The NorduGrid architecture and tools

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The NorduGrid project designed a Grid architecture with the primary goal to meet the requirements of production tasks of the LHC experiments. While it is meant to be a rather generic Grid system, it puts emphasis on batch processing suitable for problems encountered in High Energy Physics. The NorduGrid architecture implementation uses the Globus Toolkit™ as the foundation for various components, developed by the project. While introducing new services, the NorduGrid does not modify the Globus tools, such that the two can eventually co-exist. The NorduGrid topology is decentralized, avoiding a single point of failure. The NorduGrid architecture is thus a light-weight, non-invasive and dynamic one, while robust and scalable, capable of meeting most challenging tasks of High Energy Physics.

1. Introduction

The European High Energy Physics community is in the final stages of construction and deployment of the Large Hadron Collider (LHC) - the world biggest accelerator, being built at the European Particle Physics Laboratory (CERN) in Geneva. Challenges to be faced by physicists are unprecedented. Four experiments will be constructed at the LHC to observe events produced in proton-proton and heavy ion collisions. Data collected by these experiments will allow for exploration of new frontiers of the fundamental laws of nature, like the Higgs mechanism with possible discovery of the Higgs boson; CP-violation in B-meson decays; supersymmetry; large extra dimensions and others. One of the greatest challenges of the LHC project will be the acquisition and analysis of the data. When, after a few years of operation, the accelerator will run at its design luminosity, each detector will observe bunch collisions at a rate of $4 \cdot 10^7$ per second. A set of filter algorithms, implemented in hardware and on state-of-art programmable processors, aims to reduce the event rate to less than 1000 events per second for final storage and analysis. The equivalent data volume is between 100 MByte/sec and 1 GByte/sec. Each experiment is expected to collect 1 PByte of raw data per year. The two LHC general purpose experiments, ATLAS and CMS, have each more than 150 participating institutes distributed all over the world. 2000 physicists per experiment contribute to the development of hardware and software and they expect to have almost instantaneous access to the data and to a set of up-to-date analysis tools.

1.1. The NorduGrid Project

In order to face the computing challenge of the LHC and other similar problems emerging from the science communities the NorduGrid project also known as the Nordic Testbed for Wide Area Computing was set up. The goal was to create a GRID-like infrastructure in the Nordic countries (Denmark, Norway, Sweden and Finland) that could be used to evaluate GRID tools by the scientists and find out if this new technology could help in solving the emerging massive data and computing intensive tasks emerging. The first test case was to be the ATLAS Data Challenge (see [1]) which was to start out in May of 2002.

As the focus was on deployment we hoped that we could adopt existing solutions on the marked rather than develop any software in the project. The available Grid middleware providing candidates were narrowed down to the Globus Toolkit™ and the software developed by the European DataGrid project (EDG) [2][3]. The middleware from these two projects however was soon found to be inadequate. The Globus Toolkit is mainly a box of tools rather than a complete solution. There is no job brokering and their Grid Resource Allocation Manager [4] lacked the possibility of staging large input and output data. The EDG software seemed to address the deficiencies of the Globus Toolkit, but were not mature enough in the beginning of 2002 to seriously solve the problems faced by the ATLAS data challenges. Furthermore it was felt that the implementation of their centralized resource broker was a serious bottleneck that could never be used in solving the large amounts of data that were going to be dealt with on a large data Grid.

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It was therefore decided that the NorduGrid project would create a Grid architecture from scratch. The implementation would use existing pieces of working Grid middleware and develop the missing pieces within the project in order to create a production Grid testbed.

2. Architecture

The NorduGrid architecture was carefully planned and designed to satisfy the needs of users and system administrators simultaneously. These needs can be outlined as a general philosophy:

- Start with simple things that work and proceed from there
- Avoid architectural single points of failure
- Should be scalable
- Resource owners retain full control of their resources
- As few site requirements as possible:
  - No dictation of cluster configuration or install method
  - No dependence on a particular operating system or version
- Reuse existing system installations as much as possible
- The NorduGrid middleware is only required on a front-end machine
- Compute nodes are not required to be on the public network
- Clusters need not be dedicated to Grid jobs

2.1. The NorduGrid System Components

The NorduGrid tools are designed to handle job submission and management, user area management, some data management, and monitoring. Figure 1 depicts basic components of the NorduGrid architecture and schematic relations between them. In what follows, detailed descriptions of the components are given.

**User Interface** (UI) is the major new service developed by the NorduGrid, and is one of its key components. It has the high-level functionality missing from the Globus Toolkit\(^\text{TM}\), namely, that of resource discovery, brokering, Grid job submission and job status querying. To achieve this, the UI communicates with the NorduGrid Grid Manager (see Section 3.1) and queries the Information System (Section 3.3) and the Replica Catalog (Section 3.2).

The UI comes simply as a client package (Section 3.3), which can be installed on any machine – typically, an end-user desktop computer. Therefore, NorduGrid does not need a centralized resource broker, instead, there are as many User Interfaces as users find convenient.

**Information System** within the NorduGrid is another key component, based on MDS\(^\text{TM}\) and realized as a distributed service (Section 3.3), which serves information for other components, such as a UI or a monitor (Section 3.4).

The Information System consists of a dynamic set of distributed databases which are coupled to computing and storage resources to provide information on the status of a specific resource. When they are queried, the requested information is generated locally on the resource (optionally cached afterward), therefore the information system follows a pull model. The local databases register themselves via a soft-state registration mechanism to a set of indexing services (registries). The registries are contacted by the UI or monitoring agents in order to find contact information of the local databases for a direct query.

**Computing Cluster** is the natural computing unit in the NorduGrid architecture. It consists of a front-end node which manages several back-end nodes, normally via a private closed network. The software component consists of a standard batch system plus an extra layer to interface with the Grid. This layer includes the Grid Manager (Section 3.1) and the local information service (Section 3.3).

The operation system of choice is Linux in its many flavors. Other Unix-like systems (e.g. HP-UX, Tru64 UNIX) can be utilized as well.

The NorduGrid does not dictate configuration of the batch system, trying to be an "add-on" component which hooks the local resources onto the Grid and allows for Grid jobs to run along with the conventional jobs, respecting local setup and configuration policies.

There are no specific requirements for the cluster setup, except that there should be a shared file system (e.g. The Network File System - NFS) between the front-end and the back-end nodes. The back-end nodes are managed entirely through the local batch system, and no NorduGrid middleware has to be installed on them.

**Storage Element** (SE) is a concept not fully developed by the NorduGrid at this stage. So far, SEs are implemented as plain GridFTP\(^\text{TM}\) servers. A software used for this is a GridFTP server, either provided as a part of the Globus Toolkit\(^\text{TM}\), or the one delivered as a part of the NorduGrid Grid Manager (see Section 3.1). The latter is preferred, since it allows access control based on the user’s Grid certificate instead of the local identities to which users are mapped.

**Replica Catalog** (RC) is used for registering and
locating data sources. NorduGrid makes use of the RC as developed by the Globus project \cite{3}, with minor changes to improve functionality (see Section 3.2). RC records are entered and used primarily by the GM and its components, and can be used by the UI for resource brokering.

2.2. Task Flow

The components described above are designed to support the task flow as follows:

1. A user prepares a job description using the extended Globus Resource Specification Language (RSL, Section 3.5). This description may include application specific requirements, such as input and output data description, as well as other options used in resource matching, such as architecture or an explicit cluster.

2. The job description is interpreted by the UI, which makes resource brokering using the Information System and RC data, and forward the job to the chosen cluster (see Section 3.4), eventually uploading specified accompanying files.

3. The job request (in extended RSL format) is received by the GM which resides on cluster’s front-end. It handles pre-processing, job submission to the local system, and post-processing (see Section 3.1), depending on the job specifications. Input and output data manipulations are made by the GM with the help of RC’s and SE’s.

4. A user may request e-mail notifications about the job status, or simply use the UI or monitor (Section 3.4) to follow the job progress. Upon the job end, specified in the job description files can be retrieved by the user. If not fetched in 24 hours, they are erased by the local GM.

In \cite{1} this can be seen in a real production environment.

3. The NorduGrid Middleware

The NorduGrid middleware is almost entirely based on the Globus Toolkit\textsuperscript{TM} API, libraries and services. In order to support the NorduGrid architecture, several innovative approaches were used, such as the Grid Manager (Section 3.1) and the User Interface (Section 3.4). Other components were extended and developed further, such as the Information Model (Section 3.3) and the Extended Resource Specification Language (Section 3.5).

3.1. Grid Manager

The NorduGrid Grid Manager (GM) software acts as a smart front-end for job submission to a cluster. It runs on the cluster’s front-end and provides job management and data pre- and post-staging functionality, with a support for meta-data catalogs.

The GM is a layer above the Globus Toolkit\textsuperscript{TM} libraries and services. It was written because the services available as parts of the Globus Toolkit\textsuperscript{TM} did not meet the requirements of the NorduGrid architecture (Section 2) at that time. Missing things included
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integrated support for the RC, sharing cached files among users, staging in/out data files, etc..

Since data operations are performed by an additional layer, the data are handled only at the beginning and end of a job. Hence the user is expected to provide complete information about the input and output data. This is the most significant limitation of the used approach.

Differently from the Globus Resource Allocation Manager (GRAM) [4], the GM uses a GridFTP interface for jobs submission. To do that, a NorduGrid GridFTP server (GFS) was developed, based on the Globus libraries [5]. Its main features which makes it different from the Globus implementation are:

- Virtual directory tree, configured per user.
- Access control, based on the Distinguished Name stored in the user certificate.
- Local file system access, implemented through loadable plug-ins (shared libraries). There are two plug-ins provided with GFS:
  - The local file access plug-in implements an ordinary FTP server-like access,
  - The job submission plug-in provides an interface for submission and control of jobs handled by the GM.

The GFS is also used by NorduGrid to create relatively easily configurable GridFTP based storage servers (often called Storage Elements).

The GM accepts job-submission scripts described in Globus RSL (Section 3.4) with a few new attributes added.

For every job, the GM creates a separate directory (the session directory) and stores the input files into it. There is no single point (machine) that all the jobs have to pass, since the gathering of input data is done directly on a cluster front-end.

Input files local to the user interface are uploaded by the UI. For remote input files the GM start a download process that understand a variety of protocols: (eg. http, ftp, gridftp, rc, rsl, etc.).

Once all input files are ready the GM creates a job execution script and launches it using a Local Resource Management System (LRMS). Such a script can perform additional actions, such as setting the environment for third-party software packages requested by a job.

After a job has finished, all the specified output files are transferred to their destinations, or are temporarily stored in the session directory to allow users to retrieve them later.

If an output destination specifies a RC additional registration is performed in the replica catalog. A schematic view of the GM mechanism is shown on Figure 2.

Additionally, the GM can cache input files and let jobs and users share them. If the requested file is available in the cache, it is still checked (if the protocol allows that) against the remote server whether a user is eligible to access it. To save the disk space, cached files can be provided to jobs as soft links.

The GM uses a bash-script Globus-like implementation of an interface to a local batch system. This makes it easy to adapt the GM to inter-operate with most LRMSs.

The GM uses the file system to store the state of handled jobs. This allows it to recover safely from most system faults, after a restart.

The GM also includes user utilities to handle data transfer and registration in meta-data catalogs.

3.2. Replica Catalog

The NorduGrid makes use of the Globus RC, which is based on an OpenLDAP server with the default LDAP DatabaseManager back-end. There are no significant changes introduced into the original Globus RC objects schema. Apparent OpenLDAP problems with transferring relatively big amounts of data over an authenticated/encrypted connection were fixed partially by applying appropriate patches, and partially by automatic restart of the server. Together with a fault tolerant behavior of the client part, this made the system usable.

To manage the information in the RC server, the Globus Toolkit API and libraries were used. The only significant change was to add the possibility to perform securely authenticated connections based on the Globus GSI mechanism.

3.3. Information System

The NorduGrid Information System description exceeds the limits imposed by this publication.

The NorduGrid middleware implements a dynamic distributed information system which was created by extending the Monitoring and Discovery Services (MDS) of the Globus Toolkit. The MDS is an extensible framework for creating Grid information systems, and it is built upon the OpenLDAP software. An MDS-based information system consists of an information model (schema), local information providers, local databases, soft registration mechanism and information indices. NorduGrid extensions and a specific setup, made MDS a reliable backbone of the information system. A detailed account of these modifications is given below.

A Grid information model should be a result of a delicate design process of how to represent the resources and what is the best way to structure this information. In the used MDS-based system, the information is being stored as attribute-value pairs of
LDAP entries, which are organized into a hierarchical tree. Therefore, the information model is technically formulated via an LDAP schema and the specification of the LDAP-tree.

Evaluation of the original MDS and the EDG schemas showed that they are not suitable for describing clusters, Grid jobs and Grid users simultaneously. Therefore, NorduGrid designed its own information model. While Globus and other Grid projects keep developing new schemas, the NorduGrid one is the only which has been deployed, tested and used for a production facility.

The NorduGrid model naturally describes the main Grid components: computing clusters, Grid users and Grid jobs. The LDAP-tree of a cluster is shown in Fig. 3. In this model, a cluster entry describes the hardware, software and middleware properties of a cluster. Grid-enabled queues are represented by the queue entry, under which the authuser and job entries can be found. Every authorized Grid user has an entry under the queue. Similarly, every Grid job submitted to the queue is represented by a job entry. The job entries are generated on the execution cluster, this way implementing a distributed job status monitoring system. The schema also describes Storage Elements and Replica Catalogs, although in a simplistic manner.

The information providers are small programs that generate LDAP entries upon a search request. The NorduGrid information model requires its own set of information providers, therefore a set of such programs which interface to the local system was created. The NorduGrid providers create and populate the NorduGrid LDAP entries of the local database by collecting information from the cluster’s batch system and the Grid Manager, among others, on the status of grid jobs, grid users and queuing system.

The local databases in the MDS-based system are responsible for implementing the first-level caching of the providers’ output and answering queries by providing the requested Grid information to the clients through the LDAP protocol. Globus created a LDAP back-end for this purpose called the GRIS (Grid Resource Information Service). NorduGrid uses this back-end as its local information database. Local databases are configured to cache the output of the NorduGrid providers for a certain period.

Soft-state registration mechanism of MDS is used by the local databases to register their contact information into the registry services (indices) which themselves can further register to other registries. The soft-state registration makes the Grid dynamic, allowing the resources to come and go. Utilization of the soft-state registration made it possible to create a specific topology of indexed resources.

Registries (or index services) are used to maintain dynamic lists of available resources, containing the contact information of the soft-state-registered local databases. It is also capable of performing queries by following the registrations and caching the results of the search operations (higher-level caching mechanism). The Globus developed backend for the registries is called GIIS (Grid Information Index Service). The higher-level caching is not used by the NorduGrid.
Project, and index services are working as simple dynamic "link catalogs", thus reducing the overall load on the system. In the NorduGrid system, clients connect the index services only to find out the contact information of the local databases (or lower level index services), then the resources are queried directly.

The local databases and index services of the NorduGrid testbed are organized into a multi-level tree hierarchy. It attempts to follow a natural geographical hierarchy, where resources belonging to the same country are grouped together and register to the country’s index service. These indices are further registering to the top level NorduGrid index services. In order to avoid any single point of failure, NorduGrid operates a multi-rooted tree with several top-level indices.

### 3.4. User Interface and resource brokering

The user interacts with the NorduGrid through a set of command line tools. There are commands for submitting a job, for querying the status of jobs and clusters, for retrieving the data from finished jobs, for killing jobs etc. There are also tools that can be used for copying files to, from and between Storage Elements and Replica Catalogs and for removing files from them. The full list of commands is given below:

- **ngsub** – job submission
- **ngstat** – show status of jobs and clusters
- **ngcat** – display stdout or stderr of a running job
- **ngget** – retrieve the output from a finished job
- **ngkill** – kill a running job
- **ngclean** – delete the output from the cluster
- **ngsync** – recreate the user interface’s local information about running jobs
- **ngcopy** – copy files to, from and between Storage Elements and Replica Catalogs
- **ngremove** – delete files from Storage Elements and Replica Catalogs

More detailed information about these commands can be found in the User Interface user’s manual, distributed with the NorduGrid toolkit [12].

When submitting a Grid job using **ngsub**, the user should describe the job using extended RSL (xRSL) syntax (Section 3.3). This piece of xRSL should contain all the information needed to run the job (the name of the executable, the arguments to be used, etc). It should also contain a set of requirements that a cluster must satisfy in order to be able to run the job. The cluster can e.g. be required to have a certain amount of free disk space available or have a particular set of software installed.

When a user submits a job using **ngsub**, the User Interface contacts the Information System (see Section 3.3): first to find available resources, and then to query each available cluster in order to do requirement matching. If the xRSL specification states that some input files should be downloaded from a Replica Catalog, the Replica Catalog is contacted as well, in order to obtain information about these files.

The User Interface then matches the requirements specified in the xRSL with the information obtained from the clusters in order to select a suitable queue at a suitable cluster. If a suitable cluster is found, the job is submitted to that cluster. Thus, the resource brokering functionality is an integral part of the User Interface, and does not require an additional service.
3.5. Resource specification language

The NorduGrid architecture uses Globus RSL 1.0 [4] as the basis for the communication language between users, UI and GM. This extended functionality requires certain extensions to RSL. This concerns not only the introduction of new attributes, but also the differentiation between the two levels of the job options specifications:

- **User-side RSL** – the set of attributes specified by a user in a job description file. This file is interpreted by the User Interface (Section 3.4), and after the necessary modifications is passed to the Grid Manager (GM, Section 3.1).

- **GM-side RSL** – the set of attributes pre-processed by the UI, and ready to be interpreted by the GM.

This dual purpose of the RSL in the NorduGrid architecture, as well as re-defined and newly introduced attributes, prompted NorduGrid to refer to the used resource specification language as "xRSL", in order to avoid possible confusion. xRSL uses the same syntax conventions as the core Globus RSL, although changes the meaning and interpretation of some attributes. For a detailed description, refer to the xRSL specifications distributed with the NorduGrid toolkit [12].

Most notable changes are those related to the file movement. The major challenge for NorduGrid applications is pre- and post-staging of considerable amount of files, often of a large size. To reflect this, two new attributes were introduced in xRSL: `inputFiles` and `outputFiles`. Each of them is a list of local-remote file name or URL pairs. Local to the submission node input files are uploaded to the execution node by the UI; the rest is handled by the GM. The output files are moved upon job completion by the GM to a specified location (Storage Element). If no output location is specified, the files are expected to be retrieved by a user via the UI.

Several other attributes were added in xRSL, for convenience of users. A typical xRSL file is:

```plaintext
&{(executable="ds2000.sh")
(arguments="1101")
(join="yes")
(rsl_substitution=
  ("TASK" "dc1.002000.simul"))
(rsl_substitution=
  ("LNAM"
   "dc1.002000.simul.01101.hlt.pythia_jet.17")
   (stdout=$(LNAM).log)
   (inputfiles="(ds2000.sh"
    "http://www.nordugrid.org/$(TASK).NG.sh")
   (outputFiles=
    $(LNAM).log
    rc://dc1.uio.no/2000/log/$(LNAM).log)
   (jobname=$(LNAM))
   (runtimeEnvironment="DC1-ATLAS")
```

A more detailed explanation can be found in [1]. Such an extended RSL appears to be sufficient for job description of desired complexity. The ease of adding new attributes is particularly appealing, and NorduGrid is committed to use xRSL in further development.

3.6. Monitoring

The NorduGrid provides an easy-to-use monitoring tool, realized as a Web interface to the NorduGrid Information System. This Grid Monitor allows browsing through all the published information about the system, providing thus a real-time monitoring and a primary debugging for the NorduGrid.

The structure of the Grid Monitor to great extent follows that of the NorduGrid Information System. For each class of objects, either an essential subset of attributes, or the whole list of them, is presented in an easily accessible inter-linked manner. This is realized as a set of windows, each being associated with a corresponding module.

The screen-shot of the main Grid Monitor window, as available from the NorduGrid Web page, is shown in Fig. 4. Most of the displayed objects are linked to appropriate modules, such that with a simple mouse click, a user can launch another module window, expanding the information about the corresponding object or attribute. Each such window gives access to other modules in turn, providing thus a rather intuitive browsing.

The Web server that provides the Grid Monitor access runs on a completely independent machine, therefore imposing no extra load on the NorduGrid, apart of very frequent LDAP queries (default refresh time for a single window is 30 seconds).

3.7. Software configuration and distribution

Since the Grid is supposed to be deployed on many sites, it implies involvement of many site administrators, of which not all may be Grid experts. Therefore the configuration of the NorduGrid Toolkit was made as simple as possible. It basically requires writing two configuration files: `globus.conf` and `nordugrid.conf`. The `globus.conf` is used by the
The grid-config package, which configures the information system of the Globus Toolkit from a single file. This configuration scheme was developed as a joint effort of NorduGrid and EDG and thus is not NorduGrid-specific. The nordugrid.conf file is used for configuring the various NorduGrid Toolkit components.

This approach proved to be very convenient and allowed to set up sites as remote from Scandinavia as Canada or Japan in a matter of hours, with little help from the NorduGrid developers.

The NorduGrid Toolkit is freely available via the Web site as RPM distributions, source tar-balls as well as CVS snapshots and nightly builds. Furthermore, there is a stand-alone local client installation, distributed as a tar-ball and designed to be a NorduGrid entry point, working out-of-the-box. Since it contains the necessary Globus components, it can be used to interact with other Grids as well.

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