The Next Generation
Earth System Grid Federation

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National Center for Atmospheric Research (NCAR)
Computational and Information Systems Laboratory (CISL) Seminar

April 11, 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
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 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!
ESGF Holdings are Large and Growing

- CMIP5 totals >5 PB (including replicas)
- CMIP6 totals >25 PB (including replicas)
- CMIP7 is expected to have more high resolution output & ensembles, totaling ~100 PB
- ESGF2-US will expand Federation holdings by adding other Earth science data projects for AI/ML, large ensembles, etc.

As of April 11, 2023
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 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
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
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.

Flood risk increases with water availability.
ESnet Global Connectivity

An ESnet representative is part of the new Resource & Project Liaisons group

ESGF2-US will make use of the high bandwidth between DOE labs and HPC centers

Data will be automatically migrated and cached across ORNL, ANL, and LLNL sites

Global ESnet interconnectivity—including high speed connections to London, Amsterdam, and Geneva—will enable rapid data replication across most of the Federation data nodes
Data Discovery Platform: Architecture

- **Discovery UI**
  - Search Web service
    - Data updates
    - DOI based citation guidance
    - Publication request

- **Data Retrieval**
  - Online copy
  - Archive

- **Server-Side Computing**
  - Data Extractions
    - Subsetting
    - Filtering
    - Conversion
    - Statistical summaries

- **Data Access**
  - globus
  - OPeNDAP
  - jupyter
  - docker

- **Analysis and Viz**
  - jupyter
  - docker
Outreach Activities

- Organize Webinars, Tutorials, and Bootcamps
  - Data management lessons learned
  - Ingest best practices
  - Data discovery and access

  ➜ ESGF Webinar series playlist at https://www.youtube.com/@esgf2432

- 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
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 enhance communication with interdependent projects and critical resources.
  - **Science, User & Facility Advisory Board** to evaluate and prioritize project efforts with respect to community needs.

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**ESGF Steering Committee**

- Justin Hnilo (Chair), US DOE
- Ben Evans, NCI
- Vacant, NOAA
- Sylvie Joussaume, IS-ENES
- Tseng-far Lee, NASA
- Forrest Hoffman (Ex-Officio), ORNL
- Philip Kershaw (Ex-Officio), CEDA

**ESGF Executive Committee**

- Forrest Hoffman (Co-Chair), ORNL
- Philip Kershaw (Co-Chair), CEDA
- Sasha Ames, LLNL
- Rachana Ananthakrishnan, ANL
- Laura Carriere, NASA
- Ben Evans, NCI
- Stephan Kindermann, DKRZ
- Christian Pagé, CERFACS
- Aparna Radhakrishnan, GFDL

**ESGF2-US Project**

- Forrest Hoffman (PI), ORNL
- Ian Foster (Site PI), ANL
- Sasha Ames (Site PI), LLNL
- Rachana Ananthakrishnan, ANL
- Jason Boutle, LLNL
- Nathan Collier, ORNL
- Scott Collins, ANL
- Carlos Dominguez, LLNL
- Maxwell Grover, ANL
- Robert Jacob, ANL
- Michael Kellerer, ORNL
- Jitendra Kumar, ORNL
- Lee Limoing, ANL
- Lukaaz Lacinisk, ANL
- Giri Prakash, ORNL
- Zheng Price, ORNL
- Sarath Sreepathi, ORNL
- Stephen Turosco, ANL
- Min Xu, ORNL

**DOE-BER EESSD Program Manager**

- Dr. Justin Hnilo

**Resource & Project Liaisons**

- Shreyas Cholia (ESS-DIVE), LBL
- Eli Dart (ESNet), LBNL
- Paul Durack (PCMDI & WIP), LBNL
- Chris Golaz (ESRM), LLNL
- Robert Pincus (CMIP), Columbia U

**Science, User & Facility Advisory Board**

- Ana Barros, U Illinois
- Tyler Erickson, formerly Google Earth Engine
- Rebecca Hartman-Baker, LBNL
- Deborah Kihler, USC
- Kate Marvel, Project Drawdown
- Jerry Meeth, NCAr
- Paul Ulrich, UC Davis
- Michael Wehner, LBNL
- Jill Chengzhu Zhang, LLNL

*Indicates ESGF2-US team member

Updated April 11, 2023
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*).
Data transferred to ALCF

1.5 GB/s

Data transferred to OLCF

4 to 6 GB/s

Replication to ALCF

ACTIVE, PAUSED and the latest SUCCEEDED transfers

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<th>No</th>
<th>Datasets</th>
<th>From</th>
<th>Requested</th>
<th>Completed</th>
<th>Status</th>
<th>Directories</th>
<th>Files</th>
<th>Bytes Transferred</th>
<th>Faults</th>
<th>Rate</th>
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<td>2022-05-02 09:52:03</td>
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<td>405 MB/s</td>
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Replication to OLCF

ACTIVE, PAUSED and the latest SUCCEEDED transfers

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<th>Requested</th>
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<td>1.73 GB/s</td>
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Cumulative Data Transferred Over Time

Progress of transfers
- Blue line: to ALCF
- Red line: to OLCF

Data size (TB)
- CMIP5
- CMIP6
- GPFS Errors & Unreadable Files
- Big files
- Small files
- GPFS Reconfigured

Timeline:
- Feb 13
- Feb 15
- Feb 17
- Feb 19
- Feb 21
- Feb 23
- Feb 25
- Feb 27
- Mar 1
- Mar 3
- Mar 5
- Mar 7
- Mar 9
- Mar 11
- Mar 13
- Mar 15
- Mar 17
- Mar 19
- Mar 21
- Mar 23
- Mar 25
- Mar 27
- Mar 29
- Apr 1
- Apr 4
- Apr 6
- Apr 8
- Apr 10
- Apr 12
- Apr 14
- Apr 16
- Apr 18
- Apr 20
- Apr 22
- Apr 24
- Apr 26
- Apr 28
- May 1
- May 4
Transfer Rates Over Time

Transfer rate (on an hourly basis)

- LLNL->ALCF
- OLCF->ALCF
- LLNL->OLCF
- ALCF->OLCF

>7.5 GB/s OLCF → ALCF
Atmospheric Radiation Measurement (ARM) Data Center – https://www.arm.gov/data/
Environmental Systems Science-Deep Insight for Earth Science Data (ESS-DIVE) - [https://ess-dive.lbl.gov/](https://ess-dive.lbl.gov/)
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 automatically migrate data as needed
- 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

All new **ESGF development is being performed collaboratively** with Federation partners all over the world

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 research