI-Driven High-Precision Science R&D

Vendor Partners	AI Companies, DOE & Interagency Partners

Automated labs

Testbeds for Computing & Automated Labs	Prototypes for ultra energy-efficient data centers	World's most capable LCFs to train models	IRI, ESnet, AI-enabled real-time control

ADVANCED TECHNOLOGIES & FACILITIES

AI surrogate models

Building Science & Infrastructure Of AI

Recent Workshops: Transforming the Fundamentals of Computing
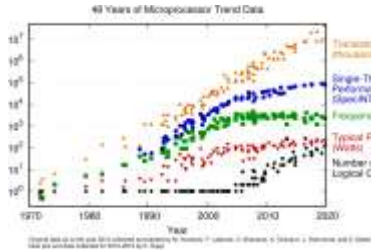
Heterogeneous, Distributed, Co-Designed, Energy-Efficient Computing and Algorithms

ASCR Workshop on Reimagining Codesign, March 2021: https://doi.org/10.2172/1822199

Quantum Computing for Biomedical Computational and Data Sciences Joint DOE NIH Quantum Roundtable March 2023: https://doi.org/10.2172/2228574
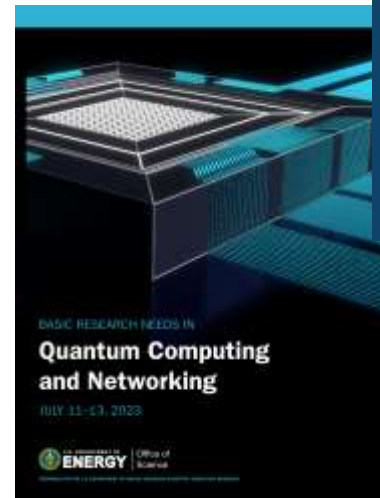
ASCR Basic Research Needs in Quantum Computing and Networking, July 2023: https://doi.org/10.2172/2001045

Recent Workshops: Empowering Science Through Data Innovations

Data, Privacy, and Scientific Integrity
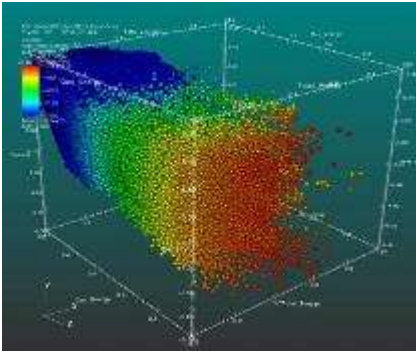
ASCR Workshop on Basic Research Needs for Management and Storage of Scientific Data, January 2022:
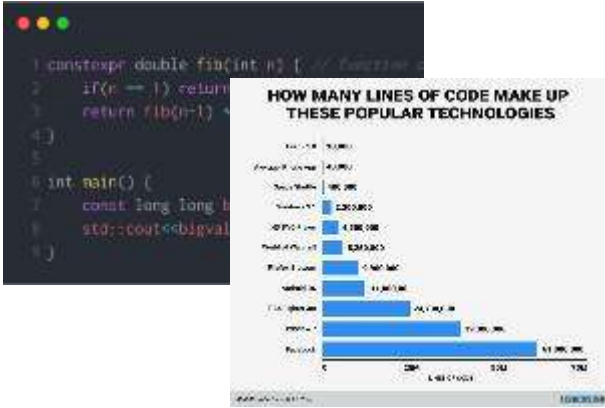https://doi.org/10.2172/1845707

ASCR Basic Research Needs Visualization for Scientific Discovery, Decision-Making, and Communication, January 2022:
https://doi.org/10.2172/1845709
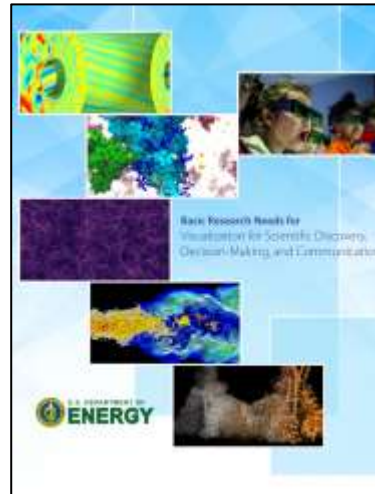
Recent Workshops: Enhancing Scientific Programming

Exploding Software Complexity

ASCR Workshop on Basic Research Needs in The Science of Scientific Software Development and Use, December 2021: https://doi.org/10.2172/1846009

DOE/NSF Workshop on Correctness in Scientific Computing, June 2023: https://arxiv.org/abs/2312.15640
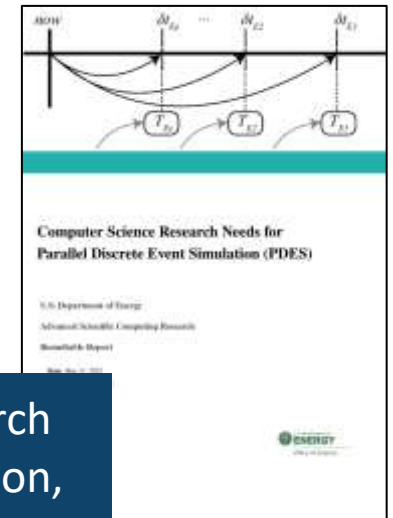
Accelerating Science from Exascale to the Edge

Scientific Computing and Networking: from Exascale to the Edge

Integrated Research Infrastructure Architecture Blueprint Activity, 2023: https://doi.org/10.2172/1984466

Roundtable on Foundational Science for Biopreparedness and Response, March 2022: Report available from https://science.osti.gov/ascr/Community-Resources/Program-Documents

Roundtable on Computer Science Research Needs for Parallel Discrete Event Simulation, 2022: https://doi.org/10.2172/1855247

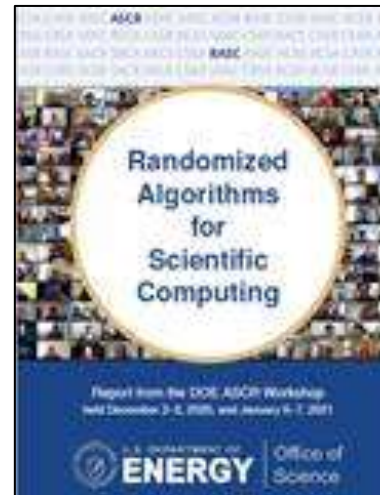# Recent Workshops: Innovating in Algorithms and Mathematics

Advanced Modeling, Simulation, and Visualization

Randomized Algorithms for Scientific Computing
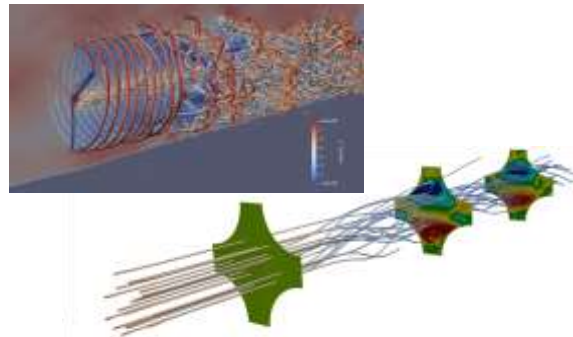
ASCR Workshop on Randomized Algorithms for Scientific Computing, January 2021: https://doi.org/10.2172/1807223

Data Reduction for Science, January 2021: https://doi.org/10.2172/1770192
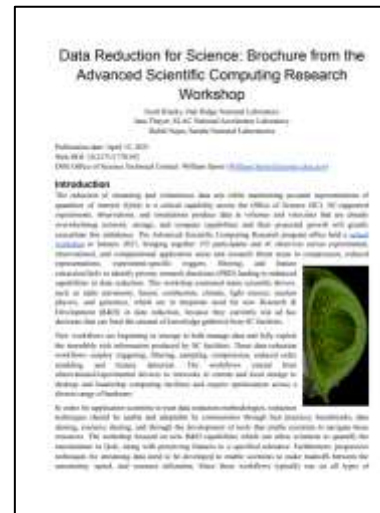
AI for Science, Energy, and Security Report

- AI for Science, Energy, and Security Report, released May 2023: https://www.anl.gov/ai-for-science-report

- Created by a confederation of laboratories, informed by a series of workshops held in 2022.

- Covers AI approaches:
  - AI and Surrogate Models for Scientific Computing
  - AI Foundation Models for Scientific Knowledge Discovery, Integration, and Synthesis
  - AI for Advanced Property Inference and Inverse Design
  - AI-Based Design, Prediction, and Control of Complex Engineered Systems
  - AI and Robotics for Autonomous Discovery
  - AI for Programming and Software Engineering
- Also covers crosscuts, including workflows, data, AI hardware, computing infrastructure, and workforce

Finding Out More About ASCR – Program Documents

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

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 ASCR 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 Communit
(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

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

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Energy.gov/science

Finding Out More About ASCR – FOAs

Browser URL: science.osti.gov/ascr/Funding-Opportunities

Funding Opportunities

Closed Funding Opportunity Announcements (FOAs)

Closed Lab Announcements

Award Search / Public Abstracts

Additional Requirements and Guidance for Digital Data Management

Announcement Archives

Computational Science Graduate Fellowship (CSGF)

Advanced Scientific Computing Advisory Committee (ASCAC)

Community Resources

Contact Advanced Scientific Computing Research

Address

solicitation. For the most current information on notices, see the DOE Grants and Contracts shows the original posting dates, changes in due dates are not track

Office of Science Guidance on Accommodating interruptions

Funding Opportunity Announcements (FOAs)

May be open to one or more types. For assistance with the Office of Science's Po Management System (PAMS) at https://p 1846 (toll-free), (301) 903-9610, or sc.pams-helpdesk

FY 2023 Continuation of Solicitation for the Office of Science Financial Assistance Program

Announcement Number: DE-FOA-0002844
Post Date: Friday, September 30, 2022
Close Date: Saturday, September 30, 2023

- Submission Deadline for Pre-Applications:
  - A Pre-Application is optional/encouraged

- Submission Deadline for Applications: Not Applicable

This FOA will remain open until September 30, 2023 or until replaced by a successor FOA. Applications may be submitted any time during that period.

> Look at the closed FOAs to see how funding has been structured in the past.

> Search non-lab award abstracts to get a sense for ongoing projects.

> The Office of Science's "Open Call" generally represents the scope interest of the various programs.

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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

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Energy-Efficient Computing for Science

Some things to think about at this workshop...

Energy-Efficient Computing – Technology Diversity is Key

2020 NSTC Advanced Computing Ecosystem Strategic Plan and industry roadmaps all stress the importance of investing in a wide variety of promising techniques post Exascale.
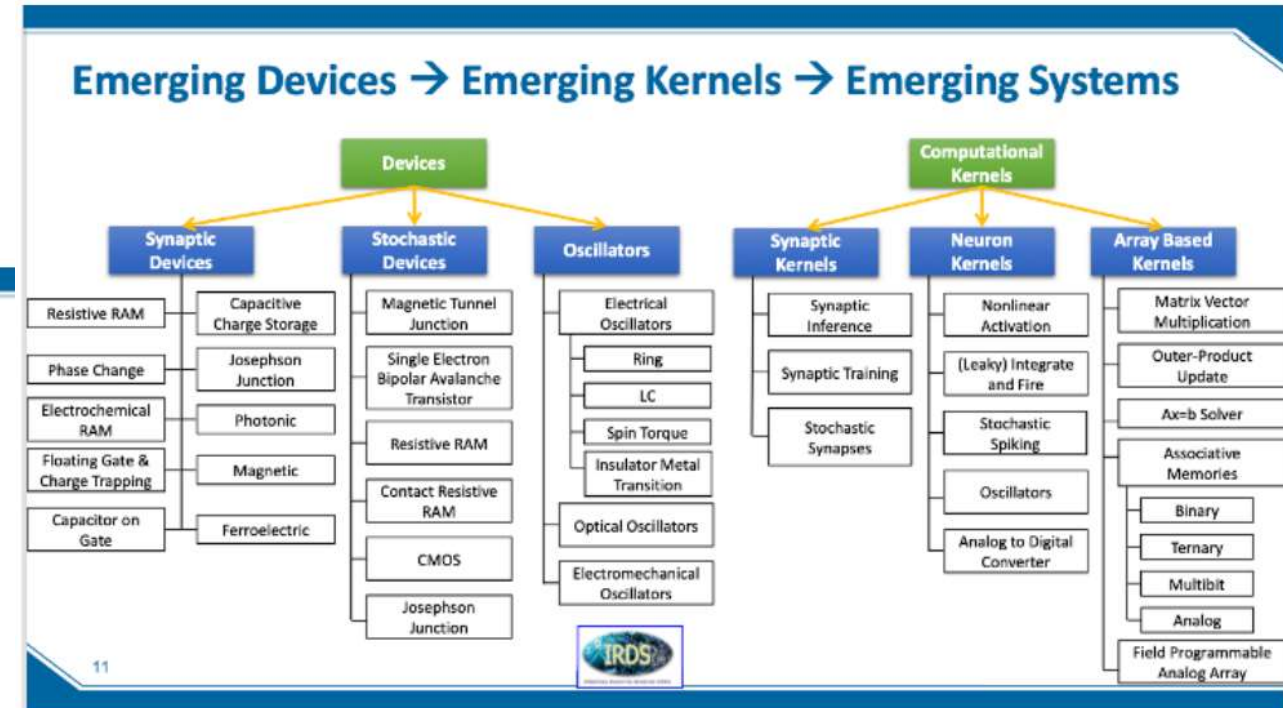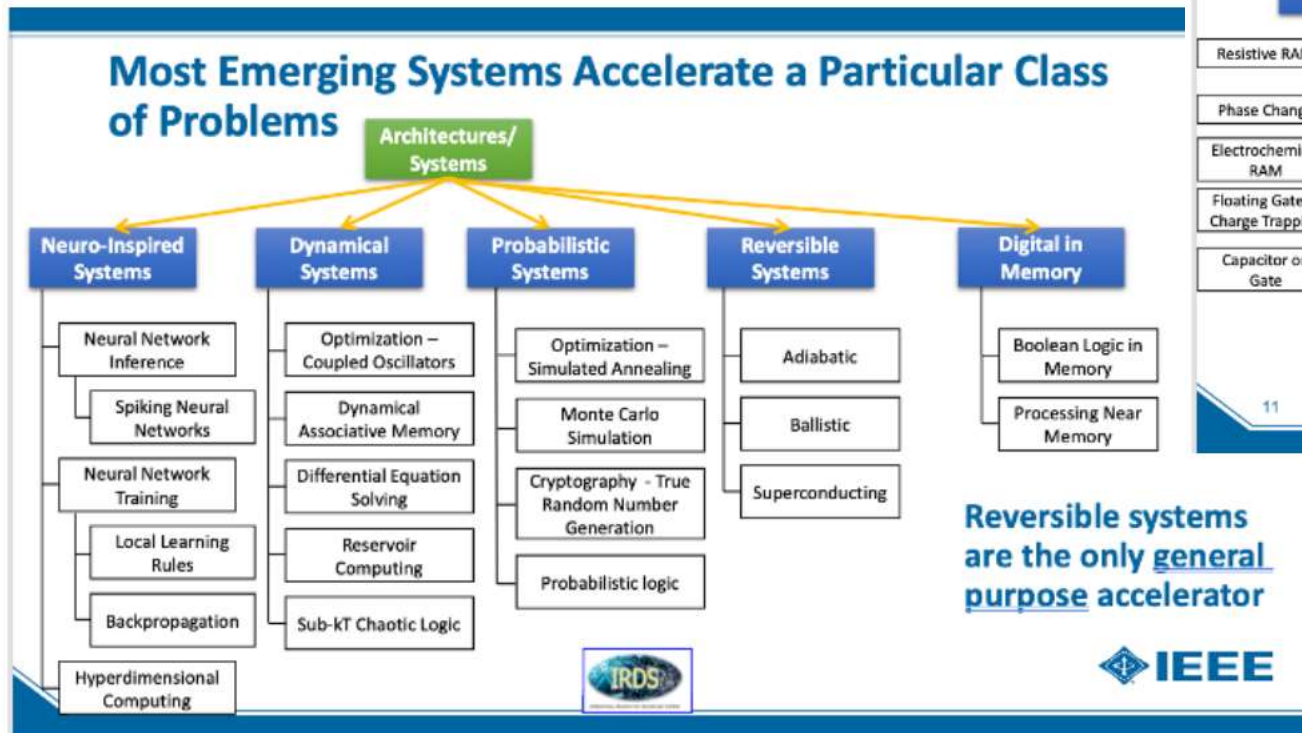
(THE INTERNATIONAL ROADMAP FOR DEVICES AND SYSTEMS: 2022; IEEE)

A holistic approach is needed, from device technologies and architectures, including both computing and memory/storage, to advanced packaging and cooling and data-center-level optimization.

Energy-Efficient Computing – What Does Each Trajectory Need?

Most Emerging Systems Accelerate a Particular Class of Problems
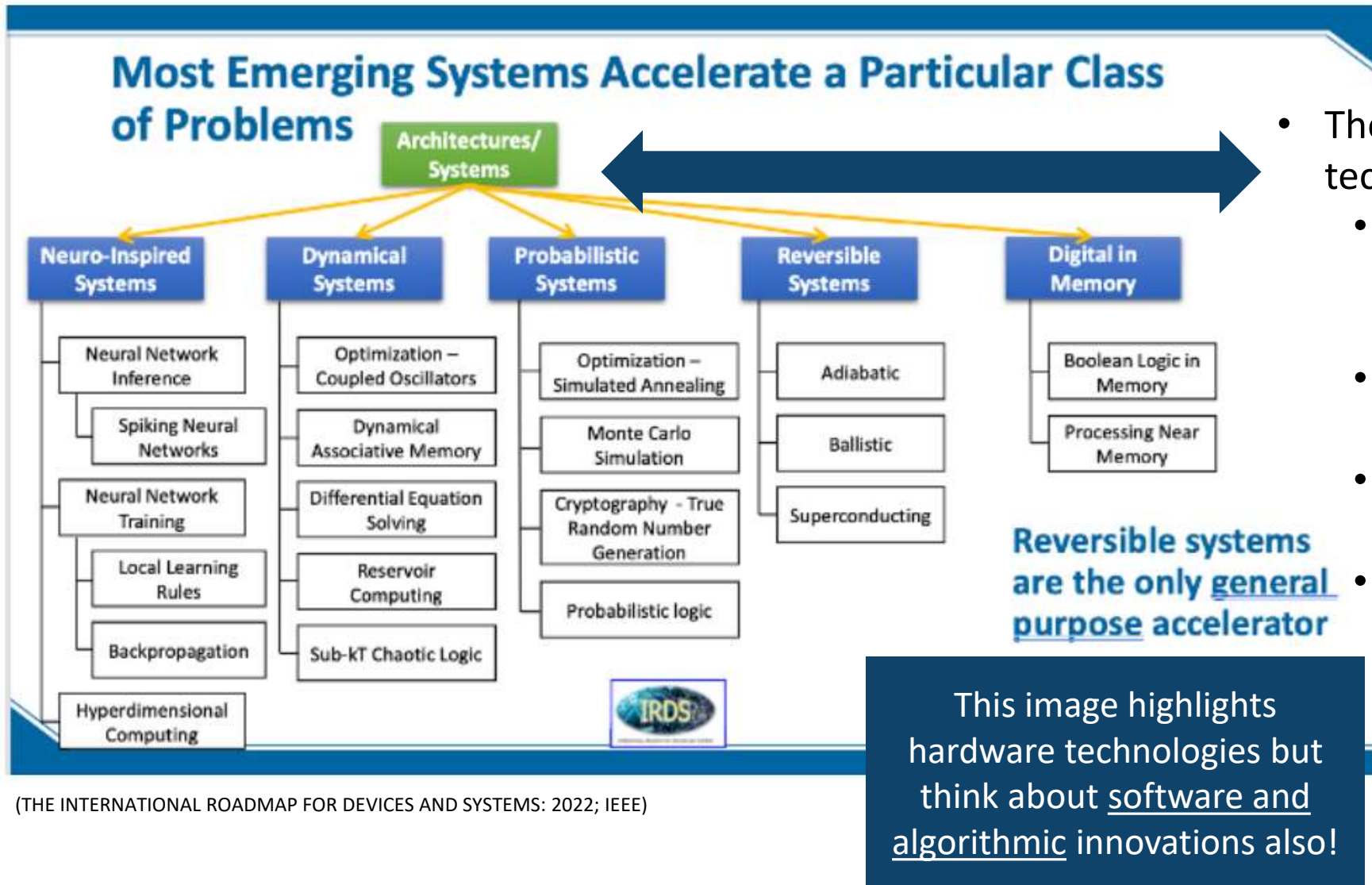
Architectures/Systems

Neuro-Inspired Systems
- Neural Network Inference
  - Spiking Neural Networks
- Neural Network Training
  - Local Learning Rules
  - Backpropagation
- Hyperdimensional Computing

Dynamical Systems
- Optimization – Coupled Oscillators
- Dynamical Associative Memory
- Differential Equation Solving
- Reservoir Computing
- Sub-kT Chaotic Logic

Probabilistic Systems
- Optimization – Simulated Annealing
- Monte Carlo Simulation
- Cryptography - True Random Number Generation
- Probabilistic logic

Reversible Systems
- Adiabatic
- Ballistic
- Superconducting

Digital in Memory
- Boolean Logic in Memory
- Processing Near Memory

Reversible systems are the only general purpose accelerator

IRDS

This image highlights hardware technologies but think about software and algorithmic innovations also!

(THE INTERNATIONAL ROADMAP FOR DEVICES AND SYSTEMS: 2022; IEEE)

- There are many potential technology trajectories, _for each_:
  - What trajectories are most interesting for scientific computing?
  - What might have an impact in the late 2030s?
  - What needs to happen for that impact to be realized?
  - What kinds of investments and partnerships are priorities?
    - Including basic research and testbeds.

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