Collaborative Climate Community Data and Processing Grid (C3Grid)

Status Report
Work Package 3 and Work Package 4

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project within the D-Grid community
promoted by BMBF

D-GRID

Reference to project plan:
This report characterizes and summarizes the steps taken and decisions made starting from the project proposal to the current status of climate data access and metadata management at the C3Grid data centres. Its focus is on the design and implementation aspect of the necessary infrastructural components in work package 3 and work package 4. The C3Grid metadata agreement (work package 3) is described in a separate report.

Abstract

Climate data is stored in distributed, heterogeneous, organizationally separated data centres. This document provides an overview of the requirements for components enabling transparent access to earth system science data products. The architectural design integrating these components is described as well as the implementation status at the German data centres. First interoperability studies with international partners are shortly mentioned.

Contents

1. Introduction

To enable grid-based climate data analysis activities, the existing climate related data archives and database systems have to provide common interfaces and access protocols. Within the C3Grid project a common infrastructure is stepwise established to access climate data of all major German earth system science institutions, including the world data centres WDC Climate, WDC RSAT and WDC-MARE as well as the DWD and several earth system science partners (MPI-M, AWI, DLR, PIK, GKSS, IFM-GEOMAR).
On the one hand, a common metadata format and (discovery) metadata exchange mechanism are defined and implemented in work package 3 (AP3). On the other hand, data supply involves complex selection and pre-processing steps, which have to be hidden behind a common data supply interface, which is implemented in work package 4 (AP4).
In this document first the basic requirements, which have to be fulfilled are characterized. Then the basic design decisions and the implementation status is described. The agreement on and adaption of a common (internationally standardized) metadata description is summarized in a separate report.

2. Requirements

2.1 Metadata Management

[M-R1] The metadata format should allow international metadata exchange (based on a common metadata schema) as well as provide the ability to describe C3Grid specific usage information (e.g. information on tools applied to produce data, data derivation information or references to C3Grid interfaces to access data).

[M-R2] The metadata exchange should be based on common, standardized protocols and available software (at client as well as server side) should be reused. The protocols should be compatible to those used in other international earth system science portal projects.

[M-R3] Metadata should allow data at different abstraction levels (e.g. dataset / experiment or data-product / project / collection), and the connection of these levels should be explicitly specifiable (e.g. to derive properties of a dataset based on its “is-part-of” relation to a collection).

2.2 Data Access and Preprocessing

[D-R1] Common well-defined interfaces have to be developed bridging the proprietary access solutions at each data provider.
[D-R2] A data-staging interface should allow to formulate specific climate data requests by users or a portal.
[D-R3] Requested data should be manageable by C3Grid middleware.
[D-R4] The final authorization decisions and user management should stay at the individual data centres.

3. Architectural Design

A survey of the existing infrastructures, and access solutions at the different data centres revealed the heterogeneity of the (meta-)data management solutions: Flat file storage with very few associated metadata is used as well as sophisticated integrated disk / tape / metadata management solutions and data warehouse implementations.
Also an evaluation of existing grid based data management solutions was done, including SRM, SRB and OGSA-DAI. None provided the necessary ability to bridge the existing platforms and data management solutions and promised to provide a common platform for C3Grid developments:

- No community agreement on SRB usage was reached. SRB would have required complex adaption steps to realize an integration into the existing systems. Also licensing issues were open for a considerable time period.
- SRM only provides a data file access solution and is not applicable for database access.
- OGSA-DAI on the other side makes only sense for database access, but also in this context would require re-implementation of great parts of the existing database access solution functionality (e.g. access wrappers).

Thus the architecture design in C3Grid is based on the idea of defining and implementing lightweight wrappers around the existing solutions with well-defined and interoperable interfaces and protocols (see Figure 1):

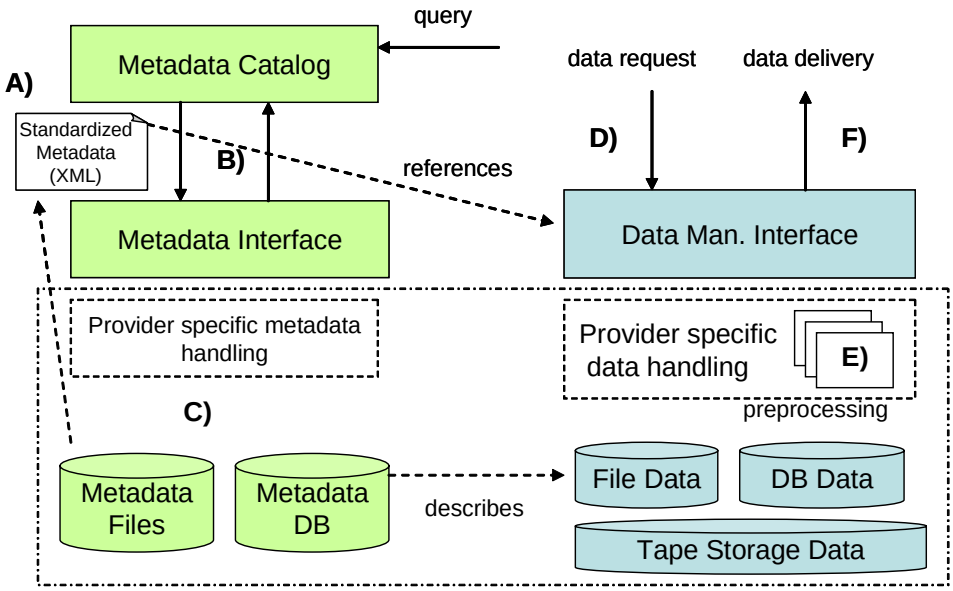

***Figure 1**: General Architecture*

Nevertheless the data providers are free to realize their data access via SRM, SRB or OGSA-DAI "under the hat" of the C3Grid interface. See e.g. the DWD implementation, which uses OGSA-DAI internally.

Design decisions for protocols, interfaces, exchange formats:
(labels correspond to tags in Figure 1)

A) As already indicated in the project proposal, ISO 19115 and its XML implementation ISO 19139 was chosen as C3Grid metadata format. Finally standardized late 2006 the ISO format provides a general description framework for geographic data products (and thus is not specific to climate data). C3Grid adaptations and usage agreements were necessary effort, which are summarized in a separate document.
B) For the exchange of metadata information the OAI (Open Archives Initiative) defined interfaces and protocol (OAI-PMH) was adopted. This approach is based on http transport of XML data and tested client as well as server software can be used. In addition this protocol is heavily used in earth system related portal systems. Thus the C3Grid implementation of OAI servers also allows for publishing metadata to other international partners.
C) The individual data centres are free in the way they implement the publishing of ISO XML documents: small centres can provide simple file based offline repositories to store their metadata, whereas large centres can implement online adaptors to extract and transform metadata in database systems on the fly.
D) Data request and data delivery interfaces were separated. For requesting data a web service interface was defined in cooperation with work package 2 which also provided a skeleton implementation of this interface.
E) Besides data access, the fulfilment of a data request in general also requires complex and flexible pre-processing to select, transform and prepare data for delivery. For this purpose general climate data analysis tools have to be triggered by a data request. The implementation is up to the individual data centre.
F) For data delivery, a common distributed C3Grid data workspace was set up based on gridftp accessible storage at each data centre. Requested data is made available in this data provider attached storage pool, which is managed by the C3Grid data management system (DMS).

Security) The design and implementation of a general security infrastructure for C3Grid is a complex task, requiring the integration of established grid security (PKI) components and protocols (GSI) on the one hand and the construction of a federated AA infrastructure (based on Shibboleth). As a very first step towards a C3grid security infrastructure the Shibboleth Identity Provider is implemented and accessible through the VO (Virtual Organisation) of the DFN-AAI. As a second step of implementing a security infrastructure data providers implemented a mechanism to map a DN (Distinguished Name) from a certificate to a local account to access data. A list of all available DNs of all registered C3Grid users is available from the C3Grid portal.

4. Implementation

4.1 Overview

In order to implement the described abstract components for data management as well as metadata harvesting each data provider has to design and realize bridging functionality to the existing infrastructure. As illustrated in the following section these existing infrastructures vary greatly in design, complexity as well as hardware and software platforms. In the following an overview is given of the major design decisions as well as implementation steps at the individual C3Grid data providers.

To enable data access for C3Grid each data provider has to realize:

- C3Grid ISO metadata descriptions of the available data sets (C3Grid ISO 19139 conforming XML files). These descriptions often can be generated automatically by e.g. applying xslt transformations to existing metadata description. In some cases metadata has to be generated by hand.
- A metadata publishing component supporting the OAI protocol for metadata harvesting (OAI-PMH, alternatively also OAI servers at partner institutions could be used.
- The C3Grid data request web service interface (see Work Package 5 for the detailed WSDL specification). Table 1 gives an overview over the currently installed versions at the data providers.
- An C3Grid data request adaptor for the request interface which does the authorization, triggers the data extraction and pre-processing functionality needed to fulfill data requests
- The C3Grid work space (disk pool) with a GridFTP data delivery interface

The pre-processing functionality at the data providers can be divided into two parts:

- Basic functionality for temporal and spatial selection and variable selection based on the CF (Climate and Forecast) standard names. This has to be implemented by each data provider.
- Advanced data provider specific functionality, like diagnosis of further CF variables, transformations and statistical analyses. This functionality development is strongly based on specific user needs and data provider infrastructure. It is designed to be dynamically extendable.

The currently available data is shown in Table 2 and the implementation status at the data providers is as follows:

- The C3Grid managed metadata is single level metadata only, describing single datasets or aggregated data, which are together accessible, e.g. a model run stored in different datasets or of a weather service product observed at different meteorological stations.
- Additional data provider specific functionality in the data access is not used at the moment.
- The authorization and security infrastructure implementation is work in progress.

Institution	Address	Version
HH	https://anticyclone.dkrz.de:9443/axis/services/C3ProviderSOAP	V0.8
DWD	http://oflsd20.dwd.de:8080/axis/services/C3ProviderSOAP	V0.8
PIK	http://c3grid.pik-potsdam.de:8080/axis/services/C3ProviderSOAP	V0.8
WDC Mare	http://ws.pangaea.de/c3grid/services/C3ProviderSOAP	V0.8
DLR-DFD	http://eridanus.caf.dlr.de:8080/axis/services/C3ProviderSOAP	V0.8
ZAIK	Test version set up	

***Table 1**: Production implementations of C3Grid data access interface at data providers.*

Data Provider	Data in C3Grid	Size	Status
WDC Climate	Model simulations IPCC-AR4 of MPI-M (ECHAM5, MPI-OM), HOAPS III	~ 63 TB	M/P (DKRZ)
DKRZ Archive			
▪ **IFM-GEOMAR**	Nemo DRAKKAR Model Simulation	~ 370 GB	M/P
▪ **GKSS**	ECHAM4 Paleo Model Simulations	~ 6.8 TB	M/P
▪ **MPI-M**	ECHAM5 IPCC-AR4 Model Simulation	~ 3.1 TB	M/P
WDC Mare / PANGAEA	Measurement Data (JGOFS, Southern Ocean)	~ 10 GB	M/P
WDC RSAT / DLR	Satellite Data (Ozone Products)	~ 60 GB	M/P
DWD	Observed Climate Time Series	~ 200 GB	M/P
PIK	Gridded Meteorological and Carbon Data (BADG, PIK-GCD, PIK-LPJ)	~ 9 GB	M/P
ZAIK / FUB	IPCC Model Simulation of DMI	~ 900 GB	M
AWI	OMIP / NAOSIM Model Simulations	~ 3 GB	Set-up

***Table 2:** Status of data supply (M: metadata available and searchable; P: selected data downloadable / prepocessing functionality implemented).*

4.2 Implementation details for DKRZ/MPI-M/M&D/IFM-GEOMAR

The implementation in HH realizes the interfaces for metadata publishing and the data request web service.

Metadata is generated offline by extracting the information from the CERA (oracle) database system, transforming it into the ISO C3Grid format and storing it in a local ISO XML repository. This metadata is then available for harvesting via the OAI-PMH protocol. The repository server was realized based on the freely available DLESE - jOAI software.

The data access web service is realized in an https secured web container and triggers the

data extraction and pre-processing functionality needed to fulfil a concrete data request. The final data result is stored in the C3Grid gridFTP workspace:

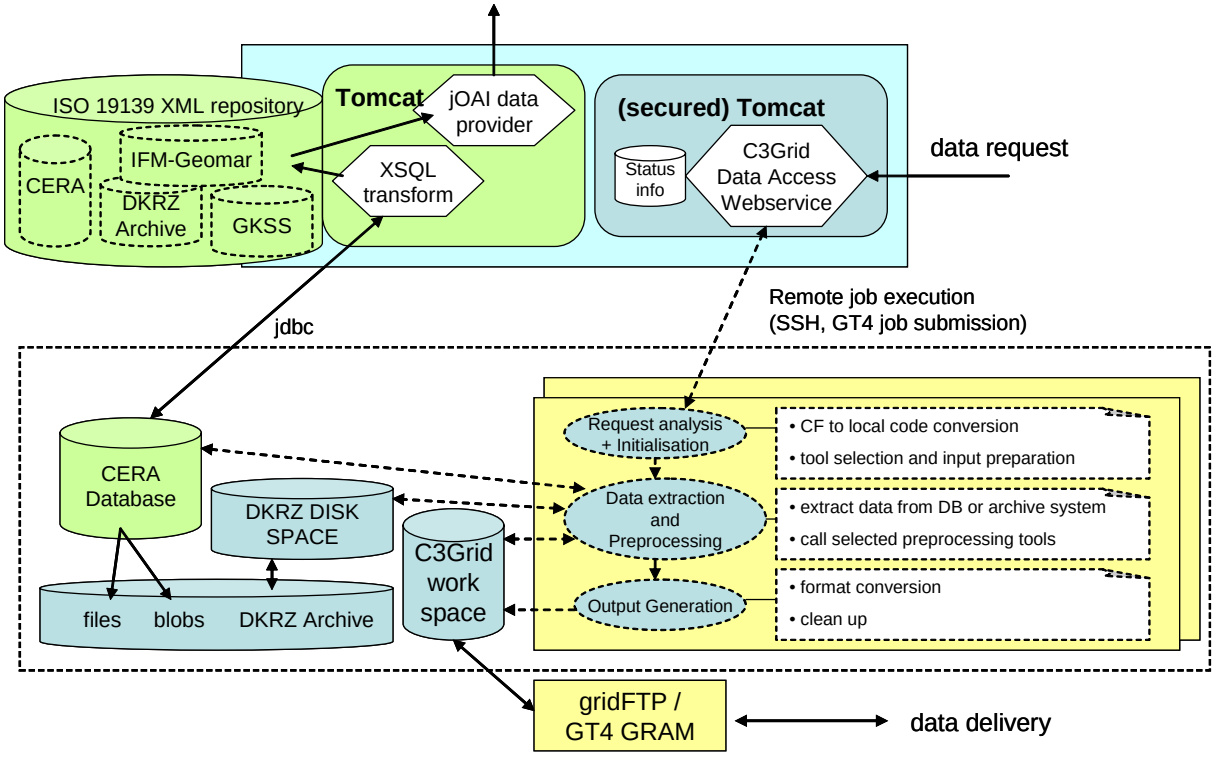

Figure 2

The basic pre-processing functionality is implemented for data stored in the CERA database of the WDCC and in the DKRZ archive, i.e. user request for spatial and temporal parts and for specific variables can be satisfied [1]. For the selection of the datasets and the pre-processing set-up, additional information (provided by CERA meta data base) is needed and several interpretation steps have to be performed before the processing, like for the mapping of the CF standard names of the user's request into local variable names or grib codes numbers of the dataset headers.
Currently, 66 ISO 19139 descriptions of aggregated data are available. These describe a data volume of about 64 TByte of IPCC data (ECHAM5 and MPI-OM model output of coupled model runs at MPI-M) and HOAPS III satellite data stored in the CERA DB and about 10.5 TByte raw data stored in the DKRZ archive from paleo-climate model run raw data of the GKSS (7 TByte), an IPCC-ECHAM5 model run raw data of MPI-M (3.1 TByte), and an OPA model run raw data of IFM-GEOMAR (0.4 TByte).
The first step of the C3Grid security infrastructure is to implement the Shibboleth Identity Provider (IdP). The access to the local LDAP information is realized in an apache2 front end. The Shibboleth is embedded in a tomcat container and controlled with a set of configuration information. As local LDAP attribute 'eduPersonEntitlement' is used for selecting C3Grid members. Within the StageFileRequest of the webservice call a DN of a certificate is delivered. With this DN a local mapping to an account is realized including an implicit authorisation.

4.3 Implementation Details DWD

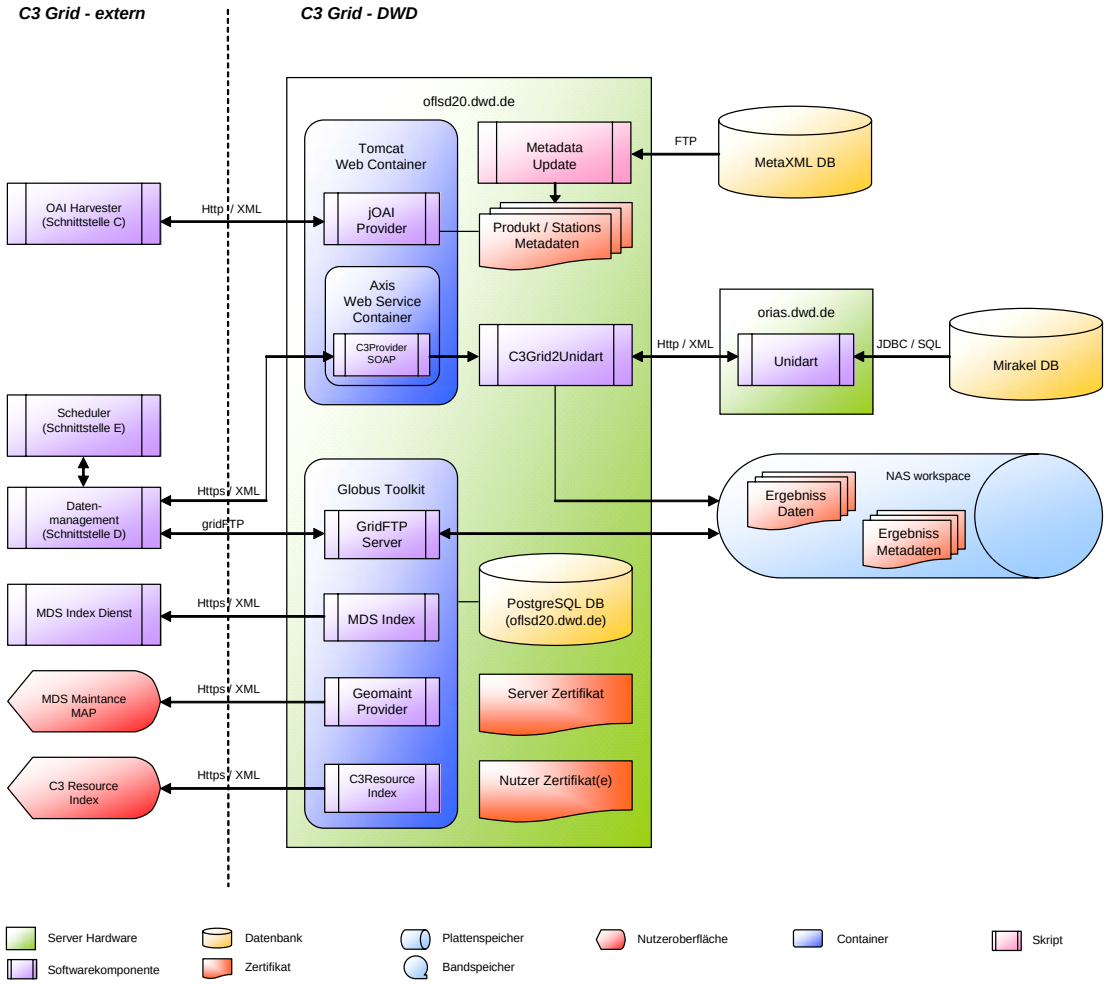

Figure 3

For the provision of meta data (interface C), the DWD uses the jOAI software. The meta data are stored in a XML database, where they are regularly recalled from. The WebService for the data providers (interface D) runs in a WebContainer on an Apache Tomcat + Axis.
For safety reasons, only a few components are located in the demilitarized zone whereas others are not visible on the Internet. It therefore is impossible to gain, for example, direct access to the DWD databases. Instead, there is an OGSA-DAI component in place which receives and responds to the requests. With a view to compatibility with the C3 Grid requirements, a 'wrapper' is being developed for this component to establish the connection to the WebService.
Some of the components, however, are still in the developing or testing stage and not yet fully operational. The structure as shown above will also undergo further changes to meet the operational requirements of the DWD.

4.4 Implementation details PIK

At PIK, the metadata publishing provider and the data access web service are implemented on a C3Grid bastion host in the demilitarized zone (DMZ) according to PIKs security policy and requirements.
Metadata for the C3Grid data sets from PIK is created using the web-based Metadata-Editor that PIK has developed and published for C3Grid (http://www.pik-potsdam.de/ops/c3grid). The metadata is stored in a local ISO XML repository on the bastion host. DLESE jOAI software is used for providing the metadata to the harvesting server.
The data access web service is implemented in a web service container, based on the skeleton reference implementation from WP2. It checks the request parameters on validity and passes the request from the DMZ on to PIK's inner network. From there the data sets in the Oracle database and / or the tape library can be accessed. The web service request and its parameters are transformed into invocations of specific access procedures. Only the data values for the requested spatial and temporal constraints is extracted, pre-processed, and afterwards transferred back to the workspace on the bastion host in the DMZ, where it can be accessed by the C3Grid Data Management via GridFTP. Additionally, the specific Use-Metadata for the created data set is derived from the original Discovery-Metadata and is also made available in the workspace on the bastion host.

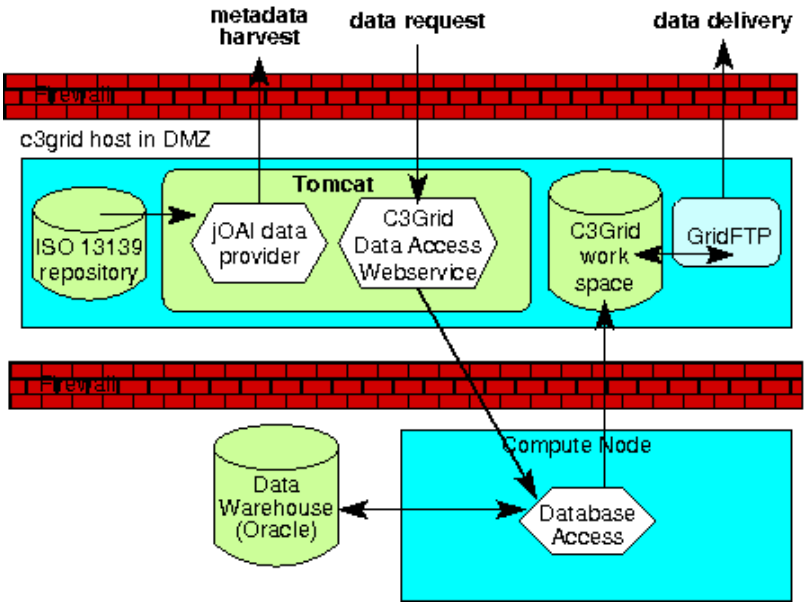

Figure 4

Based on the experiences with this implementation, a tutorial on “How to set up a C3Grid Data Provider site?” was released.
A prototype of the C3Grid XML metadata editor is available at http://www.pik-potsdam.de/ops/c3grid . The metadata editor is based on an XHtml-form using the Orbeon Presentation Server (OPS), an open source java implementation of the W3C XForms standard (http://www.orbeon.com). The internal xml-datasets are stored in the open source xml-database eXist (http://exist.sourceforge.net). The OPS-application is hosted by an Apache Tomcat 5.5.16 server under Linux.
The metadata editor enables to create new metadata from scratch and to upload existing metadata to edit them. The resulting xml metadata files can be downloaded and put into an OAI provider's metadata repository for harvesting.

4.5 Implementation details PANGAEA®

PANGAEA® - Publishing Network for Geoscientific & Environmental Data (www.pangaea.de) - is a public digital library for science aimed at archiving, publishing and distributing georeferenced data with special emphasis on environmental, marine and geological basic research. The World Data Center for Marine Environmental Sciences (WDC-MARE, http://www.wdc-mare.org) uses PANGAEA® as its data archive and distribution system.

Metadata in PANGAEA® is maintained in a relational database together with data. Preprocessed metadata records in a ISO-19115-compatible format (without static contents like data center contact information,…) are also available as XML blobs in the database for easy transformation to customized formats. On each change in the relational metadata items, corresponding XML blobs are updated by a metadata processing background queue.

On top of the XML blobs, an OAI-PMH server (own PANGAEA development) is serving new and updated XML files to C3Grid and other communities in various metadata formats (DC, DIF, ISO 19115/ISO19139). The transformation from the (proprietary) XML schema is done on-the-fly by the OAI-PMH server. For C3Grid special attention is turned on transforming PANGAEA specific variable names to CF names and other specialities of the C3Grid ISO metadata schema. The OAI-PMH server entry point is available at http://ws.pangaea.de/oai/.

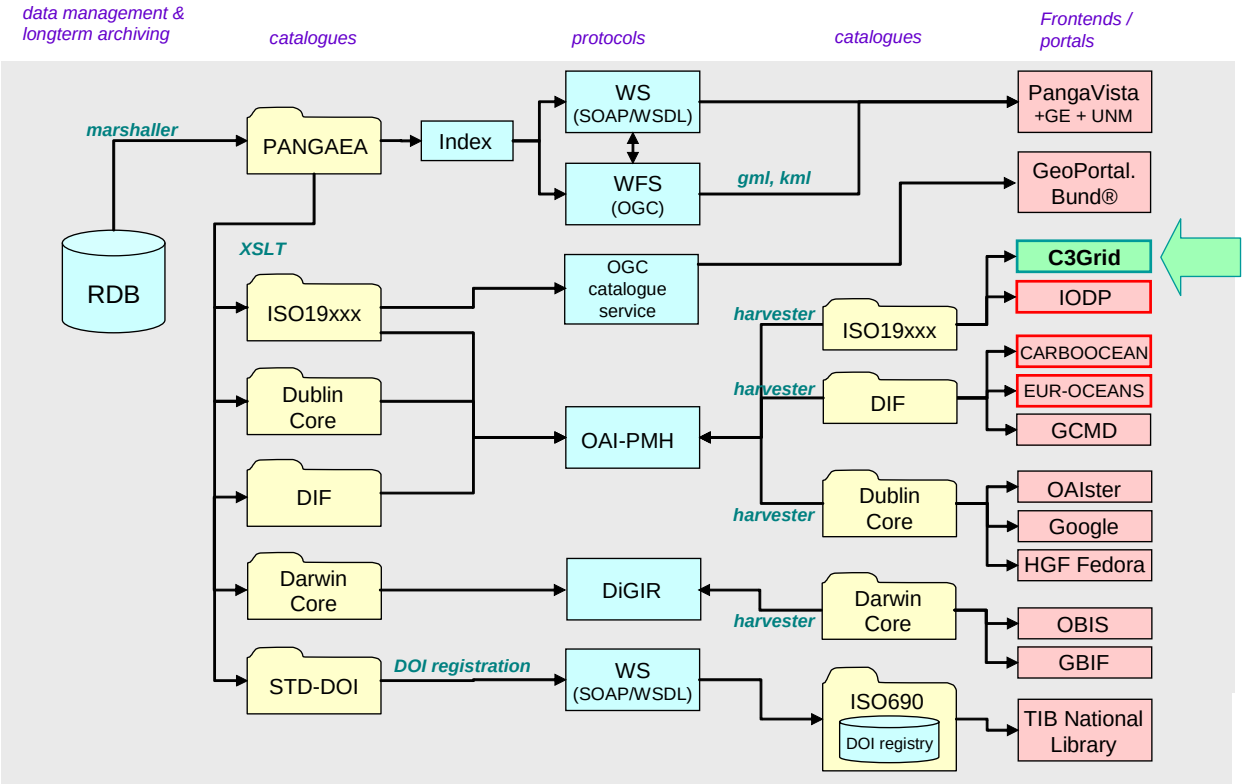

***Figure 5**: Metadata infrastructure of PANGAEA®*

All scientific data in PANGAEA® is replicated for fast access (e.g. time series) to a Sybase IQ data warehouse. The data access to the C3Grid workspace is based on the C3Grid provider template developed by ZIB and developed as a customized “FileStager” completely written in Java using the PANGAEA-specific data warehouse access web service (http://ws.pangaea.de/ws/services). This “FileStager” starts the query to the Sybase IQ data warehouse and sends the streamed result to files in the C3Grid

workspace. The C3Grid data provider web service is available at http://ws.pangaea.de/c3grid/services.

4.6 Implementation details DLR

The primary focus of WDC-RSAT is the provision of data and information on atmospheric trace gases, clouds, and the earth´s surface which are primarily gathered from satellite based sensors. The data and information products of the WDC-RSAT are archived as flat files in a directory based structure on a web server in the demilitarized zone (DMZ) of DLR, located in Birlinghoven.

The related metadata information generally results from the directory structure of the archived data and/or is covered by the data header information itself. The transforming of metadata into the ISO conform C3 Grid format is still generated offline at the moment, whereby an automatic procedure is on its way. The metadata information is archived on the web server as well and can be harvested via the OAI-PMH protocol. The installed harvesting server is based on the freely available DLESE-jOAI software.

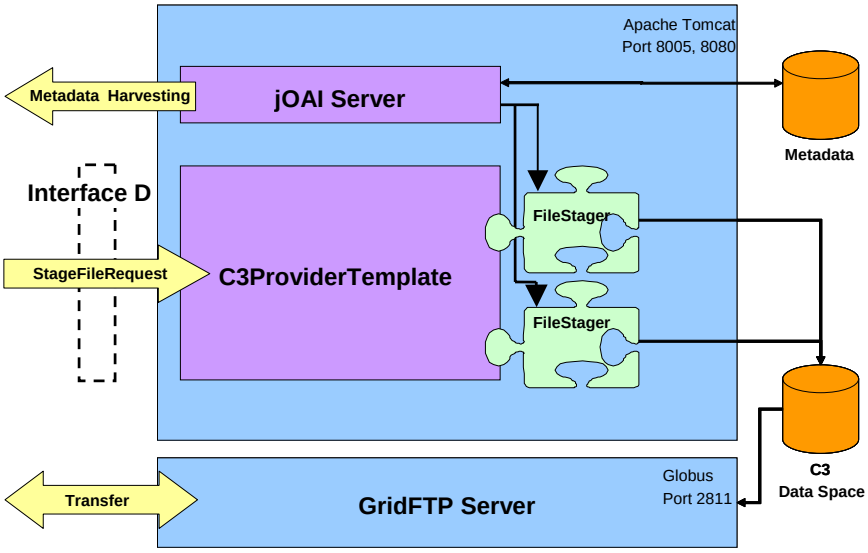

***Figure 6**: DLR implementation of C3 Interface D*

The data access to the C3-workspace is realized via a GridFTP server by using a metadata directory. The C3ProviderTemplate allows the data request from the user/portal. The requests are processed by FileStagers which store the data in the C3 data space from where they can be transferred via GridFTP and managed by the C3-Grid data management system. The FileStagers have been re-factored to be modular and extensible and to retrieve metadata from the jOAI automatically.

5. Summary

The design and implementation of the C3Grid (meta-)data publication and access interfaces was heavily influenced by the requirement to build up reusable and sustainable components which can be used in various international collaborations. Thus the metadata harvesting approach of ISO metadata descriptions is reused to publish metadata to international portals (NDG, GO-ESSP). Also an interoperability study with the EGEE

middleware was done (presented at the EGEE conference in Geneva), which makes use of the developed interfaces to publish metadata, extract data from the WDC Climate and transfer it onto EGEE resources (by GridFTP) where they can be processed making use of the gLite middleware.

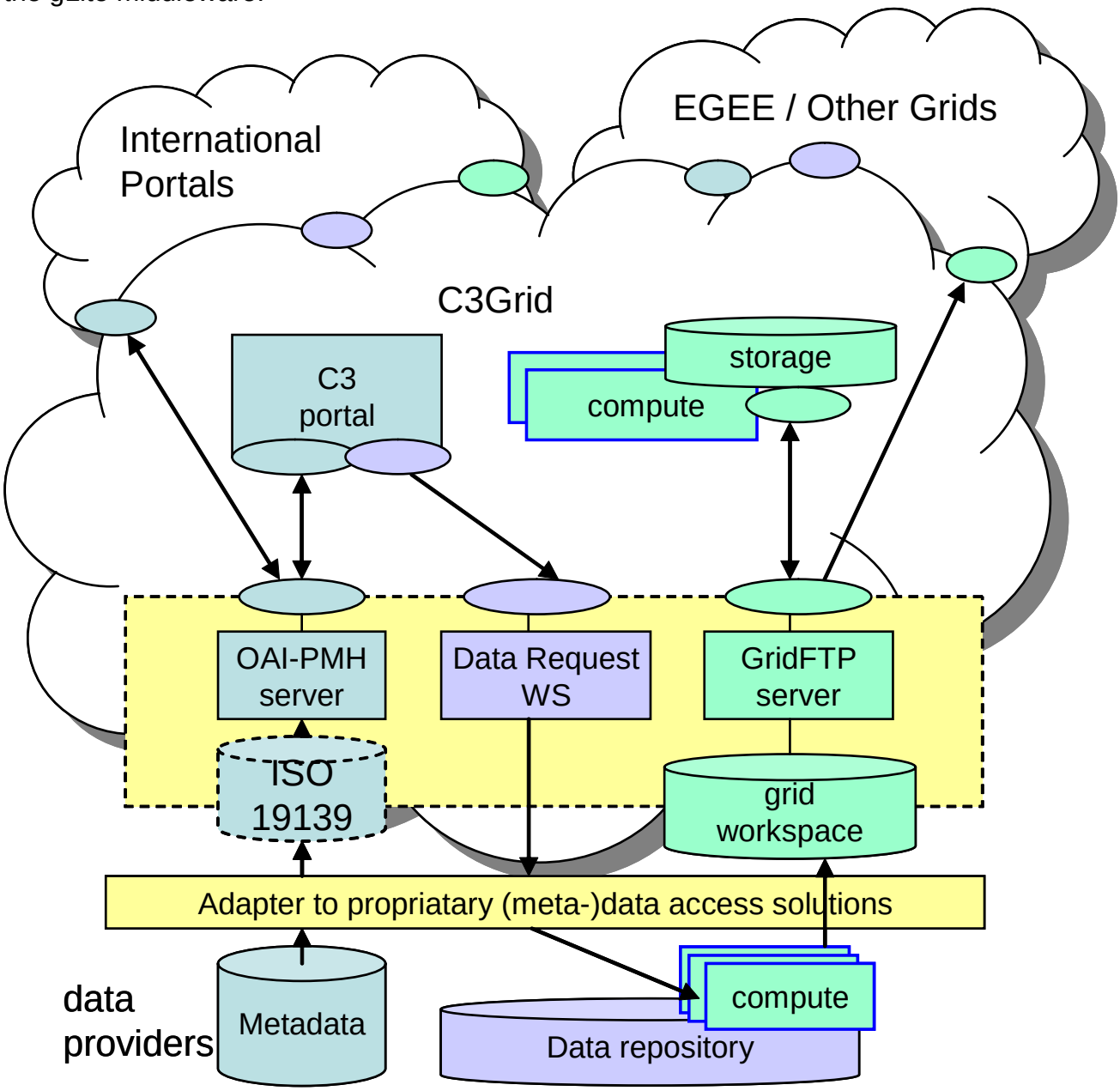

Figure 7: *Reuse of C3Grid Interfaces in international collaborations*

References :

[1] M. Stockhause :
Data Preparation (Preprocessing for Model Data)
http://www.c3grid.de/documents/DataPreparation.pdf