

Office of Science Data for Al Round Table

Implementing FAIR Data for People and Machines: Impacts and Implications
September 11, 2019

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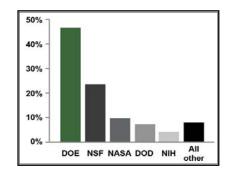
Office of Science

By the numbers

SC delivers scientific discoveries and tools to transform our understanding of nature and advance the energy, economic, and national security of the U.S.

Research

- Provides over 40% of the U.S. Federal support for basic research in the physical sciences;
- Supports over 23,000 Ph.D. scientists, graduate students, engineers, and support staff at over 300 institutions and all 10 DOE national laboratories;
- Maintains U.S. and world leadership in high-performance computing and computational sciences;
- Continues to be the major U.S. supporter of physics, chemistry, materials sciences, and biology for discovery and for energy sciences.



Support for basic research in the physical sciences by agency.

Source: NSF Science and Engineering Indicators 2012

Scientific User Facilities

SC maintains the world's largest collection of scientific user facilities (aka research infrastructure) operated by a single organization in the world, used by more than 35,000 researchers each year.



Shown is a portion of SLAC's two-mile-long linear accelerator (or linac), which provides the electron beam for the new Linac Coherent Light Source – the world's first hard x-ray, free-electron laser. For nearly 50 years, SLAC's linac had produced high-energy electrons for physics experiments. Now researchers use the very intense X-ray pulses (more than a billion times brighter than the most powerful existing sources) much like a high-speed camera to take stop-motion pictures of atoms and molecules in motion, examining fundamental processes on femtosecond timescales.



DOE Office of Science Research Portfolio*

Basic Energy Sciences

• Understanding, predicting, and ultimately controlling matter and energy at the electronic, atomic, and molecular levels

Advanced Scientific Computing Research

 Extending the frontiers of science through world leading computational science, supercomputers, and networking

Biological and Environmental Research

• Understanding complex biological and environmental systems

Fusion Energy Sciences

• Studying matter at very high temperatures and densities and the scientific foundations for fusion

High Energy Physics

• Exploring the elementary constituents of matter and energy, the interactions between them, and the nature of space and time

Nuclear Physics

 Discovering, exploring, and understanding all forms of nuclear matter



FY 2018 27 user facilities 35,000 users









































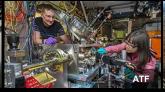










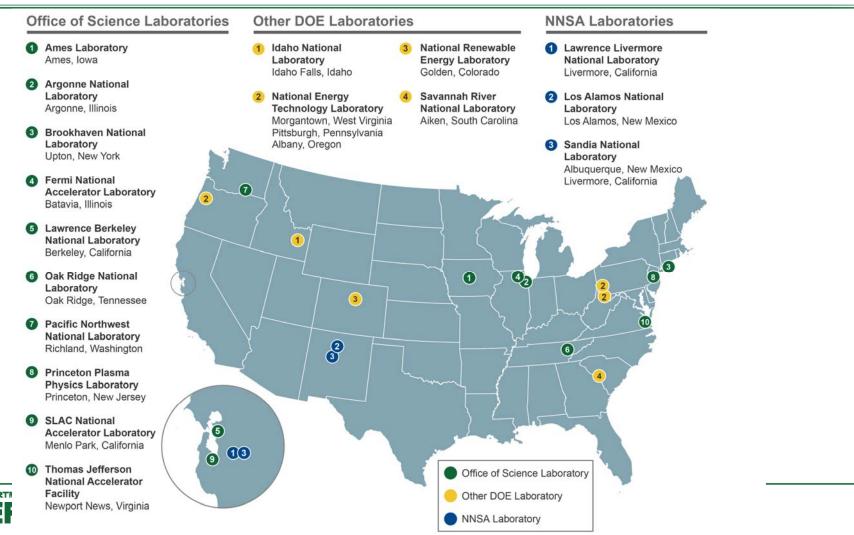






Office of Science

17 DOE National Laboratories





DOE is uniquely positioned to lead in AI/ML R&D

DOE has a unique combination of capabilities and infrastructure to lead the Nation in Artificial Intelligence (AI) and Machine Learning (ML) research and development:

- A broad mission that presents new and unique research problems on national and global scales to attract new talent.
- Sources of massive and/or complex science and engineering **data** from sensors, instruments, and from large-scale simulations.
- World-class high performance computing infrastructure capable of world-leading AI research.
- World-class high performance network infrastructure capable of integrating computing resources and data assets.
- An exceptional workforce with large numbers of scientists, computer scientists, and mathematicians currently engaged in Al and related fields.



Al Initiative



Enhance access to high-quality and fully traceable Federal data, models, and computing resources to increase the value of such resources for AI R&D, while maintaining safety, security, privacy, and confidentiality protections consistent with applicable laws and policies.

Executive Order 13859 of February 11, 2019
Maintaining American Leadership in
Artificial Intelligence

Office of Science (SC) Round Table on Data for Al

Rockville Hilton June 5, 2019

https://www.orau.gov/RTD-AI2019/

Supported by the **Office of Science Working Group on Digital Data** (SCWGDD), which includes representatives from all six SC program offices and OSTI

POC: Laura Biven (ASCR)

Participants came from 13 DOE National Labs, NIH, & NSF with expertise in Al/ML, data management, data curation, metadata, storage systems and I/O, open data, big data, data analytics, and edge computing; with ties to SC research, facilities, and community data repositories



Round Table Focus, Goals, & Context

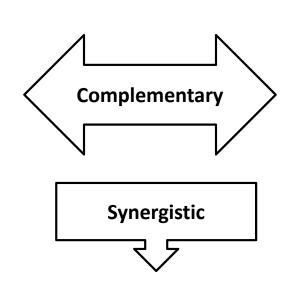
SC Round Table on Data for AI

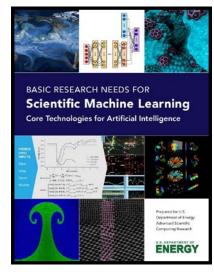
Focus:

Enhancing and enabling access to high-quality and fully traceable research data, models, and computing resources to increase the value of such resources for AI R&D and the SC mission.

Goal:

Identify key challenges/opportunities and potential next steps for the Office of Science.





AI FOR SCIENCE TOWN HALL

Al-focused workshops and round tables of sister SC program offices



Office of Science Data for Al Round Table: Challenges, Opportunities, & Enabling Capabilities

Challenges in using Al for science

Scientific data are different

There is no theory encompassing data, models, & tasks

Science applications of AI are super-

FAIR are good design principles but...

Opportunities that address challenges

Influence the development of AI tools by democratizing access to benchmark science data

Address open questions in AI with frameworks for relating data, models, and tasks

Make AI operational in science with composable services for simulation, data analysis, and AI at all scales

Capabilities to enable data enable data science, science, including Al

Data science support and incentives for teams generating data

Automated collection of metadata, provenance, & annotations at scale

Scalable, human interfaces for data

Strategic approaches to managing cost & resources



Thank you!!

SC Organizing Team

SC Working Group on Digital Data

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