

The Next Generation Earth System Grid Federation



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DOE Cybersecurity and Technology Innovation Conference

May 9, 2023



Forrest M. Hoffman, Computational Earth System Scientist

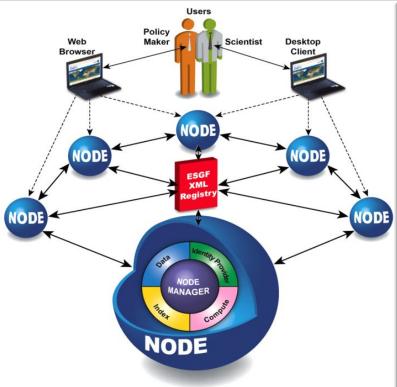
- Group Leader for the ORNL Computational Earth Sciences Group
- 34 years at ORNL in Environmental Sciences Division, then Computer Science and Mathematics Division, and now Computational Sciences and Engineering Division
- Develop and apply Earth system models to study global biogeochemical cycles, including terrestrial & marine carbon cycle
- Investigate methods for reconciling uncertainties in
 carbon–climate feedbacks through comparison with observations
- Apply artificial intelligence methods (machine learning and data mining) to environmental characterization, simulation, & analysis
- Joint Faculty, University of Tennessee, Knoxville, Department of Civil & Environmental Engineering



ESCIP What is the Earth System Grid Federation?

- The **Earth System Grid Federation (ESGF)** is an *international consortium* and a *globally distributed peer-to-peer network of data servers* using a common set of protocols and interfaces to archive and distribute climate and Earth system model output and related input, observational, and reanalysis data
- These **Open Science data** are used by scientists all over the world to investigate consequences of possible climate change scenarios and the resulting Earth system feedbacks





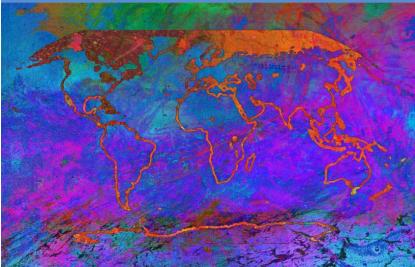
Logos represent primary international contributors: US Department of Energy, NASA, NOAA, NSF, European IS-ENES Project, and Australian NCI



- The United Nations' Intergovernmental Panel on Climate Change (IPCC) Sixth Assessment Report from Working Group I was released on Monday, August 9, 2021
- All of the climate and Earth system model simulation output underpinning this report was produced by modeling centers participating in the World Climate Research Programme's (WCRP's) sixth phase of the Coupled Model Intercomparison Project (CMIP6)
- Nearly all of that model output was stored in and distributed to researchers via ESGF
- Data are about the future of life on Earth!



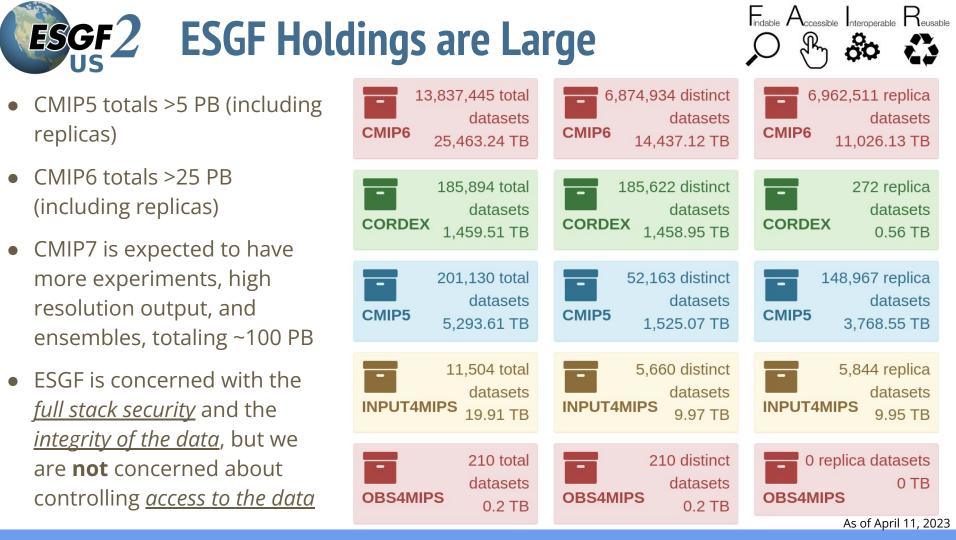
Climate Change 2021 The Physical Science Basis





Working Group I contribution to the Sixth Assessment Report of the ergovernmental Panel on Climate Change



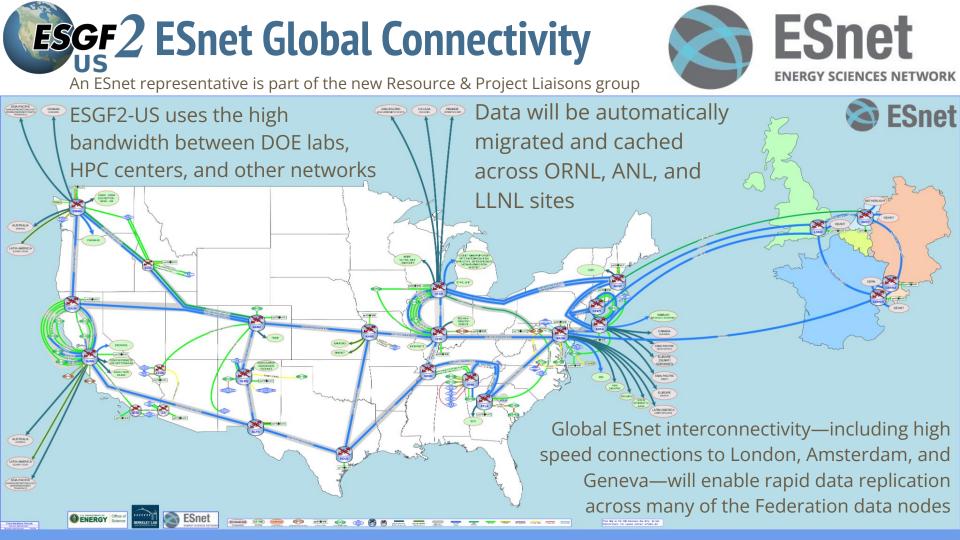




DOE's Current Earth System Grid Federation

- Primary server at LLNL
- LLNL replicates data from the global Federation when possible (primarily up to daily output)
- Independent data node at ANL





ESGF2 Web-based Search Interface

- A new multi-faceted search interface, called Multigrid, replaces old interface and adds some requested features
- Requires users to understand simulation experimental design and controlled vocabulary

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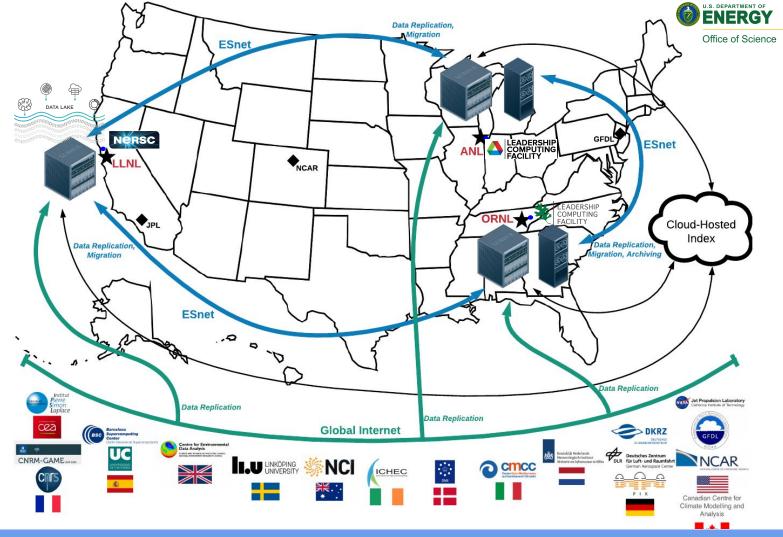
ESGF2 A New Consortium Project in the USA

- New team from Oak Ridge National Laboratory, Argonne National Laboratory, and Lawrence Livermore National Laboratory proposed to modernize the data backplane based on the Globus platform
- ESGF2-US proposal was reviewed by panel of 8 scientists in August 2021, and was **selected for funding** by the US Department of Energy starting in FY2022
- In **collaboration with international partners**, the project is developing and will deploy a new architecture based on the *Future Architecture Roadmap*
- In addition, ESGF2-US will develop new data discovery tools and data access interfaces, server-side computing (subsetting & summarizing), and user computing (Kubernetes & JupyterHub) with improved user & system metrics
- ESGF2-US added a Resource & Project Liaison group and a Science, User & Facility Advisory Board and will offer a help desk/user support



DOE's Next Generation Earth System Grid Federation

- As many as three nodes co-located at DOE's major computing facilities
- Replicating data from the global Federation
- Providing cloud indexing and tape archiving





Design and implementation principles

• Open architecture and protocols

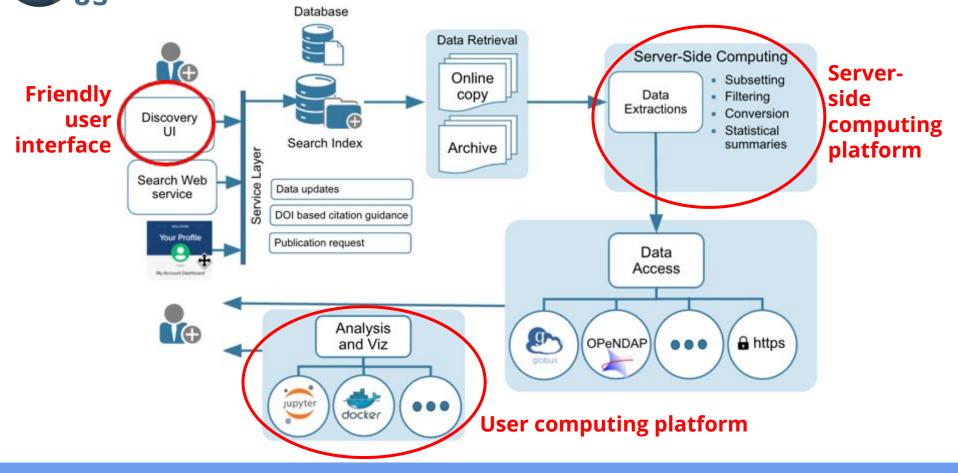
- Enable substitution of alternative implementations
- Leverage **highly available and scalable** central services from Globus
 - Reduce complexity, increase reliability, provide economies of scale
- Use proven, modern security technologies and practices
 - Integrated access control; protect against attacks and intrusions
- **Use case approach** to design, implementation, and evaluation
 - Ensure that solutions meet real user needs
- Integrated instrumentation
 - Metrics drive data management, data access features, capability development
- Focus on **performance** to deal with big data
 - High-speed data transfer, search, server-side processing

ESCIP Enabling a new level of research productivity

Logging in with her **institutional credentials**, Samantha is presented with **new data, code, and** papers relevant to her current research. Intrigued by a new report on extreme precipitation events, she examines a **Jupyter notebook** that implements the method used. Wondering how this method would work with higher-resolution E3SM data, she quickly locates required datasets and runs the notebook on a subset. Results are promising, so she shares them with collaborators via ESGF2-US federated storage, and they agree that a larger ensemble analysis is called for. ESGF2-US confirms that the full ensemble data are available at OLCF, so they submit a request to execute the analysis there. Within 24 hours, results have been published to ESGF2-US for broader consumption, along with the notebook used to produce and validate the results.



ESGF2 Data Discovery Platform: Architecture





Organize Webinars, Tutorials, and Bootcamps

- Data management lessons learned
- Ingest best practices
- Data discovery and access
- → ESGF Webinar series playlist at <u>https://www.youtube.com/@esgf2432</u>

Hackathons and Workshops

- Data standards
- Data node deployment and user compute resources
- Hold at large relevant conferences, e.g.,
 AGU Fall Meeting, EGU, and AMS Annual Meeting
- Organize and host annual
 ESGF Developer and User Conferences
- → Ninth ESGF Developer and User Dual-Hybrid Conference held January 18–20, 2023

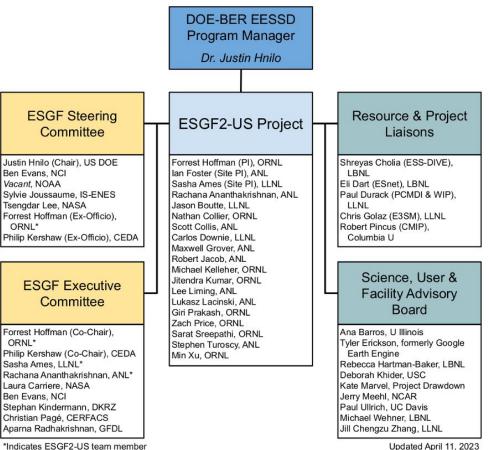




Ninth ESGF Developer and User Conference, held jointly between Oak Ridge National Laboratory (USA) and Toulouse (France), January 18–20, 2023

ESGF2 ESGF and ESGF2-US Project Governance

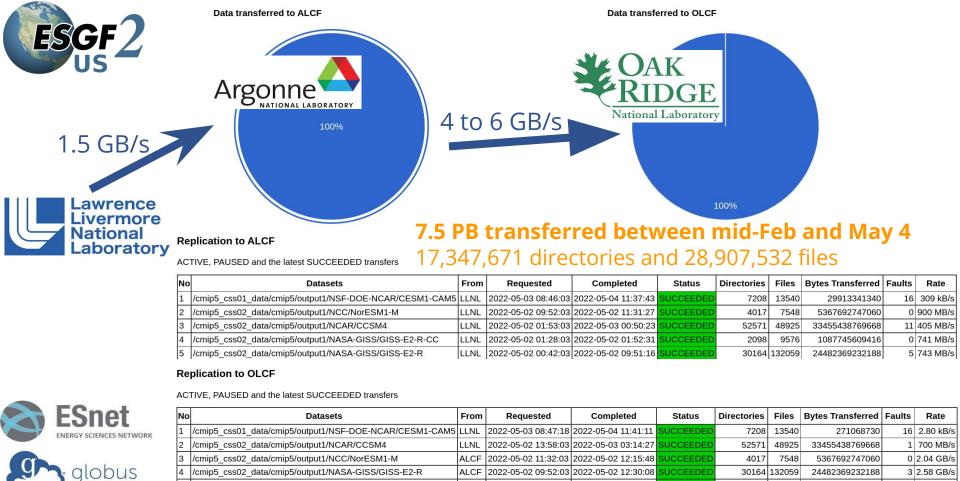
- ESGF is governed by an international **ESGF Executive Committee** that meets monthly
- The **XC** is directed by the **ESGF Steering Committee (SC)**, composed primarily of sponsoring agency representatives
- The ESGF2-US Project added
 - **Resource & Project Liaisons** group to 0 enhance communication with interdependent projects and critical resources
 - Science, User & Facility Advisory Board to 0 evaluate and prioritize project efforts with respect to community needs



*Indicates ESGF2-US team member



- In the US, LLNL operates the primary ESGF node, which replicates much of the CMIP6 and related model output from around the globe
- Since the data at LLNL are contained only on spinning disk, we decided to replicate the **entire ~7.5 PB collection of data** to Argonne National Laboratory (ANL) and Oak Ridge National Laboratory (ORNL)
- Solution: Use Globus to transfer all the data over ESnet
- We used custom Globus scripting (*thanks to Lukasz Lacinski*), ESnet network monitoring and diagnostics (*thanks to Eli Dart*), DTN and GPFS optimized configurations (*thanks to Cameron Harr and others*), and debugging and problem-solving (*thanks to Sasha Ames, Lee Liming, and others*)



ALCF

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https://dashboard.globus.org/esgf

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As of May 4, 2022

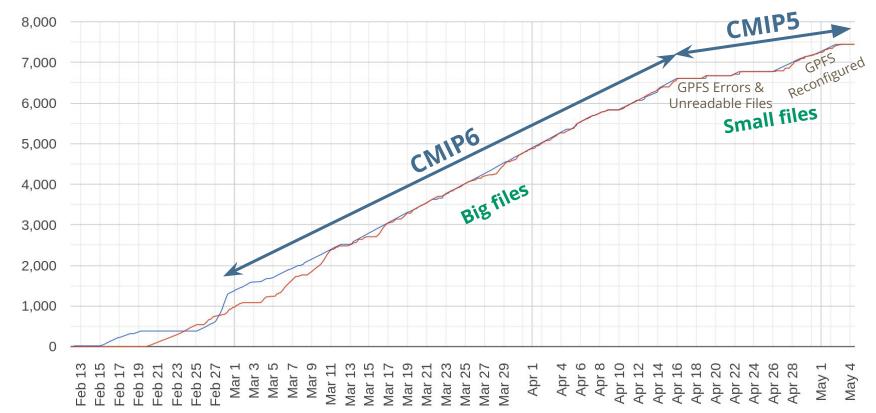
0 1.73 GB/s

1087745609416

ESGF2 Cumulative Data Transferred Over Time

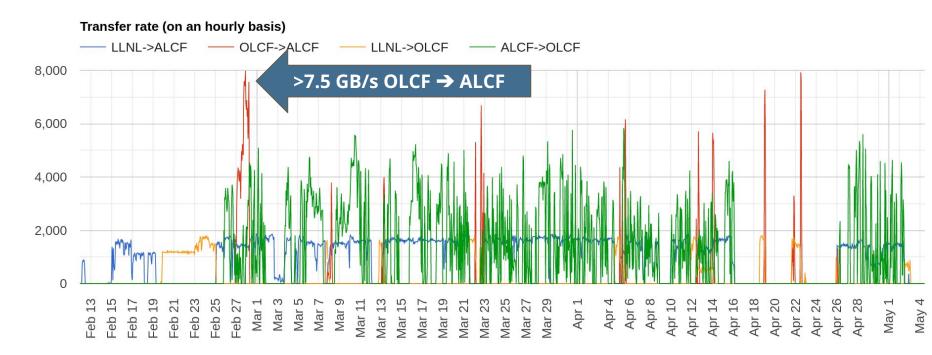
Progress of transfers



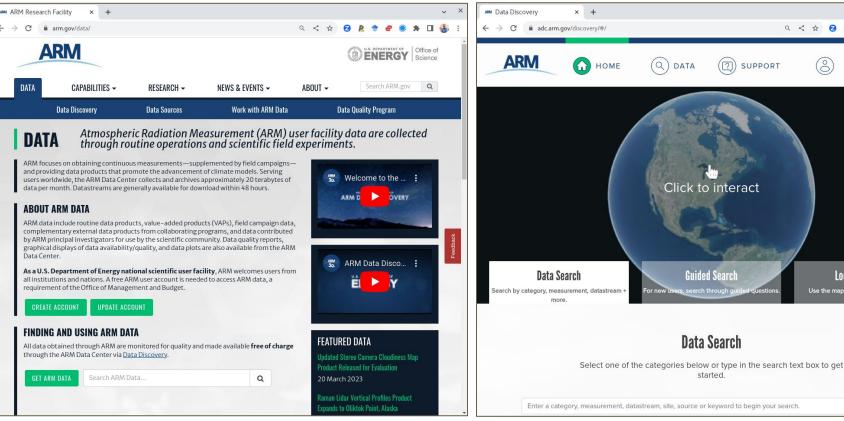


Data size (TB)









Atmospheric Radiation Measurement (ARM) Data Center – https://www.arm.gov/data/

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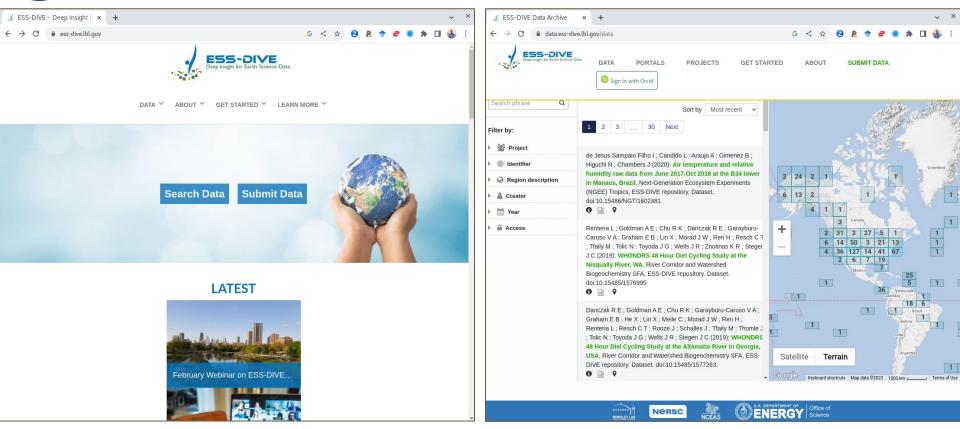
Location Search

Use the map to search by site or facility.

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SUPPORT

ESCIP 2 ESS Deep Insight for Earth Science Data (DIVE)



Environmental Systems Science-Deep Insight for Earth Science Data (ESS-DIVE) – https://ess-dive.lbl.gov/

ESCIP A Unified Data Framework for DOE BER (RFI)

DOE's Biological and Environmental **Research Advisory** Committee (BERAC) is collecting information on ways to integrate existing data activities based on charge from Undersecretary of SC

Federal Register

PDF

https://www.govinfo.gov/content/p kg/FR-2023-04-17/pdf/2023-08029. pdf

Webpage

https://www.federalregister.gov/do cuments/2023/04/17/2023-08029/a -unified-data-framework-for-doe-bi ological-and-environmental-researc

Federal Register / Vol. 88, No. 73 / Monday, April 17, 2023 / Notices

management and analysis within a unified framework. DATES: Written comments and information are requested on or before

messaging and training are not

In order to examine this trend within

initiative. CNA, in conjunction with the

Programs Division (MFP), propose the

information collection, "Marine Corps

program awareness, preferences for

identifying, from the perspective of

Marines, the reach of current LMS

understand which LMS activities and

as serve as a baseline data for future

in accordance with the standards of

Instruction 6490.16. Affected Public: Individuals or

Annual Burden Hours: 2,262.

Number of Respondents: 9.048.

Average Burden per Response: 15

Responses per Respondent: 1.

Alternate OSD Federal Register Liaison

[FR Doc. 2023-08050 Filed 4-14-23; 8:45 am]

A Unified Data Framework for DOE

Science, Department of Energy (DOE).

Officer, Department of Defense.

DEPARTMENT OF ENERGY

Biological and Environmental

ACTION: Request for information

on biological systems, bioenergy,

environmental science, and Earth

framework that links or integrates

existing data activities within BER.

inform and recommend to BER a

strategy for next-generation data

Information produced in response to

this request may be used by the BER

Advisory Committee (BERAC) to help

SUMMARY: The Biological and

Annual Responses: 9,048.

Frequency: Once.

Kayyonne T. Marston,

BILLING CODE 5001-06-P

Dated: April 12, 2023.

households

minutes

Research

LMS activity effectiveness evaluations

practice framework prescribed by DoD

This survey will assist MFP in

safety devices and locations, and the

place of safety in Marine Corps culture.

Safety Needs Assessment" survey. This

voluntary survey examines current LMS

the Marine Corps and gather relevant

baseline data for the larger DSPO

Marine Corps Marine and Family

resonating with Marines.

October 31, 2023. ADDRESSES: Interested persons may submit comments by email only. Comments must be sent to BEBACBFI science.doe.gov with the subject line "BER unified data".

FOR FURTHER INFORMATION CONTACT: Requests for additional information may be submitted to Dr. Tristram O. West. (301) 903-5155, Tristram.west@ science.doe.gov.

SUPPLEMENTARY INFORMATION: A charge efforts and the acceptability of potential was issued from the Director of Office LMS activities. The results of the survey of Science on October 13, 2022, to the will be used by MFP and DSPO to better BER Advisory Committee (BERAC) to (1) review the existing and anticipated messages resonate with Marines, as well capabilities in data management and supporting infrastructures that are relevant to the breadth of BER science and (2) recommend a strategy for nextgeneration data management and analysis within a unified framework. The Director's charge letter may be found here: https://science.osti.gov/ber/ berac/Reports/Current-BERAC-Charges. Information collected through this request for information, in addition to other informational sources, may be used by BERAC to recommend strategies to further integrate and strengthen BER's data infrastructure in support of BER research. It may also be used by the BERAC in fulfilling its October 13, 2022. charge from the Director of the Office of Science to recommend a strategy for next-generation data management and analysis within a unified framework.

Request for Information

The objective of this request for information is to gather current and future science questions within BER's mission space that would require a more integrated data infrastructure for data AGENCY: Office of Biological and Environmental Research (BER), Office of access, processing, and use spanning more than one research area. Current BER research areas are provided online https://science.osti.gov/ber/Research. Supported research includes Atmospheric Science; Earth and Environmental Research (BER) Program, Environmental System Modeling: as DOE's coordinating office for research Environmental Science; Bioenergy and Bioproducts: and Plant and Microbial Genomics, Current data archives and system science, is seeking input on the activities that support BER research need and the structure of a unified data areas include, but are not limited to. ARM https://www.arm.gov/, ESS-DIVE https://ess-dive.lbl.gov/, ESGF https:// esgf.llnl.gov/, KBase https:// www.kbase.us/. NMDC https:// microbiomedata.org/, MSD-LIVE https://msdlive.org/, and JGI https:// jgi.doe.gov/.

Information is specifically requested on how a more unified data infrastructure may better facilitate current or future science questions, and what components or technologies are needed to develop a more unified data

infrastructure. Answers or information related, but not limited, to the following questions are specifically requested: 1. Do you conduct research in one of

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the BER research areas (i.e., Atmospheric Science: Earth and Environmental System Modeling: Environmental Science: Bioenergy and Bioproducts; or Plant and Microbial Genomics) and, if so, which area(s)? Please limit additional detail on your area(s) of research interest to a brief paragraph.

2. What new or existing research area might benefit from improvements in data availability or access across research areas, potentially enabling scientific breakthroughs-and why? 3. What data improvements, including those of accessibility and integration. could facilitate new or existing research or scientific breakthroughs? a. Are there current data sets that should be linked or integrated into existing data infrastructure to facilitate existing or new research? If so, which data sets should be so linked or

integrated and why? b. Are there current barriers to accessing or integrating data from (a) different DOE sources (e.g., ARM, JGI, ESS-DIVE, MSD-LIVE) or from (b) different sources separately maintained by DOE and another Federal agency? If so, what are those barriers and how might they be addressed to allow for improved data access and integration?

c. What data infrastructure improvements would best support model-experiment feedbacks; facilitate data synthesis and analysis for multidisciplinary research; and enable application of advanced statistical techniques, including artificial intelligence and machine learning? Please include a brief explanation as to how each identified improvement would support each of these listed tasks

d. What current barriers need to be addressed in developing a unified infrastructure to promote greater use by a more diverse community of users, with a focus on improving diversity, equity, and inclusion within data usage and application?

While the questions provided above can help guide thinking on this topic, any input is welcome that may assist BERAC in developing a next-generation data infrastructure in support of BER mission science. The information provided through this request will assist





A Unified Data Framework for DOE Biological and **Environmental Research**

A Notice by the Energy Department on 04/17/2023

This document has a comment period that ends in 176 days. (10/31/2023)

Notice

1 comments received. View posted comments

PUBLISHED DOCUMENT

AGENCY:

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Office of Biological and Environmental Research (BER), Office of Science, Department

of Energy (DOE) ACTION:

Request for information

SUMMARY:

The Biological and Environmental Research (BER) Program, as DOE's coordinating office for research on biological systems, bioenergy, environmental science, and Earth system science, is seeking input on the need and the structure of a unified data framework that links or integrates existing data activities within BER. Information produced in response to this request may be used by the BER Advisory Committee (BERAC) to help inform and recommend to BER a strategy for next-generation data management and analysis within a unified framework.

DATES:

Written comments and information are requested on or before October 31, 2023.

DOCUMENT DETAILS Printed version: PDF

Publication Date: 04/17/2023

Agency: Department of Energy

Dates:

Written comments and information are requested on or before October 31, 2023

Comments Close: 10/31/2023

Document Type: Notice

Document Citation: 88 FR 23415

Page: 23415-23416 (2 pages)

Document Number: 2023-08029

ESCIP Summary and Integration Activities

- The next generation Earth System Grid Federation (ESGF2-US)
 - Will be designed for an **order of magnitude increase in data sizes**
 - Will be highly available, scalable, and fast
 - Will have improved **data discovery and sharing tools**
 - Will offer **server-side computing** for derived data
 - Will offer **user computing capabilities** (e.g., JupyterHub/JupyterLab) near the data
 - Will be developed collaboratively with **international Federation partners**
- All new **ESGF development is being performed collaboratively** with Federation partners all over the world
- ESGF2-US is integrated with **DOE Earth & Environ. Systems Modeling projects** and with international **WCRP CMIP activities**, including serving on multiple Task Teams for CMIP7
- ESGF2-US aims to add **new data projects** to support large-scale AI/ML data, multi-agency model intercomparisons, and model benchmarking
- **User computing** approaches initiated in the commercial cloud and deployed through on-premise cloud infrastructure will likely facilitate more rapid research and discovery