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GridPP: Meeting the Particle Physics Computing Challenge

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GridPP: Meeting the Particle Physics Computing Challenge

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GridPP is a £33m, 6 year project, funded by PPARC that aims to establish a Grid for UK Particle Physics in time for the turn on of the CERN Large Hadron Collider (LHC) in 2007. In phase 1, the project established a large-scale prototype Grid across the UK. The project has now entered phase 2, and is developing the prototype testbed into a production service. LHC computing technical design reports and the necessary baseline services are reviewed. The steps necessary to establish a system of sufficient functionality, robustness and scale are described in order to meet the Particle Physics Computing Challenge.

1. Introduction

In 2007, following more than ten years of preparatory work, the Large Hadron Collider (LHC) at CERN, Geneva will start to collide protons with an energy equivalent of 7 trillion volts to recreate the conditions that prevailed in the universe at the earliest moments of the “Big Bang”. A billion interactions will be generated every second and amongst them perhaps one event will involve the production of a Higgs boson, responsible for the intrinsic mass of all the other fundamental particles. This will rapidly decay and its daughter particles will be detected in massive twenty metre high detectors with up to twenty million readout channels.

The data will be efficiently filtered using dedicated electronics, but the data rates will still be enormous with around 10 PetaBytes of data produced each year from each of the four experiments. Thousands of physicists from all around the world will be eager to analyse the first data. Tens of millions of lines of analysis code will be written and more than 100,000 processors will be required, operating continuously over many years. This is the nature of the LHC Computing Challenge. The overall requirements are huge: in 2008, corresponding to the first full year of data taking, CPU capacity of 140 million SPECint2000 (140,000 3 GHz processors), 60 PB of disk storage and 50 PB of mass storage will be needed.

Particle physicists have chosen Grid technology to meet the LHC computing challenge; this is a hardware and software infrastructure that provides dependable, consistent, pervasive and inexpensive access to high-end computational capabilities. The system must allow sharing of data between thousands of scientists with multiple interests; link major and minor computer centres across the globe; ensure all data is accessible anywhere, anytime; grow rapidly, yet remain reliable for more than a decade; cope with different management policies at different centres; ensure data security; and be up and running routinely by 2007. The Grid is a practical solution to meet this and many other challenges in various areas of science, as part of the UK’s e-Science programme. Here we concentrate on the scale of the infrastructure, the tests that have been performed in recent months, and the plans for the second phase of the GridPP project, going from prototype to production.

In September 2001, the UK defined its aims in e-Science and the GridPP1 project commenced. It aimed to develop a highly functional prototype Grid deployed across the UK, consisting of more than 1000 CPUs, capable of accessing a PetaByte (PB) of data linked to computer centres around the world. This was achieved by the GridPP collaboration via a Grid deployed at institutes across the UK. The UK Grid is integrated seamlessly with the international LHC computing Grid project. This prototype is now of significant scale with more than 10,000 CPUs linked and able to access 5 PB of data across more than 100 institutes worldwide. This is illustrated in a snapshot of the LCG map (appended), monitored via the Grid Operations Centre at the Rutherford Appleton Laboratory (RAL). Sites across Europe are linked to those in the Far East and North America. This prompted The Economist to declare the LCG the World’s Largest Grid in October 2004. The UK is the biggest single contributor to the LCG, with more than a fifth of the Grid's processing power at its 16 sites. In addition 4 sites linked via the UK e-Science National Grid Service are using much of the same middleware to provide a service for a wide range of academic research projects. September 2004 saw the start of the GridPP2 project, aiming to produce a production Grid in the UK with 10,000 CPUs.

1.1 Prototype Deployment

The prototype system was intensively tested during 2004 through a set of planned stress tests by each of the 4 LHC experiments. Individual experiments accumulated up to 400 CPU years' worth of test data, with individual jobs running for up to a day and a peak load of almost 6,000 simultaneous jobs achieved in August 2004. The tests enabled the experiments to conclude that the Grid provided the necessary functionality. The power of the Grid resource discovery method was illustrated in July 2004 when 300 new CPUs at RAL were brought online and automatically discovered and fully used within 8 hours, accessed via the Grid middleware.

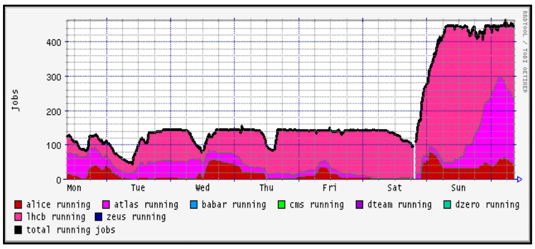


Figure 1: Startup of Grid Production indicated by the increase of jobs at the UK Tier-1 Centre in July 2004.

1.2 Middleware

Middleware is the key to a successful Grid; for LCG, the initial software stack of more than one million lines of code was developed and tested in conjunction with the European DataGrid and Enabling Grids for E-sciencE (EGEE) projects, building upon earlier work by the US-based Globus and Condor projects. This enables a user anywhere in the World, armed with his/her virtual passport (a digital certificate) to submit an analysis job to a Workload Management System (WMS). As a member of a recognised experiment (or Virtual Organisation, VO), the job will run a few minutes later on any of the sites with pre-installed VO-specific software and the required hardware for the job. This is a powerful generic methodology, applicable in many branches of science and industry, where access to large-scale computing resources are required, typically with demanding timescales, across the globe.

To submit a job to the Grid, firstly the user describes the needs of their job using a Job Description Language and submits it from a User Interface (UI) node to a WMS node. The WMS then matches the job's needs to the sites available and submits the job to the most suitable site. This matching process can take into account the location of the data that the job needs to analyse as well as the characteristics of the site (number of free CPUs, free storage space etc). The job then runs on the selected Compute Element (CE). After the job has completed, the small output files from the job are transferred back to the WMS ready to be collected by the user, while larger files may stored on a Storage Element (SE) and their location registered in the LCG File Catalogue (LFC). All changes to the state of a job are recorded in a database on the WMS. The user can interrogate this database in order to ascertain the current status of their jobs.

An SE does not necessarily *store* files, it may just *manage* the files in the mass storage system; the obvious exception being a disk-only SE which typically stores the files that it manages on its own disk. This architecture is very flexible because the higher-level middleware can access several types of SEs, and the SEs can manage different types of storage. The end user typically sees only the Logical File Name, LFN. This name is the "abstract" name, which refers to the file "on the Grid". The LFN contains no information about the physical location of the file.

1.3 Future Directions

The choice of middleware in this infrastructure is recognised to be of primary importance to all the experiments. A high-level assessment has been provided in the context of previous developments within GridPP, LCG and EGEE. This is summarised in Table 1 (appended). The definitive statement of requirements for LHC experiments is contained in the LCG Technical Design Report. An LCG sub-group (the Baseline Services Group) has worked to establish the set of fundamental services necessary to support the LHC experiments and it is these to which GridPP contribute and adhere. These services address 15 general requirement areas. The table summarises how these requirements can be met by the various software stacks.

The LCG software stack is built from components drawn from VDT and the European DataGrid project, with some other smaller additions. It forms the basis of the current production services for many sites participating in LCG including all the sites in the UK. As components of the EGEE/gLite middleware become mature they will be added to or replace components of LCG, but it is recognised that no single middleware development project will provide all the solutions necessary to meet global requirements of adequate production quality on the timescale of LHC. Rather, the solution will be built by integrating modules best matched to requirements and sourced from a number of projects. Gaps will be filled be complementary, small-scale developments.

The LCG/EGEE projects, by drawing from multiple sources to make the best matches to requirements, are already integrating a viable middleware stack and deploying, operating and monitoring this at a global scale. This is achieved through very extensive validation, testing and close cooperation with development teams. The LCG/EGEE middleware stack is seen as the only viable solution for GridPP, given the scale of the requirements and the constraints. With particular focus on the LHC experiments, this forms the basis for Grid computing to meet the forthcoming challenges. We believe that this middleware stack forms a good basis for other experiments as has been demonstrated by other non-LHC experiments and other scientific areas.

1.4 Grid Efficiency

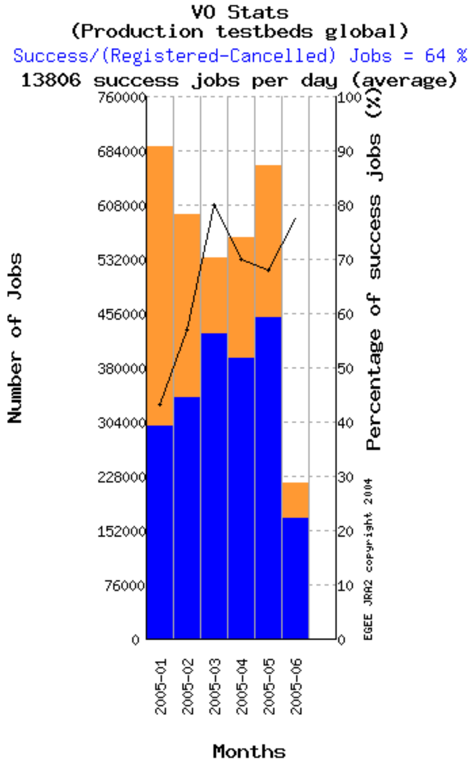


Figure 2: EGEE Overall Quality Assurance Metric for the first half of 2005. The total number of jobs per month is indicated by the blue histogram. Successful jobs are indicated by the red histogram. The line indicates the percentage success rate of the WMS.

The efficiency of the system is not optimal, but has been improving during the first half of 2005. This is illustrated in Figure 2, which shows the percentage of successful jobs recorded in the WMS database.

The data should be handled with care: an end user may see either a worse efficiency if jobs failed for non-WMS reasons e.g. data management problems or may improve their efficiency by e.g. choosing selected sites according to the Site Functional Test (SFT) performance index or deploying an agent to initiate real jobs on worker nodes where the agent succeeded. The LHC experiments are able to select sites to improve their efficiency. In the LHCb case an agent is deployed such that the initial script success is not a significant issue. Following these sorts of approaches, acceptable (>90%) throughput is possible for each of the experiments as of June 2005, but the inherent complexity of the system is apparent and many operational improvements are required to establish and maintain a production Grid of the required scale.

1.5 Baseline Services

The LHC experiments have recently expressed their priorities with respect to 15 baseline services [1]. These are summarised in the table below where A represents high priority and mandatory; B indicates that standard solutions are required, but experiments could select different implementations; and C indicates it is desirable to have a common solution, but not essential. The priorities reflect the effort the experiments have made in a given area in the absence of “off the shelf” solutions. The combined responses of the experiments can be used to categorise the priorities the experiments attach to establishing standards in a given area and are highlighted accordingly in Table 2.

Service	*ALICE*	*ATLAS*	*CMS*	*LHCb*
Storage Element	A	A	A	A
Basic transfer tools	A	A	A	A
Reliable file transfer service	A	A	A/B	A
Catalogue services	B	B	B	B
Catalogue and data management tools	C	C	C	C
Compute Element	A	A	A	A
Workload Management	B/C	A	A	C
VO agents	A	A	A	A
VOMS	A	A	A	A
Database services	A	A	A	A
Posix-I/O	C	C	C	C
Application software installation	C	C	C	C
Job monitoring tools	C	C	C	C
Reliable messaging service	C	C	C	C
Information system	A	A	A	A

Table 2: Priorities associated by the LHC experiments to the LCG baseline services [1].

1.6 LCG Technical Design [2]

The LCG baseline services should be viewed in the context of the LCG Technical Design Report. Here, the worldwide LHC Computing Grid includes LCG, the Open Science Grid in the US, and the Scandinavian NorduGrid: these three Grids comprise the total Grid resource available to each of the experiments.

In terms of future directions, each of the large LHC experiments must interface their software to the Grid; this is being developed as part of the LCG project. All experiments require a single VO operating across all flavours of Grid, along with a well-defined way to specify roles, groups and subgroups via VOMS (Virtual Organisation Membership Service). Services to support long-lived agents running in user-space for file transfer or job submission, for example, are expected to be provided at the sites. The experiments expect a standard interface for Grid access to SEs; it is envisaged this will be provided via a Storage Resource Management (SRM) standard interface. The interface must support usage quotas. In addition, it is expected that an SE will provide POSIX-like access to files for applications and present a single, logical file name space. All experiments expect to have an experiment-specific central data catalogue containing the LFN with corresponding metadata. In addition, three experiments expect that there will be a local file catalogue that will map the LFN to physical files. LHCb are currently planning to use a centralised catalogue (but expect replica(s) to be hosted to provide redundancy) to fulfil this functionality. CMS foresees it will perform data location through a two-tier service with a local component that publishes local file blocks and a global component that caches their locations, as used in the Globus Replica Location Service (RLS). All experiments expect a reliable file transfer to be provided via the Grid.

The experiments require a common interface to the CE, with the possibility to autonomously install application software and to publish VO-specific information. Worker Nodes (WNs) must present a standard environment configuration. LHCb, in particular, wish the WNs to have outgoing local and global network access for the site. There is a strong preference, from all experiments, that there should be an outbound network connection from the WNs, or at least the appropriate tunnelling mechanism. Some experiments request that a 'pilot agent' mechanism (an agent that runs basic tests on a WN before downloading a job from WMS to execute) be allowed. It is also required that a reliable WMS be provided. The main requirements are that it must be able to efficiently exploit the distributed resources; that it is able to cope with the foreseen job submission frequency; that it is able to handle bulk job submission; and that it supports usage quotas and prioritisation. It is important that the WMS has a reliable information system for the WMS matching and resource monitoring service that includes a connectivity matrix between all CEs and SEs to be available for match making. There should be a consistent schema across Grids for job monitoring, accounting and error reporting and the WMS should reliably report at least the exit code of the application. These considerations place significant constraints upon middleware providers.

In the following sections we summarise some of the key middleware components being used by the LHC experiments in the context of their large-scale computing requirements. These illustrate where the divergences in approach arise in the development of their extensive technical designs. By understanding the approaches taken by each of the experiments, the LCG and GridPP deployment teams are able to respond more effectively to their needs.

1.7 ALICE Computing [3]

The AliEn (AliCE Environment) framework has been developed with the aim of offering to the ALICE user community a transparent access to computing resources distributed worldwide through a single interface. The system is built around Open Source components and uses Web Services and standard network protocols. Less than 5% is native AliEn code (mostly PERL scripts), while the rest of the code has been imported in the form of Open Source packages and modules. The AliEn workload management system is based on the so-called ‘pull’ approach. The AliEn components incorporate significant middleware functionality: the ALICE approach is that when a standard Grid service is found to provide the same, or better, functionality than an ALICE-specific one, its adoption will be considered in order to reduce the maintenance load and increase portability and robustness of the ALICE computing environment.

The ALICE TDR emphasises the view the end-user physicist will have of the data using the ROOT system, employed widely in particle physics for analysis. An AliRoot framework has been designed whose basic design principles are re-usability and modularity, with the objective of minimising the amount of unused or rewritten user code and maximizing the participation of the physicists in the development of the code.

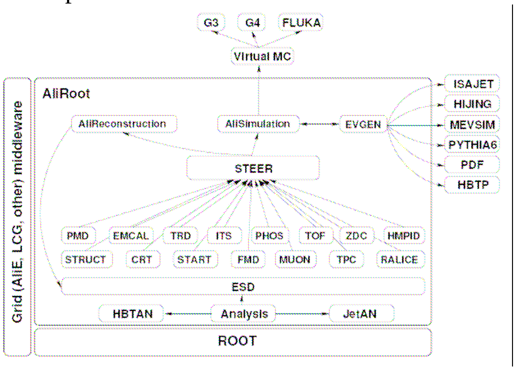


Figure 3: Schematic view of the ALICE AliRoot framework.

1.8 ATLAS Computing [4]

ATLAS has adopted the Workload Management Systems from elsewhere, enabling ATLAS developers to concentrate on the final distributed data management system for LHC startup, Don Quijote 2 (DQ2). The scope of the system encompasses the management of file-based data of all types (event data, conditions data, user-defined file sets containing files of any type). The requirements, design and development of the system draw heavily on the 2004 Data Challenge experience gained with the Don Quijote and Grid middleware components underlying it. DQ2 carries over the basic approach of layering a stable and uniform experiment-specific system over a foundation of third-party software (Grid middleware, common projects). The approach is well suited to supporting more than one Grid infrastructure.

The present DQ consists of three main components: a uniform replica catalogue interface fronting Grid-specific replica catalogue implementations; a reliable file transfer service utilising a MySQL database to manage transfers using GridFTP and SRM; and Python client tools for file lookup and replication. Figure 4 shows the major catalogues in the system and the interactions with DQ2 and user applications (production operations and end users). Initial implementation choices for the current prototype are also shown. The complexity of the architecture communicating with a series of external databases is apparent, but the approach enables developments on separate Grids to be integrated and assessed. Higher level web services to search within the production databases are provided via AMI (the ATLAS Metadata Interface).

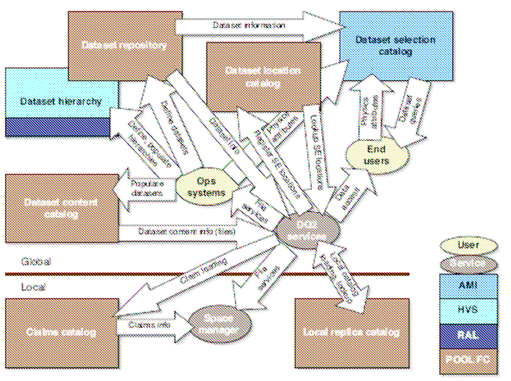


Figure 4: Architecture of the ATLAS DQ2 distributed data management system.

1.9 CMS Computing [5]

The CMS computing environment is a distributed system of computing services and resources that interact with each other as Grid services. The key components are the workflow management and data management systems. The guiding principles are to optimise for read access and bulk datasets; minimise the dependencies of the jobs on the Worker Node (WN); allow for provenance tracking (addressed via a parameter set management system); ensure site-local configuration information is discoverable on the worker node; and, trade reduced functionality for simplicity. The components of the workflow management system will support all the necessary workflows for data (re-)reconstruction, calibration activities, Monte Carlo production, Analysis Object Data (AOD) production, skimming and general user analysis and are shown below.

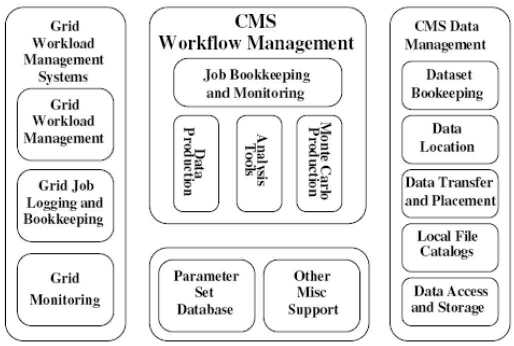


Figure 5: CMS Workflow Management components.

1.10 LHCb Computing [6]

LHCb uses the DIRAC (Distributed Infrastructure with Remote Agent Control) system to coordinate its production. The jobs sent to the LCG RB do not contain an LHCb job, but execute a simple script, which downloads and installs a standard DIRAC agent. Since the only environment necessary for the agent to run is the Python interpreter, this is possible on all the LCG sites. This pilot agent is configured to use the hosting WN as a DIRAC CE. Once this is done, the WN is reserved for the DIRAC WMS and is effectively turned into a virtual DIRAC production site for the time of reservation. This way allowed for efficient use of the LCG resources during the Data Challenge 2004 (over 5000 concurrent jobs at peak) with a low effective failure rate, despite the rather high intrinsic failure rate of LCG (about 40%) at the time of initial testing. Such a combined push-pull system represents an efficient mechanism to deliver an effective production computing system for the benefit of the experiment.

GridPP Status

In the course of meeting the deployment requirements of the experiments, numerous issues have been identified that are now being addressed as part of GridPP2 planning in order to establish the required resource for particle physics computing. Further site and middleware validation tests are needed in order to improve the overall Grid efficiency. Each experiment needs to develop an individual application interface: in this regard it is noteworthy that the system developed for the large LHC experiments has been shown to work effectively for other less resource-intensive applications. Addressing analysis group computing within the experiments, developing distributed file and database management systems, installing and validating experiment software, setting up production accounting systems, and creating an environment where everyone can share resources are all areas requiring further development.

In GridPP1, 88% of the 190 milestones were completed and all 44 monitoring metrics were within specification at the end of the project. No milestones were missed and most of those outstanding were superceded by more detailed planning in GridPP2. The aim of GridPP2 is to deliver a "Production Grid": a robust, reliable, resilient, secure, stable service delivered to the end-user applications. The Collaboration aims to develop, deploy and operate a 10,000 processor, multi-PetaByte Grid in the UK. To this end, the new project is more complex with 262 high-level milestones and 98 monitoring metrics currently defined. Approximately 20% of the way through the project, GridPP2 has already met 21% of its original targets with 86% of the metrics within specification. This is illustrated in the Project Map summary relating to the current deployment status (appended). It can be seen that the current deployment scale in terms of CPU is OK, but the declared disk resources are low. This reflects difficulties in developing and deploying SRM-compliant storage interfaces up to this point. Noteworthy high-level progress has been made in terms of:

- release of the gLite 1 middleware components in April, with version 1.2 currently being deployed and tested for robustness within the experiment teams;
- a "get fit" plan described elsewhere [7], enabling deployment performance to be tracked;
- completion of Service Challenge 2, addressing networking between CERN and the UK Tier-1, with 60 TB of data transferred over a ten-day period in April;
- 100 sites simultaneously passing the site tests (SFTs) in June, indicative of improvements of the underlying methods for rollout across the LCG worldwide infrastructure.

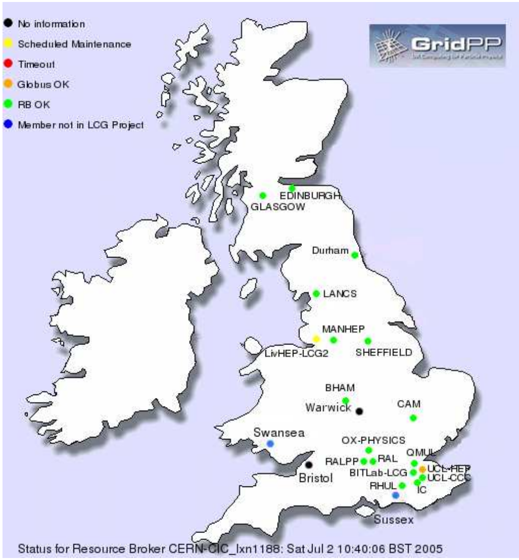
Issues arising are a long-term concern in providing hardware at the UK Tier-1 in 2007-08; short-term concerns are the under-utilisation of resources and the initial deployment of Tier-2 resources (only supported directly in the second phase of GridPP). The imminent Service Challenge 3 addressing file transfers for the experiments provides a backdrop to a further series of deployment tests. Tests of the prototype so far have given us some confidence that the final system will be capable of providing the required resource for LHC and other experiments' data analysis - in this way we plan to meet the LHC Computing Challenge but we do not underestimate the scale of the problems ahead.

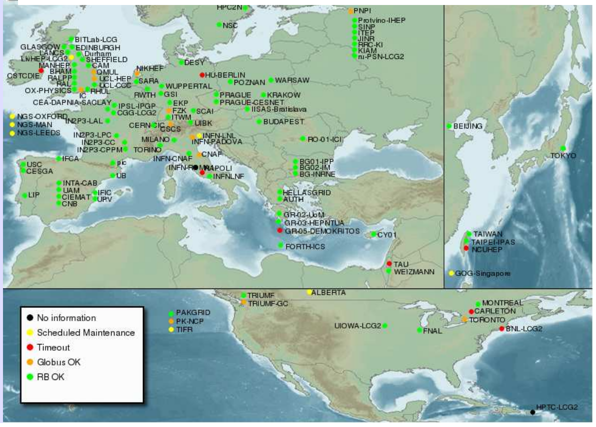
References

[1] "LCG Baseline Services Group Report", http://cern.ch/LCG/peb/bs/BSReport-v1.0.pdf. Computing Technical Design Reports are in http://doc.cern.ch/archive/electronic/cern/preprints/lhcc/public/
[2] "LHC Computing Grid Technical Design Report", lhcc-2005-024.pdf, 153pp.
[3] "ALICE Computing Technical Design Report", lhcc-2005-018.pdf, 114pp.
[4] "ATLAS Computing Technical Design Report", lhcc-2005-022.pdf, 248pp.
[5] "CMS: The Computing Project Technical Design Report", lhcc-2005-023.pdf, 169pp.
[6] "LHCb Computing Technical Design Report", lhcc-2005-019.pdf, 117pp.
[7] "Grid Deployment and Operations", J. Coles, AHM 2005 proceedings.

Total CPU	Maximum	Average	Free	Running Jobs	Waiting Jobs	Storage Available [TB]	Storage Used [TB]
2966	3145	2802	1666	843	31	74.28	16.54

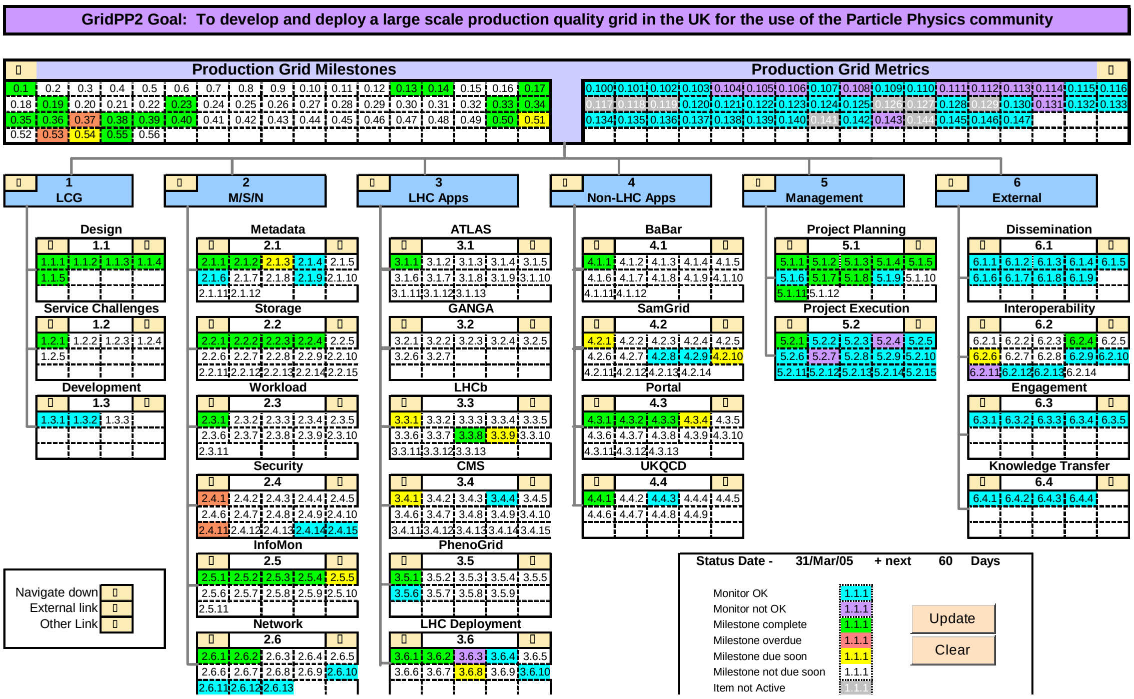
Status of the Grid in July 2005. The table shows the number of UK CPUs, jobs and storage available or used. Green sites indicate the location of the resources available to the CERN resource broker, in the UK (left) and worldwide (below).





Status of the GridPP2 project as represented in the summary table of the Project Map in July 2005. This follows assessment of the Grid deployment metrics and milestones and a review of the first quarterly reports of 2005 in six high-level areas.

Metric OK	Metric not OK	Tasks Complete	Tasks Overdue	Tasks due in next 60 days	Items Inactive	Tasks not Due	Change Forms
84 (86%)	14	54 (21%)	4	12	8	192	5



Requirement	OMII	VDT/GT	LCG/gLite	Other	Comment
1. Storage Element			Yes	SRM via dCache, DPM or CASTOR	LCG includes Storage Resource Management capability
2. Basic File Transfer	Yes	GridFTP	Yes		LCG includes GridFTP
3. Reliable File Transfer			File Transfer Service		FTS is built on top of GridFTP
4. Catalogue Services		RLS	LCG File Catalogue, gLite FireMan		Central catalogues adequate, high throughput needed
5. Data Management tools	OMII Data Service (upload / download)		LCG tools (replica management)		gLite File Placement Service under development
6. Compute Element	OMII Job Service	Gatekeeper	Yes		LCG uses Globus (GT2) with mods
7. Workload Management	Manual resource allocation & job submission	Condor-G	Resource Broker		RB builds on Globus, Condor-G
8. VO Agents					Perform localised activities on behalf of VO
9. VO Membership Services	Tools for account management, no GridMapFile equivalent	CAS	VOMS		CAS does not provide all the needed functionality
10. DataBase Services				MySQL, PostgreSQL, ORACLE	Off–the-shelf offerings are adequate
11. Posix-like I/O			GFAL, gLite I/O	Xrootd	Application access to data
12. Application Software Installation Tools		PACMAN	Yes		Tools already exist in LCG-2
13. Job Monitoring		Monalisa, Netlogger	Logging & Bookkeeping service, R-GMA		
14. Reliable Messaging					Tools such as Jabber are used by experiments (e.g. DIRAC for LHCb)
15.Information System		MDS (GLUE)	Yes	BDII	LCG based on BDII and GLUE schema

Table 1: Middleware components categorised according to the LCG baseline services. The 15 high-level experiment requirements are compared to the functionalities offered in the OMII, VDT(Virtual Data Toolkit, incorporating Globus and Condor components), LCG/gLite and other middleware sources. The comments reflect the status of deployment. The colours indicate the priorities associated by the four LHC experiments with respect to common solution being required (green indicates high priority, amber medium, and red low) as of July 2005.