

Intelligent Data Networking for the Earth System Science Community

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Abstract

Earth system science (ESS) research is generally very data intense. To enable detailed discovery and transparent access of the data stored in heterogeneous and organisationally separated data centres common data and metadata community interfaces are needed. This paper describes the development of a coherent data discovery and data access infrastructure for the ESS community in Germany. To comprehensively and consistently describe the characteristics of geographic data, required for their discovery (discovery metadata) and for their usage (use metadata) the ISO standard 19115 is adopted. Webservice technology is used to hide the details of heterogeneous data access mechanisms and preprocessing implementations. The commitment to international standards and the modular character of the approach facilitates the expandability of the infrastructure as well as the interoperability with international partners and other communities.

1 Motivation and Overview

Earth system science (ESS) research strongly depends on analysis and comparison of data. These data, resulting from observations or modelling studies, are distributed over many archives and databases. They vary highly in quality as well as in accessibility. Some of them are precisely described by corresponding metadata whereas others are described only insufficiently or not at all. Moreover the applied underlying metadata schemas and access mechanisms are heterogeneous. For these reasons, searching, finding and retrieving scientific data is often highly inefficient.

Typical scientific workflows are based on data assimilation, data validation and (model inter-)comparison studies. They often require selections of and combinations across the available distributed data sets. That is, only few variables, or spatial or temporal parts of the data are required by the scientists, usually supplemented by statistical or coordinate transformations. To extract the desired information, huge amounts of data stored across multiple data sets need

to be touched, requiring adequate tools and fast storage facilities. The analysis results could often be reused, if they were properly annotated with metadata.

Thus, the following key requirements on data discovery, access and processing in ESS can be identified:

uniform data discovery: the discovery of heterogeneous data products requires standardised data descriptions (metadata) or mechanisms to translate and correlate different annotations (metadata schemas).

uniform data access: the diversity of the existing data access solutions needs to be bridged, either by uniform access interfaces implemented at the data providers or by mediators, enabling a central access point to map data requests to the local access mechanisms.

configurable preprocessing: to reduce the amount of data which has to be transferred, preprocessing should be addressable as part of the data access functionality.

The German C3Grid (Collaborative Climate Community Data and Processing Grid, [7]) project addresses these problems by adopting and implementing a common metadata description format on the one hand; and by defining a uniform and intelligent data access interface, including transparent preprocessing functionalities on the other hand.

The design and implementation of a first working prototype are outlined in section 2 along with a short summary of related work. The metadata handling aspect is described in 3. Section 4 presents the intelligent data access interface and the preprocessing functionalities. The potential interoperability options and expandability of the system are discussed in section 5 and first experiences of an interface to the European grid infrastructure EGEE [4] are reported. Section 6 summarises, concludes and provides an outlook on future steps.

2 C3Grid overview and related work

The C3Grid project is a community driven project, which aims to ease the daily work of ES scientists. For this purpose an infrastructure is build up to improve the effectiveness of collaborative data analysis, i.e. data discovery, retrieval, processing and archiving. A community portal is set up as central entrance point for transparent discovery and access of data stored at the different German ESS data centres (e.g. the world data centres WDC-Mare, WDC-Climate, WDC-RSAT, the DWD Germany's National Meteorological Service, or the DKRZ's flat file archive). The conceptual strategy to realise the uniform data discovery and access is illustrated in figure 1. Univocal metadata in a iso-standardised format provided by the data providers are harvested to a common metadata repository (A in figure 1). This enables data discovery across data products from heterogeneous data sources. A well-defined data access interface is implemented at each data provider to realise transparent data access and to enable triggering of common (pre)processing facilities (B). A common distributed platform for data processing on shared resources is established, making use of grid technology. Data is always extracted along with metadata and data anal-

ysis workflows which generate new data products provide describing metadata (C). Thus, data produced in this infrastructure can be discovered, reused and archived (D). The tracked data provenance information allows for quality evaluation, traceability and reproduction of the product with different input data (e.g. for statistical analyses or to study another measurement period).

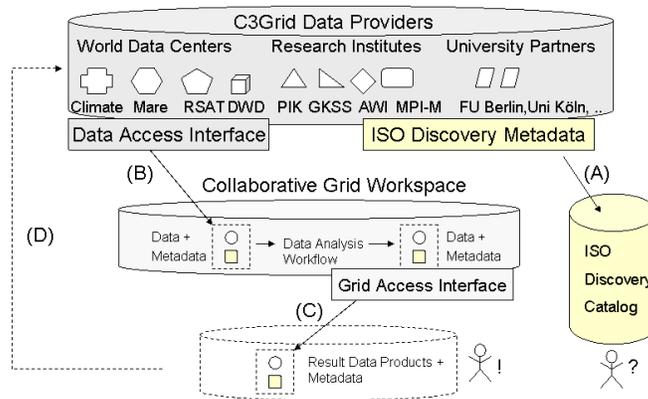


Figure 1: Data access in the C3Grid environment

2.1 Realisation

The key components of the data networking infrastructure in C3Grid are illustrated in figure 2. Besides technical reasoning the choice of the applied technology is motivated by the aim to ensure interoperability and expandability of the system. Thus, where possible the infrastructure is modular and the components are compliant to international standards.

For a uniform and comprehensive metadata description the international standard ISO 19115/19139 [9] is used. The standardised open OAI/PMH protocol [14] is used to communicate (harvest) the metadata. The harvested metadata is made searchable in a central catalogue by applying the open source Lucene [13] implementation as a search and indexing machine. A detailed description of the design of this information service, its implementation and its use through a portal is provided in [17]. The data access interface is based on webservice technology and the data and processing management builds on globus toolkit (GT4) functionality. A description of the data management and scheduling middleware in C3Grid is given in [6].

2.2 Related work

The adoption of the ISO metadata standards in C3Grid is guided by various international efforts for metadata harmonisation e.g. the world meteorological

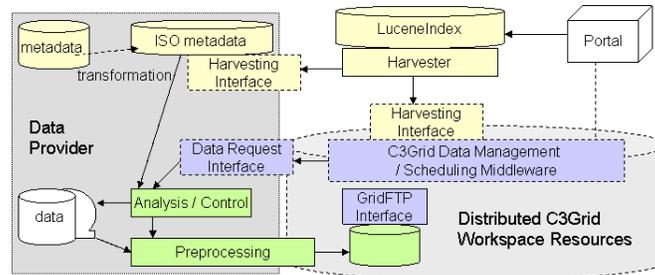


Figure 2: (Meta-)Data networking components in C3Grid

organisation WMO defines an ISO 19115 profile draft[19]. Also recently the INSPIRE project has given ISO 19115/19119 implementation recommendations [8]. On international level, the US-american Earth System Grid project (ESG, [2]) and the British NERC data grid (NDG [11]) strive for similar aims as C3Grid. The ESG implements a middleware for high-performance access and analysis of distributed climate simulation data. In the context of the UK e-science initiative the NERC data grid applies grid technology to ease and harmonise data discovery, delivery and use. However, complementary to the focus of C3Grid to implement a common metadata format (implying discovery details and some usage aspects) in these projects metadata efforts concentrate on the representation of the specifics of earth science data. The ESG defines ontological classifications for interconversion of different metadata as well as specific (use level) metadata e.g. NcML for netCDF data. NDG defines a semantic data model (Climate Science Modelling Language, CSML) based on the Geography Markup Language (GML) and a set of specific feature types. An integrated view of data discovery in ESG and NDG is reported in [12]. Also the data access solution in these projects conceptually differ from that of the C3Grid. Instead of higher level common community data access interfaces, in ESG and NDG data access is mainly file based and realised through Open-DAP and GridFTP and does not include e.g. semantic CF variable translations.

3 Metadata handling in C3Grid

As illustrated in figure 2 metadata handling in C3Grid has multiple aspects: First an agreement on a common metadata schema and its usage has to be established and conforming metadata instances have to be generated and published by each data provider. Secondly, metadata has to be adapted and generated for derived data products, protocoling the processing that has been performed on the source data. These two aspects are discussed in more detail in the following two subsections.

3.1 Discovery Metadata

For a uniform data description the C3Grid uses the recently published ISO 19115 [9] metadata standard for geographical data along with its XML schema implementation ISO 19139. The ISO 19139 metadata schema provides a rich set of tags to describe different aspects of metadata of a dataset. Yet the generality of the ISO standard and diversity of possible metadata annotations requires the derivation of a specific community ISO 19115 profile. The C3Grid profile follows the development of international profile definitions (e.g. the WMO profile) and tries to follow ISO 19115 implementation recommendations (e.g. the INSPIRE drafts).

The available aspects for data description in ISO can be categorised in:

- metadata identification and hierarchies,
- data identification (e.g. extent) and content description,
- data access information, and
- data production context description (data quality information)

Metadata entities are uniquely characterised by identifiers and can be connected hierarchically by assigning a parent identifier. Each described data resource can have exactly one parent, which is often the (physical) container of the data. Additionally other (logical) aggregate information can be attached. This potentially multi level hierarchy must be considered during the generation of data provenance information (cf. section 3.2).

The **data identification** section contains a description of the spatial, and temporal coverage (extent) of the data set as well as other basic information to uniquely identify a data resource. The **data content** of ESS data consists of (often physical) parameters as a discrete function of space and time. For the description of physical entities or real world phenomena ISO 19115 provides two possibilities: simple attribute descriptions and the definition of so called feature types. C3Grid decided to use attribute descriptions to avoid the complexity of feature types and of maintaining feature type catalogues. In C3Grid the Climate and Forecast standard names convention (CF [3]) is used to uniquely name and identify content parameters along with their physical units. Besides e.g. keywords or a free text abstract, the **data identification** and **data content** information are of central importance for data discovery.

The **data access** information characterises the different ways of access, access restrictions and access related metadata like data format and size. Herein also the reference to the C3Grid data access services (see section 4) is given.

The **quality of data** is characterised by data processing history and the original data sets. Providing this information requires basic data provenance tracking. C3Grid decided to integrate this information in the discovery metadata. Details are given in the next subsection.

Currently, two solutions are realised to generate C3Grid profile conform metadata descriptions: On the one hand automatic extraction and transformation of existing proprietary metadata formats is realised e.g. for the CERA database system (WDC climate), the PANGAEA data-warehouse system (WDC mare) and the DWD. On the other hand, previously not annotated data products have

to be made discoverable. For this purpose C3Grid developed a web metadata editor, enabling the generation of new metadata for usage in C3Grid [15]. Currently, about 250 MByte of metadata are collected for about 26700 datasets describing about 70 TByte of data in databases and 8 TByte raw data. For the future, automatic metadata extraction tools for existing flat files in netCDF/HDF and GRIB formats need to be developed and integrated. In this context a cooperation with the ESG and NDG is discussed.

3.2 Data Provenance

Data provenance can be defined as "information that helps determine the derivation history of a data product, starting from its original sources" [18]. Data provenance information can be tracked in an ISO 19139 defined data lineage description section. Each workflow within the C3Grid infrastructure records the input data as well as the processing steps, characterising the generation of the final result data sets. In Figure 3 the structure of the provenance information used in C3Grid is illustrated. Datasets are generated by a sequence of process steps. These steps have an associated time stamp, free text description, "applied tools" element, and information on the responsible author. Each step refers to its source data (set or aggregate) descriptors (metadata identifiers) and describes the performed processing in an additional process step entry in the metadata. Sources also can have subsidiary process step descriptors, extending the description process into the past.

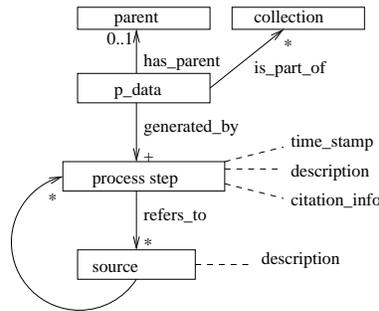


Figure 3: Provenance information for a dataset

Data provenance is of central importance for scientists to be able to evaluate and quality control data. Thus it is a key component to enable data reuse in ESS data analysis activities. In C3Grid data provenance is tracked from the very beginning. Original metadata from the archives describe e.g. the numeric model or measuring instrument with which they were generated. Data in C3Grid is always delivered along with its describing metadata. Accordingly, data analysis workflows in C3Grid have to include the functionality to update their metadata.

Currently, the generation and the update of data provenance metadata in C3Grid is realised by an adaptable set of XSLT transformations.

4 Data access and preprocessing

To allow for central transparent data access, at each data site of the German C3Grid community, an intelligent community specific interface is implemented. The interface is based on standard webservice and grid technologies. The data request is separated from actual data delivery:

- A WSDL defined data request interface allows to trigger local data access and preprocessing functionality. This community interface specifies time, space and content constraints on the data and also allows for a description of data provider supported (pre)processing options.
- The requested data is stored on storage (grid workspace) of the data provider and accessed using GridFTP. The C3Grid data management service is responsible for the data life cycle management as well as the data transport between remote sides (cf. [6]). Additionally, the grid workspaces can be accessed directly for data transfer (see section 5).

In ESS commonly only small parts of the available data of a scientific experiment are needed for an analysis or comparison (cf. fig. 1), e.g. a specific content parameter (CF). To avoid unnecessary large data transfers the data request interface allows for the specification of CFs selection as well as spatial and temporal section extractions. Also provider specific functionalities for further data amount reduction can be addressed, like a temporal or spatial mean. Currently, data can be supplied in one of the two most common data formats: GRIB or netCDF. For the provider-specific configuration of data access and preprocessing functionality, a semantic translation of the uniform C3Grid data request to the local conditions is needed. Based on metadata and local context information (like numerical model and code transformation tables), the following translations are performed:

- Translation of CF standard names into local GRIB code numbers or local variable names, and
- Selection of tool calls in terms of names, options and order.

After this the actual tool calls are executed to write a dataset along with a consistent metadata set. These are provided in the local grid workspace.

For the execution of this preprocessing functionality in the C3Grid, additional information has to be provided about:

- **The size of the derived dataset:** It can be calculated analytically as the sum of the size of each parameter (CF) which depends on the precision p of its representation (2 byte or 3 byte) and the coordinate system on which it is defined (horizontal representation: spherical harmonics or Gaussian grid, vertical: number of levels). A dataset containing n_t timesteps adds a factor of n_t and a transformation from GRIB1 to netCDF format a factor of about 2. For example a user request for a single CF parameter in 2 byte precision in one level over 20 years of modelling time reduces the data

amount from about 3.1 TByte of the whole model raw data output of a 200 years run of ECHAM5 in T63(N48)L31 resolution to 1.1 GByte (both in GRIB1 format).

- **The time for retrieval:** This depends on the one hand on the concrete user request (number of staged datasets and number and complexity of performed tool calls) and on the other hand on the working load of the local system (tape robot usage, disk and processor memory utilisation).

Since the described preprocessing can require a considerable amount of local resources for large data providers (like DKRZ, where the CERA database as well as the file archives of multiple scientific institutions are located) it is planned to modularise and 'gridify' the preprocessing in order to make use of the shared C3Grid resources (cf. fig. 2). Currently all C3Grid data providers are implementing the data access interfaces. The first C3Grid prototype successfully performs data extraction and preprocessing at specific sites.

5 Interoperability

The applied standards along with international agreements allow for interoperability with international partners at data discovery as well as data access level. The more so, as a clear trend towards support of ISO 19115 in climate grid projects and climate related portal projects can be identified. ISO conform C3Grid metadata descriptions can be harvested by partners, enabling visibility and searchability of the described data in both, the C3 and the foreign project's portals.

At the data access level, an implementation of the C3Grid data-request-webservice suffices to register as a data provider for C3Grid. Via the webservice interface the external data products can be accessed from within the C3Grid portal. Similarly, external partner organisations can directly trigger the data request interfaces at C3Grid data providers to retrieve their data. Alternatively, the C3Grid portal can be treated as a single data provider. As previously described, within the C3Grid infrastructure the requested data is made available in a so called distributed (grid-)workspace where it can be accessed via grid protocols (e.g. GridFTP) [10]. Secure data import, data processing and export on this grid-level is possible based on grid proxy certificates

Metadata exchange tests with the NDG project [11] as well as the CDP [1] portal are underway. A future metadata exchange with the GO-ESSP portal [5] is discussed. These collaborations will enable e.g. the discovery of data sets resulting from IPCC (International Panel of Climate Change) model runs at the foreign portals. A tighter interoperability experiment is realised with the European grid project EGEE [4, 16], which operates a gLite based collaborative infrastructure. A webservice interface is installed so that data, requested at the C3 portal can be automatically uploaded on EGEE storage elements. The respective metadata is filled and administered in the gLite Amga metadata catalogue. The metadata of new or processed files in the EGEE infrastructure can be logged and changed in this catalogue and are harvested by the C3 portal.

For this a ISO 19139 OAI-PMH harvesting interface for the metadata catalogue is implemented. These developments are the first step towards a uniform data workspace for European earth system science research.

6 Summary and Outlook

This paper describes design and implementation of key components of the C3Grid (meta-)data management infrastructure to enable uniform, intelligent and transparent data discovery, access and processing. The design of the system is motivated directly by the requirements of ES scientists on the one hand and on the other hand by the need for a flexible, expandable and interoperable system. Thus, the focus is on usability and the design is modular and based on international standards, where possible.

To enable consistent data discovery over a variety of distributed datacenters the data are described in a uniform format and these metadata are collected in a central searchable catalogue. As common metadata format a community profile of the ISO standard 19115/19139 is used. Intelligent and transparent data access, including preprocessing functionalities, is realised by means of a webservice interface that is implemented at each data provider. The preprocessing options include basic functionality like spatio-temporal and content selections as well as provider specific data reduction operations like statistical analysis and transformations. A first experiment to use the system to transparently exchange data and analysis tools with the EGEE infrastructure is underway. A first running prototype has proved the feasibility of the approach and the potential interoperability with other grid infrastructures could be demonstrated [16].

However, to qualify the system for the daily use of a large and diverse user community some requirements are still to be addressed. First and foremost the creation and/or translation of ISO 19139 data descriptions and the implementation of data access interfaces need to be finalised to gain experience with the system on a larger scale. To improve the performance of the system under load it is planned to modularise and 'gridify' the (pre-)processing in order to schedule it to the shared C3Grid resources. For this also a tight integration of the C3Grid job and datamanagement grid middleware components, which are currently being developed [6], is necessary. Another very important issue to be solved is a consistent security management. Here a federated approach based on Shibboleth is followed. For this also a solution for the integrated use of Shibboleth and grid security features has to be implemented.

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