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Practical Grid Interoperability: GridPP and the National Grid Service

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Abstract

In this paper, we discuss experiences with making the two large national Grids interoperable, the National Grid Service, NGS, and the UK Grid for particle physics (GridPP). We describe the current state, ongoing convergence efforts, and suggest future directions.

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1 Introduction

The two large national Grids in the UK are the National Grid Service (NGS), and GridPP, the UK Grid for particle physics, a part of the Large Hadron Collider Computing Grid (LCG). Much of the infrastructure is common, but there are important differences in how they operate. More importantly, each Grid could benefit from work done or experiences learnt in the other.

NGS consists of 4 funded sites and a growing number of partners and affiliates. It is a heterogeneous grid with different CPU architectures and OS (including prospective Windows sites) and partners which offer services not based around computation and storage (e.g., GridSAM and service hosting).

2 Comparing GridPP and NGS

2.1 Authentication

Both NGS and GridPP use X.509 certificates and Globus security (GSI) which is a derivative of X.509, so technically, NGS and GridPP are already interoperable in authentication, but there are some caveats ($\S2.1.2$). Furthermore, NGS has made significant advances in this field which we cover very briefly in this paper ($\S2.1.1$, 2.1.3, and 2.1.4).

2.1.1 Login Users in GridPP log into the User Interfaces (UIs, machines running user client software) using ssh. Thus, GridPP users must have both X.509 certificates and ssh key pairs. This is considered acceptable, since most GridPP users are familiar with both ssh and digital certificates.

NGS, in contrast, uses gsissh, that is, ssh amended to accept X.509 and GSI, thus ensuring that users only need X.509. They use X.509 certificates to log into the Grid cluster head nodes, and also run jobs from them. The process is facilitated by a MyProxy. MyProxy is used both to get a proxy to log into the head node, and to get a proxy to run jobs (and potentially to renew the proxy if the job runs longer than the proxy). The process is further facilitated by NGS' Java gsissh terminal, a Java gsissh terminal enhanced by NGS to talk to MyProxy [13].

2.1.2 X.509 The UK e-Science Certification Authority (CA) provides "medium assurance" digital certificates to Grid and e-Science users in the UK. As the only IGTF-accredited [9] CA covering the UK, it covers both user communities.

In general, each site can of course decide to trust other CAs at their discretion, but most coordinated Grids make recommendations regarding which CAs sites should trust. As a rule both Grids trust all IGTF-accredited CAs, but there are some practical differences. GridPP trusts the CA from the Fermi National Accelerator Laboratory because LCG does, despite the fact that this CA is not yet IGTF-accredited. Likewise, NGS trusts certain CAs accepted by the TeraGrid, such as the Pittsburgh SuperComputing Centre CA, to promote interoperability with TeraGrid.

We expect these will converge, as the US CAs get IGTF accredited. This is an on-going and time consuming process, and many of these CAs have for historical reasons different practices from the CAs in the rest of the Grid.

Another practical difference is that GridPP has a "catch-all" CA via LCG (namely, the CERN CA). This means that a user who does not have a "local" CA can get a certificate via this CA. NGS does not have such a facility, although could perhaps use EGEE's catch-all (CNRS France). Another possibility is to trust certain educational PKIs (Public Key Infrastructures), or commercial ones. Most NGS customers are of course covered by the UK e-Science CA, but UK scientists do collaborate with scientists from other countries who will need access to the same resources.

Finally, it should be mentioned that many novice users find digital certificates "hard to learn." Usability studies show this, also the ones performed by the NGS [14], and the NGS has done work to ease this with applets and other relatively simple java applications to ease the certificate management.

2.1.3 Shibboleth - NGS Shibboleth is being deployed by JISC to replace Athens for the higher and further education institutions in the UK. If we can make use of the UK Shibboleth infrastructure for authenticating to the Grid, then the user base becomes much larger.

This was the aim of the ShibGrid project [15] (the sister project SHEBANGS [18] looked at embedding VOMS attributes). Briefly, users log in to a portal and generate a full certificate or GSI



Figure 1: EGEE sites in April 2007

proxy transparently from a MyProxy server, and other tools enable credentials to be uploaded and downloaded from MyProxy. A second round of JISC funded projects has started follow-on work. 2.1.4 Credential Conversion - NGS

Shibboleth (§2.1.3) was built to enable users to log in to remote web-based resources using their home organisation id. However, many organisations already have an authentication infrastructure, such as Microsoft Active Directory or Kerberos. In these cases, there is a persistent (or rather, transparently renewed) token identifying the user.

The NGS has done additional work [16] to generate certificates or GSI proxies transparently using this site token. Thus, the user does not even need to go through the slightly clumsy Shibboleth process of selecting their home institution and typing their username and passwords. The site needs to run a conversion CA, also based on MyProxy, so the home token never leaves the home organisation. If this becomes wider deployed by the NGS, it can potentially make Grid access completely transparent for the user.

2.2 User Base

A simple count shows about 500 "members" of the NGS VO, of which 13 are outside the UK. Another 35 people are members of the OGF GIN ("grid interoperability now") VO which aims to make various flavours of Grid middleware interoperate. Both GridPP and NGS participate in GIN activities.

GridPP is, of course participating, in the LCG, so potentially has many thousands of users from the LHC VOs alone. In addition many non-LHC VOs are supported as part of the EGEE project (§2.2.1), including Biomedical, Astronomy and, now, industrial VOs (§2.2.3).

2.2.1 EGEE The European *Enabaling Grids for eScience*[5] project, which is now in its second phase, grew out of the European Data Grid Project (EDG), which developed the first set of testbed middleware for the European grid.

EGEE has been funded until April 2008, and a further 3 year EGEE IIII project, funded until 2011 is anticipated.

EGEE has now grown to encompass more than 32 countries, many outside of Europe, and the EGEE production grid, of which GridPP forms a part, consists of well over 200 sites (see Figure 1). The total available resources consist now of more than 37000 job slots and more than 20PB of storage resource.

With such a large production infrastructure much emphasis in EGEE is now placed on providing a production quality grid which can be reliably used by European researchers. Operations therefore play a significant role in the project, with the various monitoring systems ($\S2.7$) being actively used

by teams of *Grid Operators on Duty*, grid experts provided by the *Regional Operations Centres* (ROCs) provided by EGEE partners. GOoD teams will raise tickets against failing sites to resolve problems and can, *in extremis* suspend sites from the grid.

The tickets are channeled back through the ROCs, which play the role of co-ordinating EGEE activities and operations each region. In the UK the ROC is based at RAL and runs grid services for both GridPP and NGS, e.g., the UK/I certification authority (§2.1.2).

Work has been done to make the NGS and GridPP helpdesks interoperate; this work is complex and beyond the scope of this paper.

2.2.2 Training EGEE runs the GILDA project ([19]), which issues short lived certificates from a dedicated non-IGTF CA that can be used on a small testbed grid, run by some EGEE partners. The EGEE NA3 group at NeSC in Edinburgh run training courses for NGS as well, with certificates from another dedicated training CA.

2.2.3 Industry Through GridPP's relationship with EGEE there are extensive links to industrial partners. The EGEE Industry Forum has members from many industrial partners across Europe and has run many "Industry Days", where EGEE and grid technologies are presented to industry. EGEE's GILDA [19] testbed is used to demonstrate that grid methods are effective and to provide specialist help necessary in enabling industrial applications to run on the grid.

Recently, as a development of this process, the camont (Cambridge Ontology, [20]) and totalep (Total Oil Exploration and Production, [21]) VOs have been enabled at a number of GridPP sites. This is the first time that industrial partners have been given access to the production infrastructure of GridPP. Although the guaranteed resources available are modest, the possibility of then opportunistically using GridPP clusters when other VOs are not active is opened up.

2.3 Information System

An integral component many Grids is the Information System which gathers information from services from that Grid. It then makes this information available to clients for the purposes of determining which services are available and choosing the best services. The information servers typically publish in LDAP format, with a schema called GLUE, now an OGF standard. Both GridPP and NGS use version 1.2 [4], and although 1.3 has been finalised, there are no plans to switch to 1.3. We will need at least a clear migration path from LCG or EGEE.

Resources provide information via "Grid Resource Information Services" (GRIS) running (usually) locally to the resource, and this information is aggregated in one or more higher level server known as Grid Index Information Services (GIIS). In NGS, a single top-level GIIS is the central location to service all queries across the Grid, whereas in GridPP, the larger sites themselves can have more than one GIIS.

Prior to the launch of the NGS, various Information Systems were tested in the UK e-Science Level 2 Grid pre-production environment. Initially the Globus Toolkit Monitoring and Discover Service (MDS) [1] was used. However, the MDS at the time relied upon a client push model where the GIIS waited for information to be "pushed" by the individual GRISes and this proved to be unstable as the individual GRIS daemons were prone to locking, resulting in the catastrophic effect of freezing the top level GIIS. As an alternative, the Berkeley Database Information Index (BDII) [3] from LCG was tested and found to be a more stable model. Unlike the Globus MDS, BDII uses a server pull model, where the GIIS regularly polls individual GRISes for information. BDII proved to be far more reliable than the Globus MDS and more scalable.

As a result, interoperation between Grids running both Globus based middleware and gLite using GLUE is straightforward in terms of compatibility sharing, aggregating, and querying information.

2.4 Storage Element

Due to lack of space, we cover only the DPM Storage Resource Manager (SRM) from LCG. The NGS uses the Storage Resource Broker, which was also tried by one experiment in LCG, but in LCG it was decided to go with SRM.

2.4.1 DPM The report from the Grid Engineering Task Force [24] from an evaluation of DPM for suitability for deployment by NGS has recommended that NGS sites could deploy DPM to provide SRM interfaces to storage.

DPM is also widely deployed within GridPP, being the production SRM at 12 of the 17 GridPP Tier-2 sites. Initial deployments were on a small scale, however as GridPP Tier-2 centres ramp up



Figure 2: Total read rate with DPM

their storage in advance of LHC data, DPM is now deployed in sites managing storage of 50TB, and this will shortly rise to well over 100TB.

GridPP have also contributed to the development of DPM, and currently maintain the generic information provider plugin which allows DPM sites to correctly publish used and available storage into the BDII.

GridPP has also been very active in helping to test DPM to ensure that its performance matches the expectations, particularly those of the LHC VOs, who will need to analyse TB of data at is Tier-2 centres ([22]). This testing has shown that the read rates achieved with DPM over the LAN are good (Figure 2), but that some problems exist with trying to open large numbers of files simultaneously (Figure 3). These problems are being addressed now by the developers and tests will be repeated when a new release of DPM is available.

2.5 Computing Element

2.5.1 Resource Broker and Job Submission A resource broker presents the user with a common interface to all resources that are available to that user at any one time. The user can submit jobs to a resource broker specifying his job requirements, and the resource broker makes use of the information provided by the Information System to choose the best suited resource to send the job.

The NGS is currently trialing two resource brokers, the gLite Workload Management System and Logging and Bookkeeping Service (WMS-LB) developed by EGEE [5] and the GridWay Metascheduler [6]. The latter is in its very early stages of testing, but the NGS gLite WMS-LB (hereafter known as the NGS RB) was deployed in preproduction in March 2007, and is able to send jobs to NGS sites publishing information conforming to the GLUE schema to the NGS BDII server. Users can make use of the RB by interacting with it using the gLite client tools, typically installed on a node known as a User Interface (UI). A UI hosted at RAL is available for anyone who is a member of the NGS [8]. Alternatively, users can use an NGS RB-enabled portal such as the P-GRADE portal hosted by the University of Westminster [10]. There are also plans to support the NGS RB by the NGS Portal [11].

Currently all core NGS sites can accept jobs from users making use of the NGS RB. Work is currently under way to configure the non-core NGS sites to interoperate with the NGS RB.

The fact that the NGS RB is a component of gLite means that it can easily interoperate with



Figure 3: Open failures in rfio_open() call in DPM

Grids running EGEE middleware such as GridPP. In contrast to this, more work was required in configuring the NGS RB to work with NGS itself whose computing nodes are not based on EGEE middleware. This was as a result of the NGS RB not defaulting to a standard Globus environment if an LCG or gLite CE is not installed on the computing node, although it is planned that this will be addressed in future versions of the WMS-LB.

Transparent interoperability can be achieved on both GridPP and the NGS if, among other requirements, the following conditions are fulfilled

- An Information System is configured to aggregate information from both Grids. Presently the development NGS BDII server aggregates data from both core NGS sites and a sample subset of GridPP consisting of all GridPP resources at RAL.
- The user is authorized to use an RB which is configured to use the Information System mentioned above. Both NGS and GridPP have deployed and are using VOMS (Virtual Organization Management Service) [12] as a means of managing user authorization in the context of VOs(10). Using the VOMS hosted by Manchester, users from both the NGS VO and the DTEAM development EGEE VO are currently authorized to the NGS RB. This resource broker is additionally configured to query the development NGS BDII server described above.
- There are resources across both Grids that users from either Grid are authorized to use. All NGS core sites are configured to authorize members of the DTEAM and NGS VOS. Other VOs that are currently using GridPP will be invited to apply for access to the NGS, and when they do, their applications will be considered. On the other hand, GridPP have also agreed to authorize members of the DTEAM and NGS VOs to use their resources. However, due to a current limitation of the LCG middleware in not recognizing the new DNS style VO naming convention which the NGS VO uses, members of the NGS VO GridPP are as yet unable to use GridPP resources via the NGS RB.

At the time of writing, interoperability is possible between the NGS and GridPP but true bilateral interoperability is only possible for members of NGS or GridPP who are members of the DTEAM VO. Thus a proof of concept has been achieved showing that technically interoperability

is a possibility with the current middleware configurations, but more work is needed before true interoperability is a reality for the end users of both Grids.

2.5.2 Computing Element GridPP: The most widely deployed production compute element in gLite is the LCG-CE. This is a slightly modified version of the Globus Toolkit 2 gatekeeper, incorporating performance and security fixes.

The default job wrapper used, lcgpbs, has been modified to limit resource consumption on the gatekeeper. This is done by having a single gatekeeper process monitor all of the jobs submitted through the same resource broker for a user. The lcgpbs job manager is also able to manage jobs on clusters where the pool accounts do not share home directory spaces (this is helpful in larger clusters where, e.g., NFS scaling problems can be seen).

However, the standard GT2 pbs job manager is still available. Although it is not enabled by default, a number of GridPP sites which support the NGS have enabled it to have better compatibility with NGS job submission.

This is important because the way that certain options to the pbs and lcgpbs job managers are handled is different. e.g., the -np option (number of processes) will fork N processes within a single job slot with the lcgpbs job manager, which is often not the desired or expected behaviour for users used to the standard GT2 job manager.

However, in the longer term, the intention is to migrate to the new gLite CE. The gLite CE is based on Condor-C, which can submit jobs to all common batch systems (Torque, LSF, SGE). X509 authentication has been added to integrate with the gLite WMS-LB system.

The gLite CE also supports BLAH (Batch Local ASCII Helper) protocol, which makes it considerably easier to pass job parameters from the resource broker into the local batch system.

Despite being released in production as part of gLite the gLite CE is not yet considered stable enough for the majority of sites to use. However, as it is intended that the next major release of the gLite middleware (compiled for Scientific Linux 4) will not include support for the LCG-CE an intensive program of robustness and scalability testing is now going on.

It would seem likely that both CEs will co-exist for sometime, even if the LCG-CE is running on the older SL3 architecture.

NGS: In the NGS a standard Globus Toolkit 2 gatekeeper is deployed. The job managers vary from site to site. The list of batch systems used within the NGS include PBSPro, LSF, SGE, Condor.

Within the partners of the NGS it has been necessary to make several changes, both to how the grid middleware has been installed, either on the head node of the system or a connectivity box but also the actual software installed itself.

The connectivity boxes have been necessary particularly where we have been connecting resources which do not have good middleware support, for example Windows, SGI or Solaris systems. These connectivity systems are normally installed with a Linux variant that is Scientific Linux compatible. These are designed to be simple submission nodes for the scheduling system which is installed onto the main system as well as all the services of the middleware such as jobmanager, information server etc. This has also allowed the fears of some resource owners to be calmed. If they are unhappy with the resource utilisation of the Globus services themselves or their behaviour, for example if there was a security threat, then switching them off and removing connectivity from the cluster is merely a matter of removing a network cable.

Due to the heavy usage it has also been necessary to alter the Globus Jobmanagers. Globus 2 jobmanagers operate in a constant polling cycle which when there has been a very large number of tasks submitted can introduce a significant load onto the head node of the system, in some cases with enough submitted tasks making the system unusable. As a work around for this IO it is necessary introduce a wait period within the polling routine so that the status of the task that is connected to that instance of the running job manager is only checked once per minute. Since most tasks run within the grid operate for longer than three or four minutes then a 30 second wait was deemed acceptable. This has reduced load in some cases from approximately 75% to approximately 10% on the relevant system head node. This is an alteration that has been made to all jobmanagers for resource scheduling systems.

Other changes to jobmanagers have been made to individual systems, in particular Condor resources which have a specially altered jobmanager for situations where the pool that is being supported does not have a shared filesystem. This results in needing to alter not only the scheduler specific file 'condor.pm' but also the jobmanager.pm file to ensure that input and output files are correctly transferred between the master and workers within the pool.

2.5.3 CondorG Within the Condor eco-system Condor-G has been designed to connect a grid resource to a standard condor Condor system [2]. This includes support for native submission with the appropriate options added to the job submission script. Condor includes a different 'universe' for submission through different mechanisms. To use grid resources the user must include the 'universe = grid' in the submission script as well type of grid software that the resource has installed. For the NGS the minimum software stack the submission script looks as below for submission to the Oxford NGS-1 node (last line broken):

```
executable = /bin/date
universe = grid
grid_type = gt2
globusscheduler = grid-compute.
oesc.ox.ac.uk/jobmanager-pbs
```

Thus, users specify the exact resource that they wish the job to be run on. Within the Condor-G system itself though there is no automated way of discovering resources available to the user. It is though also possible to add options that can be passed through to the remote resources such as queue name etc. As shown above, submission to the NGS uses the basic options where queue name etc. are not necessary. However, when submitting to GridPP resources it is necessary to define the queue on the remote resource since Condor-G does not support VOMS additions to the user credentials.

2.6 Installed software

The method by which the nodes of the NGS both core and partner handle with installed software is very different. Within the NGS-1 core sites there was a conscious decision to use the system provided by Clustervision to load preinstalled software as modules which the user specifies before they then run remote jobs. This includes commercial software that requires specific licensing agreements. It should note that not all of the core sites have the same software since independent deals have been agreed by each of the four hosting institutions.

An example of the way that licensed software has been dealt with is the Gaussian computational chemistry package[7] which has been installed on the STFC node. There when each new user wants to use the package they must first locally register with the STFC e-Science group so that they can add the pool account name into a physical Unix group that has permissions to access the package. This is only a local solution, though, independent for each node since there is currently no method of propagating both the software itself and the permissions/license agreements between nodes. For open source licensed software there has been an attempt to install a common set of applications across all nodes for which the particular application is supported.

Unlike the NGS as a whole, GridPP is much more homogeneous, both in its hardware infrastructure, operating systems, middleware, and applications. Most sites are running a flavour of Scientific Linux 3 (SL3, based on Red Hat Enterprise Linux) and are currently upgrading to SL4. The gLite middleware was developed for SL3, and as of release 3.1, gLite developers are working on migration to SL4. The original LCG goals of wide portability have not been met. This affects the NGS with its more heterogeneous infrastructure.

Unlike NGS, each GridPP site supports typically only one major experiment, but provides some resources to most GridPP VOs. Various mechanisms have been invented to allow the experiments to propagate non-standard (not included in the default release) software to the sites, such as the "VO box" or "pilot jobs" which pull in applications for the real jobs. Software is always open source so there is no licencing issues, except for the "3D" (distributed database deployment) which uses Oracle.

The GridPP deployment models is based on official releases, which are then usually deployed as a "pre-production service." A deployment team is responsible for coordinating the deployment in the UK and testing the software on GridPP resources. The NGS deployment is based on the user's requirements, but also on the recommendations of the Engineering Task Force (ETF). The role of the ETF is mainly to make technical evaluations of Grid middleware, to provide guidelines for the diverse NGS sites. The NGS deployment model for the core sites could thus be brought closer to the GridPP model — or vice versa. Where GridPP has a deployment team, the NGS has the "operators", system administrators from the NGS sites, with a similar role. The NGS as a whole will need to cater for diverse sites, and GridPP could fit into this diversity. At the same time, plans should be made to test interoperability between the homogeneous core sites and the non-standard sites, insofar as they run the same services.

2.6.1 Globus The NGS makes use of the Globus Pre-WS software, Globus Toolkit 2. Since this has been unsupported by the Globus Alliance for some time, the software is currently supplied by the Virtual Data Toolkit. This includes several patches to give extra functionality. Firstly the standard version of the Globus toolkit requires a local user account and within a large multi-institutional grid this is not sustainable. The VDT system includes a patch which allows for the remote user's Distinguished Name (the name in the certificate) to be matched with a transient local pool account. This patch was originally designed by the GridPP collaboration since they have exactly the same problem.

There are plans to update this installation to Globus Toolkit 4 Pre-WS so that the upgrade path to WS based services is easier. This will be done through the use of the latest stable version of the VDT system. This will also allow for running a stable production service alongside a development environment using the WSRF based services. This can also be allowed to decide the full upgrade path dependant on real user demand.

2.7 Monitoring

NGS monitors sites using the GITS (Grid Integration and Test Scripts), developed by the NGS's Engineering Task Force. This is an active monitoring system, where jobs and services on each of the NGS sites are probed directly.

INCA has been adopted by the NGS as part of its monitoring framework. The GITS tests have been integrated within INCA and the framework implements a "some-to-all" testing model, that is, testing is performed from some (not all, but more than one) site and tests are performed against all sites.

Further work on INCA is planned to allow it to implement monitoring as specified in the NGS Monitoring Specification document [17].

A number of monitoring schemes are in place within GridPP. The first of these is the gstat monitor. This system polls the information as published by each GridPP site's BDII 2.3 and carries out basic sanity checks.

Although these checks are quite simple, as the information published by the site represents the face of the site on the grid, problems at this level can severely impact the performance of the site, e.g., if the SRM storage system end points are not properly published then jobs may not be able to store their output, leading to wasted CPU cycles. Worse, in certain circumstances a poorly configured site may affect the performance of the whole grid, e.g., if empty queues are advertised on a site which is blackholing jobs, then large numbers of jobs on the grid may disappear.

Sites are encouraged to regularly monitor their status within gstat and deal with any anomalies. In addition, as the information system snapshots the state of sites, it can be used as the basis of trend monitoring, e.g., storage use by VOs. The EGEE storage accounting system, which was developed by GridPP, uses this method to record storage uses by each VO on each site ([23]).

However, gstat is only a passive system and thus rather limited in what it can probe at a site. For this reason a much more active monitoring system, the Service Availability Monitoring (SAM) system is also deployed.

SAM tests a site actively, either by directly testing advertised services at a site, e.g., the SRM storage interface, or by submitting jobs to the site which perform basic functionality. The core tests consist of ensuring that:

- A job can be submitted successfully to the site's CE through a resource broker.
- That the version of the gLite software found on the batch worker is valid.
- That the CA certificates found on the site are valid and up to date.
- The hostname of the job's broker is defined and is consistent.



Figure 4: EGEE Sites Passing Basic SAM Tests

- That the csh environment is sane.
- That basic replica management tasks can be performed:
 - A valid host for the information system provider is found.
 - A file can be copied from the worker node to the site's storage system and registered in the file catalog.
 - The file can be copied off the storage system
 - This file can be replicated to an off site storage system.
 - The file can be deleted from both storage systems.

If any of these tests fail then the site is considered to be unavailable. If tests fail for any length of time a ticket will be raised against the site.

Experience suggests that testing sites in this way does improve sites' performance, as shown in Figure 4.

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3 Conclusion

In this paper, we have presented a whirlwind tour of getting the two national Grids, NGS and GridPP, to interoperate. We have focused the areas that are either most mature, or most urgent to resolve. Specifically, we have covered authentication, information systems, job submission and resource brokering, monitoring, and computing and (briefly) storage elements. We have outlined where we have already achieved interoperability and specific areas for further work. Future developments will see further interoperability, to the benefit of UK science.

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