

Earth System Grid Center for Enabling Technologies (ESG-CET): A Data Infrastructure for Data-Intensive Climate Research

Executive Committee:

- **Dean N. Williams** (williams13@llnl.gov), Lawrence Livermore National Laboratory, Livermore, CA, USA
- **Ian T. Foster**, Argonne National Laboratory, Argonne, IL, USA
- **Don E. Middleton**, National Center for Atmospheric Research, Boulder, CO, USA

Team:

Rachana Ananthakrishnan, Neill Miller, Argonne National Laboratory, Argonne, IL, USA

Mehmet Balman, Junmin Gu, Vijaya Natarajan, Arie Shoshani, Alex Sim, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Gavin Bell, Robert Drach, Michael Ganzberger, Lawrence Livermore National Laboratory

Jim Ahrens, Phil Jones, Los Alamos National Laboratory, Los Alamos, NM, USA

Daniel Crichton, Luca Cinquini, Jet Propulsion Laboratory, National Aeronautics and Space Administration, Pasadena, CA, USA

David Brown, Danielle Harper, Nathan Hook, Eric Nienhouse, Gary Strand, Hannah Wilcox, Nathan Wilhelmi, Stephan Zednik, National Center for Atmospheric Research, Boulder, CO, USA

Steve Hankin, Roland Schweitzer, Pacific Marine Environmental Laboratory, National Oceanic and Atmospheric Administration, Seattle, WA, USA

John Harney, Ross Miller, Galen Shipman, Feiyi Wang, Oak Ridge National Laboratory, Oak Ridge, TN, USA

Peter Fox, Patrick West, Stephan Zednik, Rensselaer Polytechnic Institute, Troy, NY, USA

Ann Chervenak, Craig Ward, Information Sciences Institute, University of Southern California, Marina del Rey, CA, USA

Abstract. For the Earth System Grid Federation (ESGF), the ESG-CET team has led international development and delivered a production environment for managing and accessing ultrascale climate data. This production environment includes multiple national and international climate projects (e.g., Coupled Model Intercomparison Project, Community Earth System Model), ocean model data (such as the Parallel Ocean Program), observation data (Carbon Dioxide Information and Analysis Center, Atmospheric Infrared Sounder, etc.), and analysis and visualization tools, all serving a diverse user community. These data holdings and services are distributed across multiple ESG-CET sites (such as LANL, LBNL/NERSC, LLNL/PCMDI, NCAR, and ORNL) and at unfunded partners sites such as the Australian National University National Computational Infrastructure, the British Atmospheric Data Centre, the National Oceanic and Atmospheric Administration Geophysical Fluid Dynamics Laboratory, the Max Planck Institute for Meteorology, the German Climate Computing Centre, and the National Aeronautics and Space Administration Jet Propulsion Laboratory.

More recently, ESG-CET has extended its services beyond data-file access and delivery to include more detailed information products (scientific graphics, animations, etc.), secure binary data-access services (based on the OPeNDAP protocol), and server-side analysis. The last capabilities allow users to request data subsets transformed through commonly used analysis and intercomparison procedures. As we transition from development activities to production and operations, the ESG-CET team is tasked with making data available to all users seeking to understand, process, extract value from, visualize, and/or communicate it to others. This ongoing effort, though daunting in scope and complexity, will greatly magnify the value of numerical climate model outputs and climate observations for future national and international climate-assessment reports. Continued ESGF progress will result in a production ultrascale data system for empowering scientists who attempt new and exciting data exchanges that could ultimately lead to breakthrough climate-science discoveries.

1. ESG Introduction

One of the most difficult challenges that climate scientists face today is managing and understanding massive amounts of global atmospheric, land, ocean, and sea-ice model data generated by complex computer simulations and collected by observations [Overpeck 2011]. Advances in collaboration technologies and high-performance computers and networks have been instrumental in allowing many different types of users access to globally shared, disparate ultrascale data sets. The advent of rapid increases in technology performance and ultrascale data repositories, coupled with the need to share information, has motivated a community of aware climate and computational scientists to develop a federated open-source system that everyone (e.g., scientists, resource managers, policymakers, citizens) can use to study climate change. Among emerging knowledge portals and collaborative environments, the Earth System Grid Center for Enabling Technologies (ESG-CET) effort—the primary contributor to the Earth System Grid Federation (ESGF) software—stands out as one of the development leaders in premier science gateways for present and future ultrascale climate holdings [Williams 2009a, Williams 2009b]. The ESGF, a coordinated international collaboration of people and institutions, works to build an open-source software infrastructure to manage and analyze Earth science data [Williams 2011].

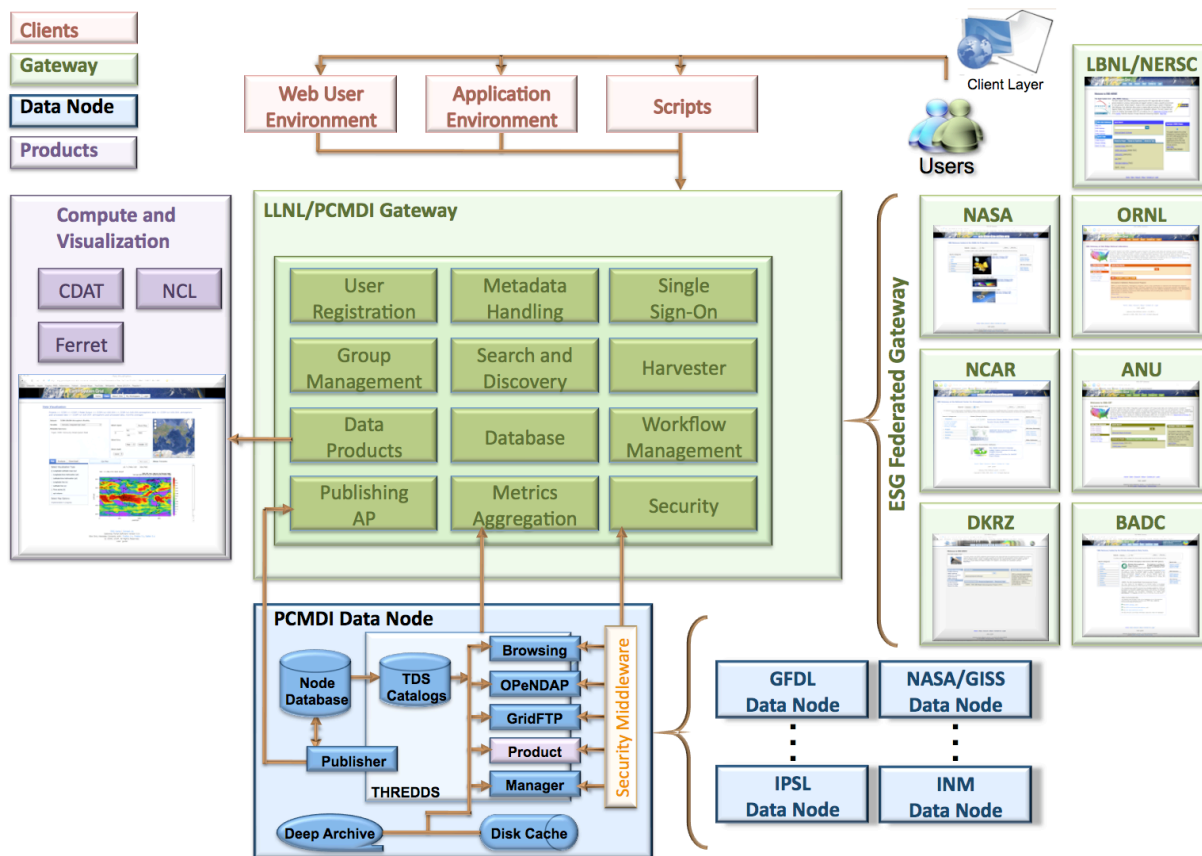


Figure 1: Users can access ESGF data using Web browsers, script, and, in the near future, client applications. ESGF is separated into gateways (green) and data nodes (blue). Gateways handle user registration and management and allow users to search, discover, and request data. Data nodes are located where the data resides, allowing data to be published (or exposed) on disk or through tertiary mass store (i.e., tape archive) to any gateway. They also handle data reduction, analysis, and visualization. ESGF currently comprises eight national and international gateways, four of which hold special status in housing CMIP5/AR5 replication data sets: LLNL/PCMDI, BADC, DKRZ, and the Australian National University (ANU) National Computational Infrastructure (NCI). Users have access to all data from the federation regardless of which gateway is used.

Funded through the DOE SciDAC-2 program with support from the Offices of Advanced Scientific Computing Research (ASCR) and Biological and Environmental Research (BER), ESG-CET efforts

extend across many national and international agencies to provide researchers with access to much needed, important ultrascale data, information, models, analysis, visualization tools, and computational resources. As a global consortium of data providers, data archives, and users—and under the governance of the Global Organization for Earth System Science Portals (GO-ESSP)—ESGF aims to develop, deploy, and maintain a software infrastructure for managing ultrascale-model output and observational data. In this infrastructure, users can access many disparate ESGF data holdings through a growing number of national and international gateways (as shown in Figure 1). By leveraging ESG-CET software components, scientists accessing portals can perform comparative analysis and visualizations across experiments. ESGF efforts require integration of software and hardware resources spread across all-important institutions carrying out climate research. The members of the U.S. contingent for ESGF include Argonne, LBNL/NERSC, LLNL/PCMDI, NASA/JPL, NCAR, and ORNL. All ESG-CET members work across institutional boundaries to contribute to the development and integration of disparate software that facilitates climate research.

The climate-science community has come to rely on ESGF to provide fundamental support for its development efforts. As evidenced by the important data sets mentioned in Section 2.1, ESGF is entrusted to unify computational and analytical climate resources under one unique and powerful knowledge-discovery enterprise system. It continues to evolve to maintain its reputation as a reliable resource for serving the climate-science community as it seeks to derive fundamental and practical understanding of the climate and climate change.

2. Data

We review briefly the data holdings maintained by ESGF and various issues associated with data access and usage.

2.1. Climate Community Data Holdings

Before accessing ESGF data holdings, users must create an account at one of eight gateway sites shown in Figure 1, with more gateways to come: **LLNL/PCMDI** (<http://pcmdi3.llnl.gov/esgcet/home.htm>); **BADC** (<http://cmip-gw.badc.rl.ac.uk/home.htm>); **DKRZ** (<http://ipcc-ar5.dkrz.de/home.htm>); **NASA** (<http://esg-gateway.jpl.nasa.gov/home.htm>); **NCAR** (<http://www.earthsystemgrid.org/home.htm>); **ANU** (<http://esg.nci.org.au/esgcet/home.htm>); **ORNL** (<http://esg2-gw.ccs.ornl.gov/esgcet/home.htm>); or **LBNL/NERSC** (<http://esg.nersc.gov/esgcet/home.htm>). This process generates an OpenID [OpenID 2011], username, and password. Once logged into the system, the user can apply for group membership to access data from a growing list of climate projects, such as the following:

- Phases 3 and 5 of the Coupled Model Intercomparison Project (CMIP3 and CMIP5, respectively)
- Community Climate System Model (CCSM)
- North American Regional Climate Change Assessment Program (NARCCAP)
- Transpose-Atmospheric Model Intercomparison Project (TAMIP2)
- Carbon-Land Model Intercomparison Project (C-LAMP)
- NASA's Atmospheric Infrared Sounder (AIRS)

These data archives will be augmented with additional observational and model-generated data sets, for example: CESM1, CCES, ARM, CDIAC, ESM and RGM, NASA satellite observation data (CloudSat, MLS, MISR, AIRS, CERES, TRMM, etc.), NOAA observation and reanalysis data, and many other data sets critical to understanding climate change [Strand 2011].

2.2. Current and Future Data Volumes

Currently, ESGF holds and disseminates data for 12 national and international climate projects, ranging from model simulations to satellite observations. Current ESGF production sites boast over 23,000 registered users and manage over 700 TB of primarily model data. The federation spans five sites in the United States, two sites in Europe, and one site in Australia. Over the years, the community of registered users downloaded over 1.2 petabytes of data.

Although ESGF has been indisputably important to CMIP, its future impact will not be limited solely to this especially high-profile project. Jointly, with other funding agencies, ESGF research scientists and software engineers are applying a diverse base of expertise to develop software and serve data that enables broader climate-research groups worldwide that access, visualize, and analyze data. ESGF is expanding climate scientists' ability to construct highly collaborative problem-solving environments and to capitalize on the availability of future integrated-but-distributed data and computers. Work to utilize high-bandwidth wide-area networks with DOE ASCR projects such as the Advanced Network Initiative (ANI)—a prototype network designed to accelerate deployment of 100Gbps technologies and Climate100—and to research, develop, and test end-to-end capabilities of the ANI tested in collaboration with the ESGF community continues [ASCR 2009, ASCR Terabit 2011, Sim 2010]. Ongoing partnerships and established relationships with a wide variety of data, research, and technology efforts (e.g., GridFTP [Allcock 2005], Globus Online [Allen 2011]) position ESGF to speed progress in climate science. Also, though ESG tools and technologies primarily benefit the climate community, they have also proved general enough to serve other scientific communities.

2.3. Technical and Legal Aspects

Data management and access includes ensuring that data is used in a legal manner. Some data must be protected from profiting agencies and groups or be protected for proprietary institutional knowledge. To guard data, the federated archive allows users to self-police by allowing them to indicate whether they are accessing data for research that is noncommercial (unrestricted use of the data) or commercial (restricted use of the data). Depending on their terms-of-use selection and the authorization access level of the data, users will be granted access. For both groups of users, the terms of use include additional legalities: users of the data will not hold individual(s), organization(s), or group(s) responsible for any errors in the models or in their output data and will appropriately credit data providers with an acknowledgment in published journals [CMIP 2011]. Technically, the security infrastructure has to reflect individual national data-access regulations as well as access constraints imposed by corresponding projects.

2.4. Data Users

Continued ESGF progress will result in a production-scale system that will empower scientists to attempt new and exciting data exchanges that could ultimately lead to breakthrough climate-science discoveries. The model joins four main physical components (atmosphere, ocean, land, sea ice). Management of the effort takes place through working groups focused on each component as well as specific application areas, including climate change and variability, chemistry and climate, biogeochemistry, and polar-climate change. The primary working groups associated with upcoming assessment reports (such as the Intergovernmental Panel on Climate Change) include Working Group I (WG I) to assess the physical scientific aspects of the climate system and climate change, Working Group II (WG II) for climate-change impacts, adaptation and vulnerability, and Working Group III (WG III) for the mitigation of climate change [IPCC 2011]. For these groups, deployed web portals (shown in Figure 1 and listed websites in Section 2) constitute the main entry points into the ESGF system and allow data users and data providers to access the full spectrum of ESGF high-level data services for publication, search, discovery, description, download, aggregation, and subsetting. In the immediate future, users will have the ability to search discover and access data directly via standalone desktop client applications.

3. Data Infrastructure

In attempting to assemble the largest-ever worldwide collection of climate science data, computational and climate scientists are coming together to work on technical challenges inherent in building a revolutionary facility with worldwide repositories as well as access systems that handle data at the exascale level. This technology is built on gateways, nodes, and associated services [Williams 2011].

3.1. Gateway Software

Multiple ESG gateways manage limited access to specified climate projects such as CMIP5, NARCCAP, AIRS, etc.). Such gateway-deployed services will include the user interface for searching and browsing

metadata, for requesting data products (including analysis and visualization tools), and in the future for orchestrating complex workflows. Because the relevant software requires considerable expertise to maintain, gateways are monitored directly by ESGF engineers. The ESGF gateway was extensively developed over the past year. Accomplishments included the major gateway releases such as the Baseline release (version 1.2.0) and the critical milestone Security release (version 1.3.0). With the Baseline release in October 2010, ESGF moved into production mode. Prior to the initial production release, in anticipation of CMIP5 data, the gateway received substantial improvements:

- Federationwide X-509 certificate and OpenID-based authorization.
- Full CMIP5 Data Reference Syntax (DRS) metadata, which provides a common naming system to be used in files, directories, metadata, and URLs to identify data sets wherever they might be located within the distributed ESGF.
- Automated Open Archives Initiative (OAI)-based federation metadata exchange using Resource Description Framework (RDF).
- Completion of basic common information model (CIM) ingestion in collaboration with NOAA/Global Interoperability Program (GIP), Earth System Curator and the U.K. METAFOR teams. This allows key data and model distinctions to be shared and understood between users of different scientific repositories.
- Streamlined gateway installation and configuration.
- Integration of MyProxyLogon WebStart application into data-download user interface.
- Capture of missing DRS attributes during the publication process.

In June 2010, ESGF upgraded the gateways to the Security release version 1.3.0. This release includes several important new features along with bug fixes:

- Upgraded Spring 3.0 Framework and Spring Security
- Improved MyProxy service for remote Globus services that stores user credentials [Novotny 2001]
- Enhanced data access and authorization workflow
- Provided a centralized gateway registry for federation support
- Improved user-registration workflow
- Integrated product service via the Live Access Server (LAS) and metrics and notification support for monitoring infrastructure usage and notifying users of data changes.
- Ability to show users the data-set version history in the user interface.

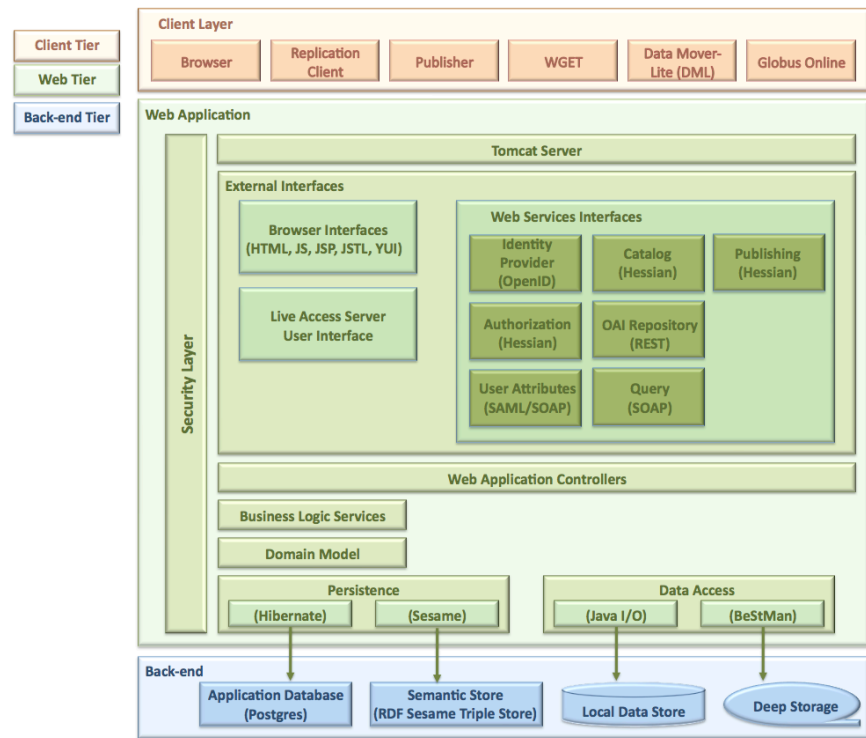


Figure 2: The gateway architecture layers

In this rapidly changing environment, the ESG-CET team has executed major overhauls of the gateway software, centralizing configuration properties outside the gateway for easier maintenance and

simplifying the customization files and improved documentation for application installation and updates. These improvements have been well received by the international ESGF community. For ESGF services provided to the end users, the gateway provides the all-important convenient, browser-based interface to data and assorted tools for analysis and visualization.

3.2. Data Node Software

Actual data holdings and the services used to access data reside on ESGF data nodes. Typically host services needed to publish data and to execute data-product requests made through a gateway that might serve data requests to many associated nodes. For example, more than 20 institutions are expected to operate nodes for the CMIP5 project. Because personnel with varying levels of expertise will operate data nodes, the software comes with exhaustive documentation and a build script for easy installation. The installation process comes in two forms: recommended (in which the data provider's name, e-mail address, institution domain name, username, and password are accepted and the system is built by using predefined and initial conditions) and custom, which gives the user complete control over the building each data-node component. There are also virtual machine versions of the data-node installation.

Collaboration with external partners such as BADC and DKRZ has accelerated and enhanced several data-node components, such as security, replication, and versioning [Kershaw 2011]. For replication, a client, shown in Figure 3, was developed to facilitate replication of data sets among ESGF mirror sites [Chervenak 2011]. This client identifies files within a data set for replication and prepares a command file for data transfer clients. After files are replicated, the replication client verifies the correctness of the scanned metadata catalog compared with that from the original publication site and publishes the replicated data set at the mirror gateway. In addition to the replication client, the data node is composed of many other software packages, web applications, and tools (see Figure 3) that work with the gateway to provide overall server-side federated functionality. The current software stack release is version 1.0.0.

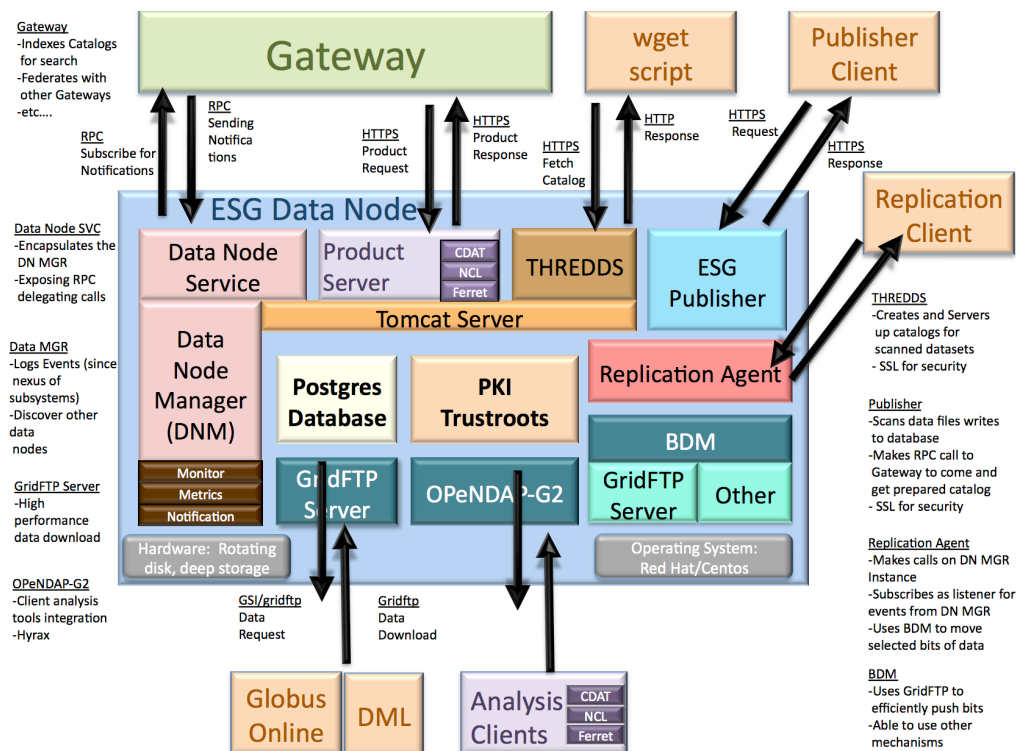


Figure 3: Architecture diagram showing the diverse, complex operations the data node performs, ESGF infrastructure To match the gateway Security release, the data node development includes several highlights:

- Simplified data node installation process. We codified the data-node installation process into an interactive script that will fully install and configure all components. Written in BASH (a Unix command shell) for portability, the script also includes flags for security management and testing.
- Revised security infrastructure for tokenless authentication through new security components such as Security Assertion Markup Language (SAML) [SAML 2011] and OpenID. The new framework uses public key encryption throughout to ensure communication and data integrity. In addition, the SAML standard is employed for information exchange among federation members.
- Secured attribute service support using SAML as the transport protocol and leveraging Yadis service. It provides secure query responses to the federated entities.
- Data reference syntax (DRS) support for file-system layout.
- Enhanced data-node metrics interface served over HTTP to show machine state. A number of aggregating interfaces provide administrators with a bird's eye view of all the machines in the system, allowing them to drill down to specific data nodes and even files, as needed.
- Stand-alone, dynamic, portable, and easy-to-use graphical user interface for publishing data to the system. It allows researchers to scan and publish large volumes of data in a single operation, thus quickly making their climate data available worldwide.
- A data-node dashboard that allows operators to monitor data nodes in real time as data are added through the Publisher. Information on disk space, CPU usage, memory, network resources, load, and peer connections are presented in a comprehensive and intuitive Web interface.

The ESGF production data services, through gateways and data nodes, span multiple domains including metadata, security, data transport, data aggregation and subsetting, usage metrics, and services monitoring. As shown in Figures 2 and 3, the cohesive integrated architecture is built in Java and Python and based on third-party software such as Globus, Tomcat servlet engine, and the Spring security framework. We are integrating the Globus Online managed data transfer service [Allen 2011] for high-speed data access, including from behind firewalls.

4. Future

ESG-CET has developed and delivered substantial community resources for the global climate- science community in time to be of use to important projects and climate assessments. We have collaborated to tackle demanding problems: new levels of metadata and knowledge handling; high-performance replication of large data; and security and virtual organization capabilities for an international federation. The current ESG-CET architecture is roughly modeled on a client-server paradigm. Multiple data nodes provide data access and computing power to execute user requests that are formulated at a central gateway. However, ESGF demands necessitate deployment of a more modern, robust, and scalable architecture because its constituency is expanding to more organizations worldwide. Also, application of the ESGF software stack to other scientific disciplines is beginning. To realize this goal, we have invested in a new ESGF architecture, envisioning a peer-to-peer system of distributed nodes. With this new model, the management of system information and the execution of data requests can be shared and spread. The distributed nodes are composed of modular, pluggable components that interact through a lightweight messaging system. They also can be easily configured to perform all functions currently entrusted separately to a data node or a gateway. The peer-to-peer node architecture is currently in the beta-test phase and is scheduled to be deployed by mid-summer.

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Participants

The ESG-CET executive committee consists of Dean N. Williams, LLNL; Ian Foster, Argonne; and Don Middleton, NCAR. The ESG-CET team is a group of researchers and scientists with diverse domain knowledge, whose home institutions include eight laboratories and two universities: Argonne, Los Alamos National Laboratory, LBNL/NERSC, LLNL/PCMDI, NASA/Jet Propulsion Laboratory, NCAR, ORNL, PMEL, NOAA, Rensselaer Polytechnic Institute, and USC's Information Sciences Institute. All ESG-CET work follows DOE open-source guidelines and is in close collaboration with the project's stakeholders, domain researchers, and scientists.

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