# The Earth System Grid Federation:

An Open Infrastructure for Access to Distributed Geospatial Data

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The Earth System Grid Federation (ESGF) is a multi-agency, international collaboration that aims at developing the software infrastructure needed to facilitate and empower the study of climate change on a global scale. The ESGF's architecture employs a system of geographically distributed peer nodes, which are independently administered yet united by the adoption of common federation protocols and application programming interfaces (APIs). The cornerstones of its interoperability are the peer-to-peer messaging that is continuously exchanged among all nodes in the federation; a shared architecture and API for search and discovery; and a security infrastructure based on industry standards (OpenID, SSL, GSI and SAML). The ESGF software is developed collaboratively across institutional boundaries and made available to the community as open source. It has now been adopted by multiple Earth science projects and allows access to petabytes of geophysical data, including the entire model output used for the next international assessment report on climate change (IPCC-AR5) and a suite of satellite observations (obs4MIPs) and reanalysis data sets (ANA4MIPs).

Keywords: Earth System Grid Federation (ESGF), peer-to-peer (P2P), Node, security, search, discovery, climate science, CMIP5.

## I. INTRODUCTION

The study of climate change, including an evaluation of its impact on Earth's ecosystem and human society, is one of the most important scientific challenges of our time. Because the physical processes governing Earth's climate are extremely

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diverse and complex, this research involves sophisticated model simulations, which generate an unprecedented amount of output data, as well as the collection of observational data from multiple sources (such as remote sensors, in situ probes, and vertical profiles) on a global scale. These data sets are managed and stored at multiple geographic locations across the globe; yet, they need to be discovered, accessed, and analyzed as if they were stored in a single centralized archive.

For over a decade, the collaborative objective has been to establish the Earth System Grid Federation (ESGF) as a leader and visionary architect for all aspects of climate data discovery and knowledge integration. From its formative years (previously known as the Earth System Grid (ESG) [1]), ESGF has demonstrated a viable path forward into the future and attracted key national and international collaborators and potential sponsors recently reaching the critical mass required to undertake fundamental data-intensive and data-driven science problems. In the climate application arena, an increasing number of projects are consolidating on the ESGF peer-to-peer (P2P) infrastructure, a next generation version of the earlier architecture, based on loosely coupled administrative relationships and light-weight protocols for unification. The new architecture allows the federation to play a stewardship role and also enables the world to better organize and integrate all climate knowledge via a cooperative federation. With that said, the ESGF P2P software has distinguished itself from other collaborative knowledge systems in the climate community, as evidenced by its widespread adoption, federation capabilities, and broad developer base. It is the leading source for current climate data holdings, including the most important and largest data sets in the global-climate community.

Through ESGF, users access, analyze, and visualize data using a globally federated collection of networks, computers, and software. In addition, an enterprise system was adopted to support international intercomparison activities of climate models and observations as well as high-profile projects involving such organizations as the Department of Energy (DOE), the National Oceanic and Atmospheric Administration (NOAA), the National Aeronautics and Space Administration (NASA), and the National Science Foundation (NSF).

#### II. ARCHITECTURE

ESGF is based on a distributed and federated software architecture (see Figure 1). The system is composed of multiple sites (called "Nodes") that are geographically distributed around the world, but can interoperate because they have adopted a common set of services, protocols and APIs. Data and metadata are managed and stored independently at each Node; yet, clients can access them as if they were held on a single global archive. Nodes can join or leave the federation dynamically, and the services and holdings that are discoverable and accessible by clients will automatically change to reflect the latest state of the system.

Internally, each ESGF Node is composed of a set of services and applications that collectively enable data and metadata access and user management (see Figure 2). The software stack includes components that were developed directly by ESGF (e.g., the Publishing program, many of the data and metadata web services, and the web portal user interface), as well as open-source, third-party applications that are commonly used in industry (Postgres, Tomcat, Solr), eScience (MyProxy, GridFTP) and the geospatial community (THREDDS, Live Access Server (LAS)). These components are logically grouped in four areas of functionality, which determine the Node "flavors" (color coded in Figures 1 and 2):

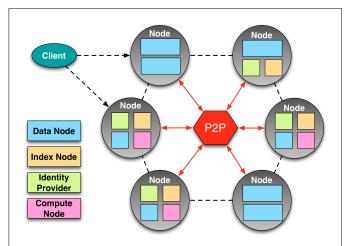


Figure 1. Schematic representation of the Earth System Grid Federation (ESGF) as a system of Nodes hosting services of four possible "flavors". Nodes continually exchange messages with each other through the peer-to-peer (P2P) protocol (here pictured as the central core of the system). A client can query any Node to access data and metadata throughout the federation.

- The <u>Data Node</u> (blue color, Figure 2) includes services for secure data publication and access. Its main components are the data Publisher application that generates the metadata catalogs, the THREDDS and GridFTP servers (with security filters at the front end) to serve the data, and the OpenID Relying Party and Authorization Service to ensure proper authentication and authorization.
- The <u>Index Node</u> (tan color, Figure 2) contains services for indexing and searching metadata, currently implemented using Apache Solr as the back-end server. The Web Portal application provides a convenient browser-based interface for system users and administrators, while the Dashboard contains utilities that monitor and report on the state of the federation. The Common Information Model (CIM) Viewer is a plugin component that retrieves and displays model metadata from CIM repository sources.
- The <u>Identity Provider</u> (light green color, Figure 2) allows user authentication and secure delivery of user attributes. It includes an OpenID Provider for browser-based authentication, a MyProxy server for requesting limited-lifetime user certificates, and Registration and Attribute Services for distributed access control.
- The <u>Compute Node</u> (purple color, Figure 2) contains higher-level services for data analysis and visualization. Currently its only components are the Live Access Server, the Ferret-THREDDS Data Server and the Ferret engine. More analysis engines (e.g., Ultra-scale Visualization Climate Data Analysis Tools (UV-CDAT)) are to be added in the near future.

Additionally, each of these flavors always includes the Node Manager, a web application that allows a Node to continually exchange service and state information with all its peers throughout the federation. Each Node can be configured during installation to have one, more, or all of the flavors, depending on the site specific needs. Furthermore, a site can combine multiple Nodes configured for different flavors, to

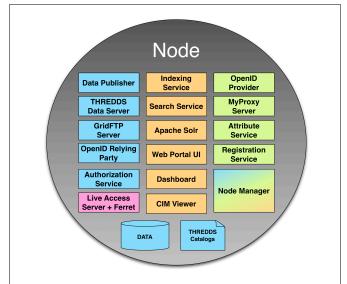


Figure 2. Software components that may be deployed onto an ESGF Node, grouped by "flavor" or area of functionality.

achieve higher performance and availability. For example, a common practice is to deploy the Index Node and Identity Provider services on one server, while keeping the Data and Compute Node services on one or more separate servers, e.g., for performance considerations.

ESGF Nodes interoperate through a set of common federation services and mutual trust relationships. A user who registers at any site can authenticate (via OpenID or a shortlived user certificate) across the entire federation because the other Nodes trust the original Identity Provider. A metadata search initiated at any Node will be distributed to all the other Nodes, and the search results will be merged before they are presented to the user. When data is accessed from a specific Node, the local Authorization Service will query the appropriate Attribute Services across the federation, to determine whether the user has been granted the necessary permissions to satisfy the local access control policies. The list of trusted Identity Providers, their Certificate Authorities, the target search Indexes, and the location of the Attribute Services are continually updated at each Node through the peer-to-peer messaging executed by the Node Manager. The net result of this setup is that a client (web browser or desktop application) can query any Node to investigate and access data and metadata holdings distributed throughout the federation.

# III. THE ESGF SOFTWARE STACK

ESGF software components are developed collaboratively by many institutions worldwide, which are funded by different agencies and programs. For the U.S., the DOE Office of Science is the lead funding agency. The software is made freely available on the ESGF github web site (http://esgf.org/gitweb, soon to be replicated to https://github.com/ESGF) under the Open Source BSD license, and it is documented for users, administrators and developers on the ESGF collaboration site (http://www.esgf.org/). The general development philosophy is to build modular components that interact with each other and with outside clients through well-defined interfaces, so that different implementations could be plugged into the system, possibly written in different computing languages (Java, Python, etc.). When possible, ESGF uses existing standards from industry (e.g., OpenID, SSL, SAML) or the geospatial community (e.g., NetCDF, CF, OPeNDAP) to maximize interoperability with other systems. Popular, freely available application servers such as Tomcat, Solr, THREDDS and LAS are integrated into the stack to avoid re-implementing a specific piece of functionality.

In this section, we describe in more detail the major components of the ESGF software stack.

# A. The Node Manager

The Node Manager is the primary coordinating software component that manages the local ESGF Node and maintains the federation's cohesion. It is an event-driven system composed of 'components' that comprise a SEDA [2] inspired *finite-state machine* (FSM). Events are routed through an arrangement of components and are transformed as they travese the FSM from start state (ingress) to end state (egress). The main components of the Node Manager implement the discovery and information dissemination protocol that keeps the federation connected and they provide the necessary routing

information used by higher-level Node services. The Node Manager is also responsible for collecting current system *health* information - i.e., system metrics - and monitoring information such as cpu, memory, and up-time information as well as quantitative information on a local Node's data holdings. The Node Manager implements *intra*-node message passing through its internal components and enables *inter*-node message passing by way of its peer-to-peer protocol implementation.

# B. The Peer-To-Peer Protocol

A key feature of ESGF is the ability for Nodes to discover each other and therefore create a single federated *dataspace* [3] that spans all participating ESGF Nodes. The resultant overlay mesh network created by the ESGF protocol allows users to interact with this singular dataspace to seamlessly query and access data. At its core, the protocol is a gossip protocol [4] with two primary purposes: as the discovery mechanism allowing Nodes to learn about each other in an unsupervised way, and as the anti-entropy [4] protocol that maintains a distributed 'database' of currently federated, participating nodes. The implementation of the gossip protocol in ESGF follows the push model [4]. Each Node views the federation as a list of other Nodes it is authorized to access, which is essentially the 'database' maintained via the anti-entropy protocol. This list is encapsulated and sent as payload within a remote event that is forwarded to peer Nodes. Nodes receive remote events and inspect the payload information. The payload is then integrated with the receiving Node's internal list, and that new list is pushed randomly to two other peer Nodes. Nodes propagate state information directly after receiving an ingress remote event. Each Node initially creates a list with a single list entry containing its own time-stamped information. As ingress events are encountered, the introduced list is merged with the local list like a vector clock [5], maximally by time.

A gossip protocol was chosen because of its simplicity, scalability, robustness and reliability "even in the most demanding settings" [6]. ESGF leverages the gossip protocol's fault tolerance to create a fully connected overlay mesh network of Nodes with no single point of failure. The federation may be partitioned into groups, and a Node may participate in any number of groups. Each group must contain at least one Identity Provider Node to service the security needs of the group's users. Each Node is bootstrapped with a prior knowledge of at least one default peer. Nodes maintain an eventually consistent data store of all the Nodes in the union of the peer groups they are members of.

Several protocol optimizations are being studied, including tuning fanout [7] and frequency and taking advantage of a push-pull interaction between Nodes. Our ultimate goal is to optimally decrease database convergence time and network overhead..

# C. Data Preparation and Publishing

The Publisher application is a Python package that is responsible for scanning data stored on a Data Node and making it available through the system. The program, which can be run from the command line or from a graphical user interface (GUI), can extract metadata from both the directory structure and filenames, and from the content of the files

themselves. Files are grouped in logical collections named *data* sets according to project-specific rules in the relevant configuration file. All information is stored in a local Postgres database and is used to generate THREDDS/XML catalogs. These catalogs contain the descriptive metadata and the URL pointers to access the data through all available protocols (e.g., HTTP, GridFTP). The THREDDS Data Server (TDS) and Live Access Server (LAS) use these catalogs to deliver data to clients for download, analysis, and visualization.

The Publisher contains prebuilt *handlers* for processing data that are stored in NetCDF format and follow the Climate and Forecast (CF) convention, a prescription for encoding richer metadata. Most of the projects that ESGF has focused on to-date mandate that data be stored as NetCDF/CF (e.g., CMIP5, obs4MIPs, ANA4MIPs). Nevertheless, the Publisher package is extensible, and custom handlers can be plugged-in to parse data that are stored in other formats or are organized on disk according to other specific directory structures.

#### D. Search Services

The ESGF search module, deployed as part of an ESGF Index Node, is responsible for making the data holdings of one or more ESGF Data Nodes discoverable and accessible by clients. Its two main features are the ability to execute distributed searches across the federation, and the support for a well-defined REpresentational State Transfer (REST) [8] API that insulates clients from the specific query syntax of the back-end metadata repository. Although the software allows for pluggable back-ends, it currently uses Apache Solr as the underlying search engine. Solr is a popular web application which is used in many commercial web sites, featuring high-performance text and faceted searching, geospatial and temporal querying, and partition of searchable metadata across multiple local indexes (cores) and distributed servers (shards).

The search module makes two high-level web services available to clients:

- The <u>Indexing Service</u> parses the metadata content available at some repository (located by its URL), and ingests it in the back-end metadata storage. To-date ESGF has focused primarily on parsing metadata from THREDDS catalogs, but support for other repositories such as GCMD archives is forthcoming. Indexing operations are subject to authorization according to the local policies established at the Index Node: the client must present a valid certificate belonging to a user that has been granted publishing rights for that specific data collection.
- The <u>Search Service</u> queries the index metadata content and retrieves matching results that include descriptive information as well as all the available data access points (e.g., HTTP, GridFTP, OPeNDAP, and LAS). The search service is invoked by clients through a REST API that includes the ability to execute free-text queries (e.g. "climate", or "surface temperature"), and to search for specific values of one or more search categories (e.g. "model = CESM and time frequency = monthly"). Among its many features, the API allows clients to search for either the latest or a specific version of the data as well as

for its replicas, plus it can target the local index only or any number of remote indexes. Response documents can be returned in either XML or JSON format.

Internally, the search module partitions its metadata space into different object types, which are stored and queried separately – a strategy we employed to optimize performance. Data sets are the unit of discovery in the system, since they contain high-level information about a collection (such as the model that generated the data, the instrument that collected it, or the collection's temporal and geospatial coverage). As such, data sets are typically returned as results matching a query. Files and aggregations represent the content of data sets, and contain the URL endpoints of all services that clients can use to access the data. Typically, a single data set contains many files and/or aggregations, so searching for datasets is much faster.

Within Solr, each object type is stored in a dedicated "core" or index, which is separately updated and queried. Additionally, the Solr setup at each Node is such that metadata is indexed into a *master* Solr instance, which is only accessible locally. The master is replicated at one-minute intervals to a *slave* Solr instance, which is accessible in a read-only fashion.

## E. Security Infrastructure

The ESGF security infrastructure [9] restricts resource access to users who have been granted the necessary permissions and it manages trust between participating parties across the federation. Permissions can be set at various levels of granularity, for example, authorizing a specific user to publish metadata to an Index Node, download specific data sets from a Data Node, or manage user permissions through a Node administrative web interface. A typical use case might limit access to a specific data collection to only those users who have subscribed to a license agreement (such as the CMIP5 Research or Commercial licenses). Other collections might be limited to a particular research group and not intended for public consumption. ESGF security allows Node administrators to maintain complete control over the local resources, while enabling federation-wide services such as single sign-on and distributed access control. This security framework is accomplished through a set of trusted Identity Providers and Certificate Authorities.

ESGF enables users and applications to authenticate through two different mechanisms. The OpenID protocol is used by humans accessing the system through a web browser. When users enter their OpenID at any Node in the federation, they are redirected to their Identity Provider (the Node where they registered), where they can sign-in using the mechanism enforced by that Provider (for example, username and password). Once authenticated, the user is redirected back to the original Node. X.509 certificates are used by programs (such as wget scripts or GridFTP) to act on behalf of a user. Before executing the program, the user requests a shortlifetime certificate from a MyProxy server that is linked to the user's Identity Provider, and thus to the user's OpenID identity. The certificate contains the user's identity and permissions, and it will be honored by all Nodes in the federation that trust the Identity Provider.

ESGF authorization is based on security policies, defined by each Node administrator, that match local to the groups and roles that are allowed to execute specific operations. Users from any site can request membership in one or more access groups (e.g., the "CMIP5 Research" or "NASA OBS" group). In addition, they are assigned one or more roles within each group (e.g., "user", "admin", or "super"). Groups may be managed by any Identity Provider in the federation, and the user attributes are made available to trusted clients through the Node's Attribute Service. When authorization is required, the local Authorization Service enforces the Node security policies by querying the particular Attribute Service in the federation that manages the configured access control group. For example, any Data Node participating in CMIP5 allows users to access the data if they have enrolled in the group "CMIP5 Research" that is administered by the Lawrence Livermore National Laboratory (LLNL) Identity Provider.

Because ESGF security is based on standards (OpenID, SSL, SAML), the security components can interoperate with trusted components from other software stacks that are based on the same standards. For example, a Java-based ESGF Authorization Service can request and consume user attributes from a remote Attribute Service part of a Python software stack, because the entire communication is encoded as SAML/XML documents that have been digitally signed. Similarly, users can authenticate throughout the federation via their OpenID, no matter what the underlying OpenID client and server implementations.

One additional benefit entailed by the pervasive security infrastructure is the ability to log detailed metrics about user requests (i.e., linking each action to a specific user identity). Currently, metrics are collected on a Data Node whenever a user initiates a data download, and then aggregated across Nodes to provide federation-wide statistics. This information can be used to push notifications about data updates and retractions. In the future, logging could be expanded to track other usage of the system such as data searches and administrative actions. Logging has also been used to hold users accountable for intentional or unintentional misuse of the system, such as for example massive data requests resulting in effective denial of service events.

# F. Web Portal User Interface

A key goal of the current ESGF development effort is to provide an intuitive, easy-to-use web portal. To this end, ESGF has adopted a modern design inspired by emerging Web 2.0 technologies. The portal makes heavy use of the state-of-the-art JQuery JavaScript libraries and Model-View-Controller (MVC) design patterns. The user interface (UI) also conforms to the overall ESGF philosophy of decoupled software components that accommodate a more dynamic user experience. Services of other components (e.g. search and node manager components) may be utilized via Ajax-style HTTP calls. The web UI materializes a variety of ESGF-supported services through the browser: administrative and user account management interfaces, collection and file-level search and discovery, the dashboard service, the LAS visualization engine, and the CIM viewer. The first two

features are briefly described in this section, the others later on in this paper.

The *user account and administrative component* delivers a clear, concise means for users and administrators to manage personal information and security aspects of the portal. Users may view and edit personal attributes and apply for group memberships that grant access to restricted data. Administrators are provided with tools that interface to the security infrastructure services allowing them to authorize group access to specific data holdings.

Search and discovery mechanisms are presented to the user via the search component of the web portal (see Figure 3). The search component is presented as a single composite page, which eliminates the clumsy "back-and-forth" navigation offered by static pages. Initially, a user may search the data holdings at the *collection* level. Here, the user has many search options. The sidebar widget on the left side of the page presents a configurable list of facets, which allow users to constrain their search results through categorization. Search constraints can also be added via the free text search bar. Furthermore, users may take advantage of the temporal and geospatial (based on Google Maps) search overlay widgets by searching for data measured or simulated at specific times or in specific geographical locations, respectively. The state of the search (i.e. the current constraints applied by the user) is shown prominently in the upper left corner of the page and may be changed at any time. Important information about the results is viewed through the portal search component.

Each data set contains a comprehensive metadata summary outlining descriptive information about the data set. The CIM viewer, which provides richer and more detailed metadata about climate models, may also be invoked. Additional information associated with a data set, such as a technical report, may also be accessed. Finally, the LAS browser visualization tool may be invoked to visualize details of the data sets. For file access, the search component uses a "shopping cart" approach commonly deployed by e-commerce sites. The user needs only to select a collection-level data set (via the "Add to Cart" link) and navigate to the "Data Cart"



Figure 3. The ESGF web portal exposes a friendly user interface for searching, including the capability to specify free text, facet options, and geospatial and temporal constraintss.

tab. The collections previously chosen are displayed in this tab and may be quickly expanded to their *file*-level data holdings. These files may then be downloaded using different methods, which are discussed in the next section.

#### G. Data Access

By default, every Data Node is configured to serve data through the following access types:

- <u>Direct browser</u> access is provided by the TDS and allows users to download files via simple HTTP hyperlinks.
- <u>OPeNDAP</u> access is also provided by the TDS. The Open Data Access Protocol provides an abstraction level on top of the files allowing users to tailor data selection by variable, temporal or geospatial coverage. ESGF provides aggregations for variables that are normally split in files of no more than 2 GB to simplify access.
- Wget Scripts, contrary to other access mechanisms, are not tied to the Data Node hosting the data, but to an Index Node implementing the search API, which was extended to return a BASH script that simplifies data retrieval. The user can thus access any file in the federation without knowing where the file is stored or even what it is named. The script encapsulates calls to the wget utility—hence the name—and adds functionality such as: certificate verification, retrieval and renewal; download continuation, verification via MD5 checksums and verification results caching; download structure generation via the facets results; file overflow check (if the query resulted in a set of files larger than the maximum number allowed per script); and script auto-update and remote file changes check.
- <u>GridFTP</u> access uses a special protocol based on FTP to allow for a high-performance, securly authenticated, and reliable data transfer. Within ESGF, the most common use of GridFTP is for data replication, where bulk data is replicated across Nodes. This feature requires higher access permissions for the user, including write access to the ESGF Data Node, and typically is restricted to administrators.

Furthermore, a Data Node can be configured to allow other optional data access methods:

- Globus Online [10] is a hosted service that provides reliable and managed file-transfer capabilities over GridFTP. The web portal component includes a preliminary integration with Globus Online. A user can choose to have Globus Online either transfer the items in their data cart to another server or download them to their local machines. Users must install Globus Connect on their machines to upload and download data locally.
- The <u>Live Access Server</u> (LAS) is a highly configurable, freely available open source web application that allows users to visualize and compare data on-the-fly, perform basic analysis, and download results in various file formats. New capabilities were implemented for reading THREDDS catalogs, managing the data selection UI for large collections, and generating distributed products to ensure a seamless and efficient integration of LAS into the ESGF software stack. In general, LAS can create the configuration it needs directly from THREDDS catalogs and the underlying NetCDF data sources. However, within ESGF, LAS was enhanced to build its configuration

from the enhanced metadata in the THREDDS catalogs that are generated by the Publisher application. Search interface tools allow the user to quickly identify and select the data sets of interest. Once a set is selected and the user has transitioned to LAS, the LAS UI limits the available data sets to those preselected in the browsing session from the ESGF search interface. In this way, the user is not overwhelmed with tens of thousands of data sets while performing advanced visualization and analysis on the data of interest.

#### H. Dashboard

The Dashboard is the distributed monitoring system of ESGF. It is responsible for collecting historical information about the status of the federation in terms of:

- *Network topology* (peer-groups composition)
- *Node type* (host/services mapping)
- Registered users (including their Identity Providers)
- Downloaded data (both at the Node and federation level)
- *System metrics* (e.g., round-trip time, service availability, CPU, memory, disk, processes, etc.)

From an architectural viewpoint, the ESGF Dashboard is composed of the following three parts: the information provider, the dashboard catalog, and the user interface.

The *information provider* represents the system's backend and is responsible for retrieving and storing all peer-to-peer metrics. The information provider strongly interacts with the node manager to synchronously retrieve updated snapshots of the federation's status and stores them in the dashboard catalog. This module can easily be extended to collect new metrics, by implementing additional sensors associated to new classes of information.

The *dashboard catalog* is a temporal database (running on top of a Postgresql RDBMS) used by the information provider to persistently store the five classes of information previously mentioned. It manages historical information with a *per-site* and *per-metric* configurable time-window.

Finally, the user interface (see Figure 4) is a web



Figure 4. The dashboard screen indicating location, composition and status of all nodes in the "esgf-prod" peer group.

application that exploits the MVC design pattern. It relies on strong adoption and implementation of Web 2.0 concepts such as mash-up, Google maps and permalinks. It provides several views at four different (hierarchical) granularity levels: federation, peer-group, host and service. These views provide charts and summaries about the service availability, the round trip time between pairs of nodes, the host status, and other information. The views, which can be customized (at the presentation level) by the end user, are delivered in different ways (charts, tables) and formats (XML, CSV, JSON), and can be easily exported (both with and without authentication) in other web-applications, by exploiting the permalink feature implemented into the Dashboard module.

# I. CIM Viewer

The Metafor Common Information Model (CIM) [11][12] is an ontology designed to become the standard for climate modeling related metadata. The CIM software eco-system is composed of several applications and services that collectively support a wide range of functionality: the ontology itself; validation; search; dissemination; and integration with other platforms such as the ESGF web front-end. For example, the CMIP5 questionnaire is a web based interactive tool for creating CIM documents describing climate models that contribute to CMIP5, and captures information about how those climate models were set up to run simulations for CMIP5 experiments. The CIM web services backend was implemented according to the Service Orientated Architecture (SOA) paradigm using the Python language, and following a REST architectural design. The web services support a diverse array of CIM resources, including documents, validation reports, queries, identifiers, and controlled vocabularies. The lightweight Javascript CIM Document Plugin Viewer is a platform independent web-based client used to display CIM documents from within a generic portal environment, such as for example the ESGF web portal. Currently it provides the basic capability to display one CIM document at a time. It will be extended with more advanced capabilities to take information from multiple CIM documents and merge them together into a cohesive and meaningful presentation.

# IV. EXAMPLE USE CASE

A typical use case scenario that exercises the ESGF system is that of a climate scientist who wishes to analyze the predicted change in some physical field (for example, the "Sea Surface Temperature") in the next 20 years under different emission scenarios. The scientist would start his workflow at any of the ESGF P2P Nodes, and use the search interface to select monthly average data sets from the CMIP5 project that contain the field in question. Because of the distributed nature of the system, the search results would contain data sets that are stored across four continents and tens of Data Nodes. To reduce the number of results returned, the scientist could additionally select a specific model (e.g., "GFDL-ESM2M") and/or a specific emission scenario (e.g., "1% CO2 increase"). Each data set result would contain a link to the LAS server, which the scientist could click to visualize the field over the surface of the Earth, or create a line plot versus time, latitude or

longitude. Another link would display the detailed metadata describing both the model and the experiment that were used to generate the output. Once the scientist decided that he indeed located data relevant to his research, he could either download the files from the browser interface (if only a few), or click on the "wget" link to generate a script that he would run on his desktop to download all the files at once. At this point, he would be able to use his analysis package of choice (e.g., UV-CDAT, IDL, MatLab etc.) to take a more in-depth look at the data. Later, the scientist might decide to expand his analysis to include more models and/or scenarios. Instead of clicking many times on the browser UI, he could leverage the ESGF back-end web services to write a simple program that loops over all the models and experiments, generating constrained URLs that can be invoked to obtain the wget scripts programmatically. Additionally, the scientist could decide to compare the model predictions to the current available observations. To do so, he would just need to execute a new search that contained the exact same parameters, but requested data from the obs4MIPs project. The observational data sets could be downloaded, visualized and analyzed just like the model output.

Overall, this example use case shows how the ESGF system enables unprecedented capabilities for scientists to discover and access data, which were either completely unavailable before, or would have taken weeks if not months to perform across disparate and disconnected systems.

# V. APPLICATION AND OPERATION

From the beginning, the primary focus of ESGF has been to provide the IT infrastructure in suport of CMIP5, the Climate Model Intercomparison Project, phase 5. CMIP5 is a global effort coordinated by the World Climate Research Programme (WCRP) that involves tens of modeling groups spanning 19 countries. CMIP5 designed several decadal and century experiments that all models run to assess the future state of the Earth's climate and ecosystem and to understand the complex processes in play during simulated changing climate. These experiments include economic and human development scenarios, Green House Gases emissions and/or concentrations, idealized experiments, and quantifying the predictability of the climate system at the decadal scale. When completed, the CMIP5 data archive will total upwards of 3.5 petabytes, stored across 15 Nodes on four continents (North America, Europe, Asia, and Australia). In order to facilitate access and to secure the long-term preservation of this invaluable data store, ESGF plans to replicate 1.5 - 2 petabytes of data at five major data centers: LLNL (U.S.), BADC (U.K), DKRZ (Germany), ANU (Australia), and the University of Tokyo (Japan).

Alongside the CMIP5 model output, ESGF provides access to the <u>obs4MIPs</u> data sets. These are satellite observations from several NASA missions that have been purposedly formatted to allow easy comparison with models: they have been converted from the original HDF/EOS format to NetCDF/CF, averaged as monthly means, and regridded over global grids from the original satellite swaths. In addition, the system provides access to scientific Technical Notes, authored by the data processing engineering teams in collaboration with the mission scientists. These Technical Notes contain invaluable information on how to use the observations for comparing and validating models.

obs4MIPs also includes the CFMIP-OBS data set, which contains observational data and diagnostics about clouds and cloud-related processes. These data can be of great value for climate prediction over a wide-range of space and time scales: for numerical weather predictions, for climate prediction at seasonal to decadal timescales, and for the prediction of the long-term climate response to anthropogenic perturbations at the global and regional scales. This stems from the strong interaction of clouds with the global Earth's radiation balance, the local energy balance, the atmospheric circulation and the hydrological cycle.

Another such effort in support of CMIP5 is <u>ANA4MIPs</u>, which allows users to find and download reanalysis data via ESGF. Through reanalysis climate scientists are continually updating gridded data sets that represent the state of the Earth's atmosphere and incorporating weather observations and numerical output of weather predictions. To enhance climate science resources, five participating reanalysis institutions have agreed to host the following primary reanalysis data sets on ESGF Nodes: (1) MERRA (NASA/GSFC), (2) CFSR (NOAA/NCEP), (3) Interim (ECMWF), (4) 25 (JMA), and (5) 20CR (NOAA/ESRL). These reanalysis data will be translatted to the NetCDF/CF format for greater CMIP5 compatability.

Additionally, CMIP5 has become the benchmark standard that other similiar Earth science projects have leveraged in order to make their data accessible to users under a distributed and integrated infrastructure. Some of the most prominent examples are:

- <u>CORDEX</u>: The COordinated Regional climate
   Downscaling EXperiment is a WCRP-sponsored program
   aimed at producing an improved projection of regional
   climate change worldwide for input into impact and
   adaptation studies. CORDEX will use the multiple forcings general circulation models (GCMs) from the
   CMIP5 archive to generate an ensemble of dynamic and
   statistical downscaling models. The amount of data
   managed by the system is expected to be comparable to
   that of CMIP5.
- <u>TAMIP</u>: Transposed-AMIP is a WCRP endorsed activity to run climate models in weather-forecast mode. This activity will primarily focus on analyzing the accuracy of climate models by comparing hindcasts run by those models with observational data.
- GeoMIP: The Geoengineering Model Intercomparison Project is a WCRP-endorsed project aimed at analyzing the effects of manipulating an environmental processes by implementing one or more large-scale geoengineering technologies.
- PMIP: The Paleoclimate Model Intercomparison Project is a WCRP endorsed project designed to evaluate how accurately climate models reproduce climate states that are radically different from those of today. The third phase of this project (PMIP3) shared some experiments with CMIP5 but proposes an additional set of paleo-climate experiments.
- <u>LUCID</u>: The Land-Use and Climate Identification of robust impacts project explores how robust hanges in land cover—that is, those above the noise generated by model variability—affect model output.

All these projects rely, at least partially, on the CMIP5 archive. By providing their results over the same platform they guarantee that users can find, use, and share their data in a standardized manner, thus minimizing the amount of time employed in non-core activities.

Other non-CMIP5 projects that leverage ESGF include:

- <u>CSSEF</u>: Sponsored by DOE's Office of Science, the Climate Science for a Sustainable Energy Future project is developing a new climate-modeling methodology to reduce uncertainty through the provision of a test bed.
- <u>CMDS</u>: The Coastal Marine Discovery Service is a NASA-sponsored activity aimed at providing Global Information System visualization capabilities for prominent OPeNDAP-accessible oceanic data sets.

#### VI. USABILITY, PERFORMANCE AND RELIABILITY

At the time of this writing, the ESGF P2P system has been under development for approximately two years, and deployed operationally for several months – first opened only to early adopters, more recently to the community at large.

Users have in general been very appreciative of the new system, praising the responsiveness, completeness and consistency of the search results across Nodes in the federation. In particular, the so called "power-users" are making extensive use of the back-end search services that allow them to query and generate data download scripts programmatically for different sets of constraint parameters. Other facilities such as the LAS, the CIM Metadata Viewer, and the Dashboard are providing users and administrators with functionality that simply did not exist before.

One early problem detected on the system was the excessive memory usage of the TDS when indexing very large collections of thousands of catalogs, which made the data download services unavailable for long periods of time. This problem seems to have been solved with the latest TDS release. Other aspects of the system that demanded particular attention, but has become progressively more reliable as the system evolved, include the coordinated installation of the several software components, the federated security infrastructure, and the client-side support for data download (i.e., the wget scripts, which must be made to work on a large variety of user operating systems).

Because the system is globally distributed, software integration and updates can be challenging. Time zone coordination across modeling and data centers must be done with the upmost care, as to not disrupt or hinder the scientific community from their research activities. These changes in the system mandate a commitment to backward compatibility for all federated services, as the typical lag time for an update across all Nodes in the federation may span several weeks. It also requires a careful job of testing and documenting each release—a process that admittedly is still under improvement today.

# VII. COMPARISON WITH EXISTING SYSTEMS

The ESGF P2P infrastructure is only one of many systems, currently operational throughout the world, that are devoted to enable web-based access to scientific data. Many of these

systems have great merits, offering functionality that partially overlaps and sometimes extends that of ESGF. However, ESGF certainly stands out for its federation capabilities, size of data holdings, broad developer base, extended adoption, and most notable data holdings (i.e., CMIP5, obs4MIPs, ANA4MIPs).

A few of the most noticeable examples of other science data systems include:

- The NASA <u>Global Change Master Directory</u> (GCMD) is a well-established clearinghouse for geo-scientific metadata records based on the popular DIF metadata standard.
- The <u>British Atmospheric Data Center</u> (BADC) is a Python-based infrastructure that shares many technologies with ESGF, and is interoperable based on common APIs and trust relations.
- The <u>NOMADS</u> network of NOAA sites is serving a plethora of heterogeneous Earth datasets via TDS servers and OpenDAP, sometimes enhanced by a Live Access Server.
- The USGS Geo Data Portal provides access to climate datasets and derivative products through standard OGC protocols.
- The Mercury system is a web portal deployed at ORNL that provides extensive metadata capabilities and data access for DOE observations and models.
- The <u>Planetary Data System</u> (PDS) is deployed at NASA and other international Space centers, is based on a federation model similar to ESGF, and uses some of the same search technology such as Solr.
- The <u>Regional Climate Model Evaluation System</u> (RCMES) provides a common data model for accessing model and observational climate datasets at regional scale.

All these systems were developed largely independently based on different sources of funding, and to fulfill specific institutional and science domain requirements. Despite its current fragmentation, the geo-informatics community is realizing the need for a cohesive approach and increased interoperability to meet the challenges of globalization and ever-increasing data volumes. For long-term survival of ESGF, collaborations with many of these groups and others are well underway. Primarily engagement of all interested parties include an open software engineering process that will promote the definition of common APIs, the adoption of re-usable and modular software components, and the expanding suite of capabilities (e.g., Machine learning, visualization, graph analysis, etc.) available to all science communities.

# VIII. FUTURE DIRECTIONS

Many challenges remain for climate scientists, and new ones will emerge as more and more data pour in from climate simulations run on ever-increasing high-performance computing (HPC) platforms and from increasingly powerful, higher-resolution satellites and instruments. From these current and future challenges, ESGF envisions a scientific data universe in which data creation, collection, documentation, analysis, preservation, and dissemination are expanded not just to benefit the geoscience community, but also for other scientific domains, such as biology, chemistry, energy, fusion, and materials. By combining with other disciplines, ESGF

seeks to strengthen the entire scientific community with advances that will be beneficial for all. In addition to our trademark advances in data preparation, search and discovery, data access, security, and federation—as mentioned in this paper—we will focus our efforts on expanding into the new areas of data mining, provenance and metadata, workflows, HPC, data movement, and data ontology. Furthermore, we intend to fully explore the possibility of providing a configurable and scalable ESGF environment that can be easily deployed on the Cloud, so that resources and services can be instantiated on demand for specific short-lifetime projects, or to meet other requirements such as high availability, extended storage, and elastic allocation of computing processes. As future computing platforms, satellites, and instruments expand and reach extraordinary speeds and levels, we anticipate that in the coming decade ESGF software will migrate from managing petabytes to zettabytes of federated data. To prepare for such an expansion—with continual delivery of a comprehensive end-to-end solution for the overall increase in scientific productivity—ESGF is also partnering with private industry in an effort to make substantial investments in data-driven software and technologies paramount for future computing platforms and ultrascale data archives.

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