The Grid2003 Production Grid: Principles and Practice

The Grid2003 Project
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Abstract

The Grid2003 Project has deployed a multi-VO, application-driven grid laboratory ("Grid3") that has sustained for several months the production-level services required by the physics experiments of the Large Hadron Collider at CERN (ATLAS and CMS), the Sloan Digital Sky Survey project, the gravitational wave search experiment LIGO, the BTeV experiment at Fermilab, as well as applications in molecular structure analysis and genome analysis, and computer science research projects in such areas as scheduling. The deployed infrastructure has been operating since November 2003 with 27 sites, a peak of 2800 processors, work loads from 10 different applications exceeding 1300 simultaneous jobs, and data transfers among sites of greater than 2 TB/day and has met essentially all is performance targets. We describe the principles that have guided the development of this unique infrastructure and the practical experiences that have resulted from its creation and use. We discuss, in particular, application requirements for deployment and configuration of grid services, the Grid3 monitoring infrastructure, application performance and metrics, and operational experiences including a summary of lessons learned.

1 Introduction

The Grid2003 Project [1] has deployed for the first time a persistent, shared, multi-virtual organization (VO), multi-application grid laboratory capable of providing production level services for large scale, data-intensive science applications. The project was organized by representatives of the U.S. "Trillium" Grid projects: the GriPhyN virtual data research project [2], the Particle Physics Data Grid (PPDG) [3], the International Virtual Data Grid Laboratory (iVDGL) [4], and the U.S. ATLAS and U.S. CMS Software and Computing Projects [5, 6] of the Large Hadron Collider (LHC) program [7] at CERN [8]. The planning process converged with a set of principles to build an application grid laboratory ("Grid3") that would provide:

- a platform for experimental computer science research for participants in GriPhyN and other grid research projects
- the infrastructure and services needed to demonstrate LHC production and analysis applications running at scale in a common grid environment
- the ability to support multiple application groups, including those from the Sloan Digital Sky Survey (SDSS) project [9] and the Laser Interferometer Gravitational Wave Observatory (LIGO) [10] which are core participants in iVDGL, and extending to others as needed.

A set of specific and quantitative goals were defined for Grid3, comprising performance targets using well-defined metrics. The timing of the initial deployment coincided with preparations for demonstrations at the SC2003 conference in Phoenix (November 15-21, 2003) [11]. The deployed infrastructure continues to operate today, and has met almost all of its performance targets. We view this as a significant step forward in terms of our ability to create and operate persistent shared grid-based cyberinfrastructure.

In the rest of this paper, we present in turn the overarching project requirements (Section 2) , application requirements (Section3), grid design (Section 4), application results (Section 5), milestones and metrics (Section 6), and lessons learned (Section 7).

2 Project Requirements

The following requirements and constraints were considered in defining the project:

- A simple grid architecture linking execution and storage sites, services for monitoring, information publication and discovery, and operations should accommodate several grid application frameworks.
- The middleware would be based on the Virtual Data Toolkit (VDT) [12] which provides a platform of services from the Globus Toolkit [13], Condor [14], GriPhyN, PPDG, as well as components from other providers such as the European Data Grid Project (EDG) [15]. Packaging, installation and configuration should be simple and easy for grid facility

administrators with a minimal, well defined interfaces: batch queues (use existing facility configurations), information service providers, and storage elements.

- Efforts should be made to "federate" with other Grid projects where possible, in particular the LHC Computing Grid Project (LCG) [16] and also the NSF TeraGrid.
- Experiment groups should be able to run their applications effectively on *non-dedicated* resources, including resources not controlled by their VO. In addition, applications must be able to install and publish themselves dynamically, thereby imposing minimum requirements on grid facility managers.
- Data replica location services such as RLS [17] should be provided by the individual VOs; other data management services such as Storage Resource Manager (SRM) [18] and dCache [19], may be used as required by the VOs.

3 Application Requirements

Grid3 was aligned with specific application milestones (such as LHC data challenges) as detailed below. Additional requirements were supplied by the milestones for the participating grid projects. This alignment with the milestones of external projects helped to ensure strong participation.

3.1 ATLAS Challenge Problems

The ATLAS application focused on Monte Carlo simulations of physics processes occurring in high energy proton-proton collisions of the LHC. Datasets which recorded the simulated response of the ATLAS detector to these collisions were used as input to event reconstruction and analysis algorithms.

The application workflow consisted in several steps and was implemented using Chimera virtual data tools [20, 21] and other services in the VDT. The first step was to generate the physics processes with the Pythia [22] program to simulation and record them into a replica location service (RLS). Next, the GEANT-based [23] core simulation package, built from official code releases from software repository at CERN and packaged with grid-based installation scripts, created dataset pieces of varying size, the average output file being ~2 GB. All data produced were to be archived at the Tier1 facility at Brookhaven National Laboratory (BNL). Files from this cache were to be reconstructed at CERN, producing samples ready for physics analysis. Output from CERN needed to be replicated back to BNL for high level analysis using the DIAL program [24].

3.2 CMS Challenge Problems

In July 2003 the CMS Collaboration began producing events for the 2004 data challenge. Fifty million events with minimum bias pile-up at a beam luminosity of $2x10^{33}$ are needed in the final sample. Creating CMS detector simulation currently consists of 3 steps: (1) event generation with Pythia, (2) event simulation with GEANT -based simulation application, and finally (3) reconstruction and digitization with the additional pile-up events. The sample of simulated events will be accumulated at CERN for primary reconstruction, but will be distributed in real time to Tier1 and Tier2 centers for calibration and toy analysis. The software suite includes MC_RunJob [25] a CMS tool for job specification, which specifies CMS Production jobs by reading input from a database of input parameters.

3.3 Cluster finding in SDSS

SDSS contributed two challenge problems. The first is a search for clusters of galaxies in the SDSS data resident in data catalogs. The software involves creation of workflows with several thousand processing steps to be organized by Chimera virtual data tools. The second was a pixel-level analysis of astronomical data such as analysis of cutouts of images about galaxies with the aim of adding more information to existing catalogs. Others included search for near earth asteroids in the SDSS data, which calls for transferring out complete SDSS images in search of highly elongated objects.

3.4 Blind Gravitational Wave Searches

The LIGO demonstrator project was to conduct an extensive, all-sky, blind search for continuous wave (pulsar) signals in the LIGO S2 data set. Each search requires that a conventional binary short Fourier transform (SFT) data file be accessible and contain the frequency band that the target signal spans during the observation time. Additional data files that contain the ephemeris data for the year must be present, which must be staged from LIGO facilities to Grid3 sites using GridFTP. We expect to publish the location of the staged data (on average estimated to be 4 GB per job) in a Globus RLS server so that its location is available to the job. The last job in the workflow stages the output results back to the LIGO facility and update entries in a database. Each workflow instance will run for several hours on an average process and will producing output to be copied back to LIGO facilities. The GriPhyN-LIGO working group developed the necessary infrastructure using Pegasus and Chimera to generate the workflows.

3.5 CP Violation in Heavy Quark Decay

The BTeV Grid-3 challenge problem was to demonstrate an integration of BTeV Monte Carlo simulation of charge-parity violation (CP) with GriPhyN virtual data tools. The clarity of the Chimera virtual data toolkit as a BTeV physics interface and the scalability of these tools for large Monte Carlo generation were be tested with data challenges run at the scale.

The workflow processing time is about 15 seconds per event on a 2GHz machine, translating into a typical request for 2.5 million events generated with 1000 10-hour jobs across the Grid-3 testbed.

3.6 Computational Chemistry and Biology

SnB [26] is a computer program based on the Shake-n-Bake algorithm [27], a dual space direct-methods procedure for determining molecular crystal structures from X-ray diffraction data. Traditional direct-methods procedures are amenable to high-resolution structures on the order of 100 atoms. The application requirements on Grid3 sites were minimal; a grid template-based portal would be used for job submission.

GADU [28] is a Genome Analysis and Databases Update Tool for the Mathematics and Computer Science division at Argonne National Laboratory.

3.7 Computer Science Challenge Problems

Computer science groups worked closely with experiment developers to provide application middleware components and services (such as Chimera and Pegasus, Globus client libraries, Condor-G, and RLS) as necessary for their grid-based application frameworks. Various computer science groups are also using Grid3 as a vehicle for research studies. In addition, the following three demonstrators were provided.

Studies of Data Transfers over the Grid. An important metric was to establish reliable data transfers between sites on Grid3 at sufficient scale. A Java-based plug-in environment (Entrada) was developed for this purpose to generate simulated traffic between a matrix of sites in periodic fashion [29]. No special requirements on Grid3 sites.

NetLogger instrumented GridFTP. NetLogger was used to instrument the GridFTP server and the Globus URL copy program. Two levels of instrumentation were to be implemented. The default level which generates NetLogger events at program start, end, and on errors. The detailed instrumentation level generates NetLogger events for all significant I/O [30].

The Exerciser. A backfill application provided by the Condor group [14] to test the status of the batch systems and operation of each Grid3 site. The application runs repeatedly with a low priority at 15 minutes intervals, introducing no special requirements for Grid3 sites.

4 Grid Design

The applications and experiment priorities and software described above served to guide the deployment and configuration of grid services for Grid2003. A simple two-tier approach was taken: each resource (compute, storage, application, site, user) was logically associated with a VO. At each site, a core set of grid middleware services with VO-specific configuration and additions were installed, with registration to a VO-level set of services (such as index servers, grid certificate databases). Where appropriate, VO-level services were combined into top layer services at the iVDGL Grid Operations Center (iGOC), providing monitoring applications, display clients, and verification tasks an aggregate view of the collected Grid3 resource and performance. Six VOs (U.S. ATLAS, U.S. CMS, SDSS, LIGO, BTeV, and iVDGL) were configured for Grid2003. Policies were implemented at the local batch scheduler level (OpenPBS, Condor, and LSF were used) and Unix group accounts for each VO.

4.1 Site Installation Procedures

Procedures for installation, configuration, post-installation testing, and certification of the basic middleware services were devised and documented. The Pacman [31] packaging and configuration tool was used extensively to facilitate the process. A Pacman package encoded the basic VDT-based Grid3 installation which included:

- The Globus security infrastructure (GSI), GRAM and GridFTP services;
- Information service based on the Globus MDS, with registration scripts to top level VO-specific information index servers.
- VO specific information providers.
- Cluster monitoring services based on Ganglia, with provisions for hierarchical grid views
- Server and client software for the MonALISA agent-based monitoring framework

Conventions were documented to provide grid facility administrators and operators with uniform instructions for with the goal of obtaining a consistent Grid3 environment over the heterogeneous sites. In particular, information providers for site configuration parameters reporting application installation areas, temporary working directories, storage element locations, and locations of installed VDT software were included. We found that only few extensions to the GLUE MDS schema were necessary.

4.2 Monitoring and Information Services

The software installed on Grid3 sites included components necessary to gauge overall behavior and performance of the grid and its applications. These included a number of packages which sensed monitoring data and made it available to a distributed framework of services and client tools. Specific choices for information providers were made by considering a list of interesting grid-level (such as overall resource availability and consumption) and VO-level (e.g. aggregate CPU usage) performance indicators. Requirements were also drawn from auditing, scheduling and debugging considerations. These were classified, rated in term of importance and urgency and listed, together with preliminary deployment considerations.

The framework was built by adapting existing monitoring applications into simple architecture, supplying missing parts as necessary. Figure 1 shows the components of the framework, organized using the classification suggested by the GMA working group of the Global Grid Forum. Producers are elements that provide the monitored information, consumers use this information and intermediaries have both roles, usually adding some aggregation or elaboration.

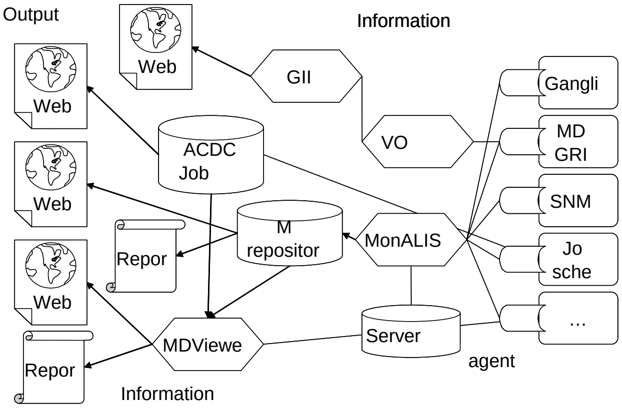

Figure 1 Grid3 monitoring architecture showing information providers and consumers, and the data flows between them.

Some of these components are located on Grid3 sites, some in central servers and some are the clients of the users accessing the information. An aggregated summary of the data was centrally available, while more detailed or streams of updates are available from the sites. The main components of the monitoring framework are:

- MDS: part of the Globus Toolkit, MDS is directory service for configuring distributed computations. In addition to site configuration information, monitoring information is provided. A schema extension, producers (MDS Information Providers) and intermediaries have been developed to use this framework in Grid3.
- Ganglia [32]: it is a open source tool to collect cluster monitoring information such as CPU and network load, memory and disk usage. The Ganglia collected information is available through web pages served at the sites, a summary[1] of it is available in a central server at iGOC and intermediaries have been developed for it too.
- MonALISA[33][2]: Monitoring Agents in a Large Integrated Services Architecture, is a monitoring tool to support resource discovery, access to information, and gateways to other information gathering systems. It plays a big role in the information gathering for Grid3. The MonALISA client allows access to both the central repository as well as the servers at the sites through a nice graphic interface. New MonALISA agents were developed to collect VO specific and other Grid3 relevant information.
- Central repository: the MonALISA web repository, integrated with MonALISA, collects its information in a central server at the iGOC, storing it in a round robin-like database, and makes it available through the web. It is possible to display the data on web pages, traditional or WAP, and to access it through web services.
- ACDC Job Monitoring[3]: the Advanced Computational Data Center (ACDC) at the University of Buffalo has developed job monitoring applications which collect information from local job managers through grid-submitted jobs. Statistics and job metrics are collected and stored in a web-visible database, available for aggregated queries and browsing.
- “Site Status Catalog”[4]: it is a Grid2003-developed application that periodically tests all the sites and

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[1] The Grid3 Ganglia front-end is located at: http://gocmon.uits.iupui.edu/ganglia-webfrontend/

[2] The Grid3 MonALISA web front end is located at http://gocmon.uits.iupui.edu:8080/index.html.

[3] The ACDC job monitor is located at: http://acdc.ccr.buffalo.edu/statistics/acdc/fullsizeindexqueue.php.

[4] The Grid2003 site catalog is located at http://www.ivdgl.org/grid2003/catalog/.

replicates centrally some critical information. A web interfaces provides a list of all the Grid3 sites, their location on a map, their status and other important information.

- MDViewer: the Metrics Data Viewer program [34] is a open source project developed within Grid2003 that allows analysis and display of collected metrics information. It provides an API for manipulating, comparing and viewing information and a set of predefined plots, parametric in arbitrary time intervals, sites and VOs, tailored to Grid2003 project needs.

In the monitoring and analysis system of Grid3, different paths allow collection of similar information, providing crosschecks to verify the correctness of the data collected. A coordinated system has been deployed adapting and combining the different monitoring tools. The information producers collect the information close to its source, a common intermediary defines a uniform way to represent and access the data, and the information is centrally collected to produce aggregated information, statistics and documents. Client consumers can access centrally stored data or data from participating sites (for more detailed information) in a uniform manner. in a uniform way.

4.3 Virtual Organization (VO) Management

In order to simplify user access to Grid3 resources, and to reduce the burden on grid facility administrators, the project chose to deploy the Virtual Organization Management System (VOMS) provided by the EDG project [15]. In addition, group accounts were used at cites with a naming convention for each VO. Local grid map files were generated by calling an EDG script which contacted each of the VOMS servers for the VOs.

4.4 Support and Operations

The deployment and operation of the Grid3 environment required a number of centralized support activities. The iVDGL iGOC [35] hosted centralized services for the project, including the Grid3 Pacman cache design and support, the top-level GIIS server, the Site Status Catalog, the central repositories for MonALISA and web services Ganglia. A simple trouble ticket system was used intermittently during the project. An acceptable use policy modeled after the LCG was adopted.

5 Results

As stated, the Grid2003 Project was organized to meet several strategic project goals, including "Provide the infrastructure and services needed to demonstrate LHC production and analysis applications running at scale in a common grid environment." Figure 2 shows the integrated and differential Grid3 usage (in CPU-days, by VO) over selected time periods in Fall of 2003. Both U.S. ATLAS and U.S. CMS were able to run production systems at scale during this period using shared facilities. Note that the experiments continued to exercise production on Grid3 with an average of 700 CPUs in daily use.

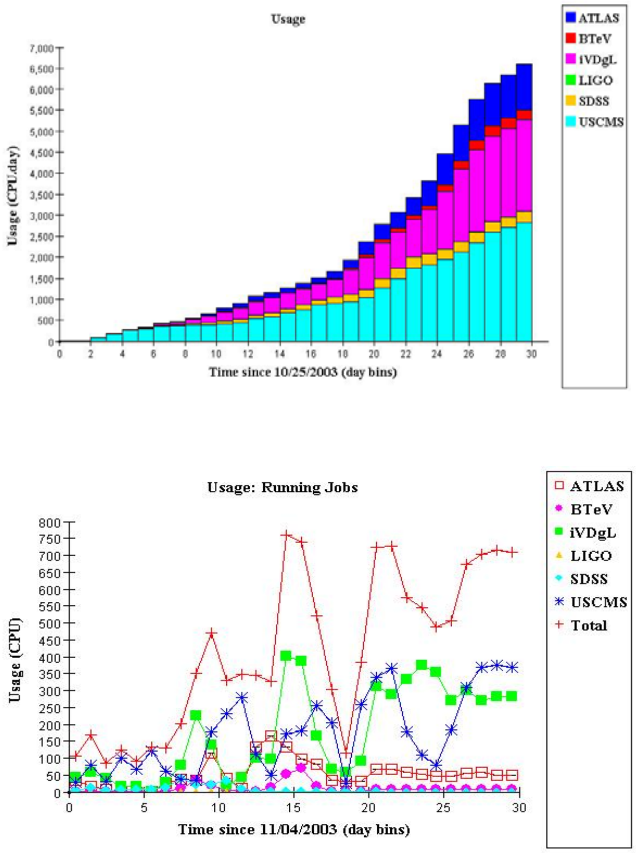

Figure 2 Integrated and differential CPU usage during and following SC2003, organized by Virtual Organization.

5.1 U.S. ATLAS GCE and DIAL

ATLAS deployed a grid-enabled application package GCE-Server [36] on 22 of the Grid3 sites. Automatic (user-level) installation tools based on Pacman were developed, and effectively used the Grid3 GLUE schema extensions for application installation attributes. Client hosts (GCE-Client) were installed outside Grid3 for job submission. More than 5000 jobs (Geant3 based simulation followed by reconstruction) were processed on about 18 large computing sites, with total data I/O of about 1.1 TB (the results are summarized in Figure 3). A dataset catalog was created for produced samples, making them available to the DIAL distributed analysis package. Figure 3 displays the (background free) results indicating prominent, four electron signal peaks which were reconstructed from the produced Higgs datasets. The produced datasets were stored at BNL as part of the grid jobs, and continue to be analyzed by DIAL developers and the SUSY physics working group.

We observed a significantly high failure rate of approximately 30%, where failures were defined jobs experiencing errors in any step of the processing sequence which prevent perfect completion (pre-stage, job execution producing the output files, post-stage to the final storage element at BNL, and registration to RLS). Approximately 90% of the failures were caused by problems at the computing site: disk filling errors, gatekeeper overloading or network interruptions. Our software did not handle the nightly roll over the worker nodes at ACDC gracefully, and so jobs still running were crashed and had to be re-processed.

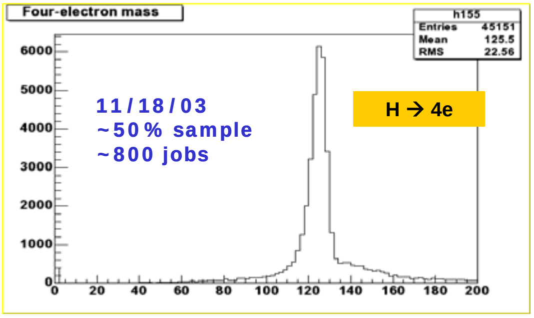

Figure 3 Simulation of Higgs decay into four electrons and detection by the ATLAS detector from Grid3 produced datasets.

5.2 USCMS MOP Production

U.S. CMS used Grid2003 resources to produce simulated events for the upcoming CMS data challenge. U.S. CMS ran a GEANT3 based, statically linked FORTRAN application called CMSIM and a GEANT4 based, dynamically linked, C++ application called OSCAR. The simulations were at first primarily test samples designed to demonstrate the scaling and reliability of the system, but not saved for physics analysis. Since SC2003 U.S. CMS has successfully used Grid2003 resources on 11 sites to simulate more than 1 million GEANT4 full detector simulation events for the CMS physics groups. Computing usage since the middle of November is shown in Figure 4 and Figure 5. In general, the efficiency to run on Grid2003 resources is roughly as high as the original U.S. CMS production grid, once the sites have been fully validated. The official OSCAR production jobs are extremely long and not all sites have been able to accommodate running them.

The rate of CMSIM to successfully complete is approximately 70%, which is consistent with the US-ATLAS estimates. We have yet to do a calculation of the percentage of OSCAR jobs which complete. One aspect we have noticed is that jobs often failed with site configuration problems, or failed in groups from site service failures. We saw fewer random job losses and more frequently a disk would fill up or a service would fail and all the jobs submitted to a site would die. The service level monitoring needs to be improved and some of the services need probably to be replaced. For example, the resource reservation available through the SRM based storage element service would have prevented a variety of storage related service failures.

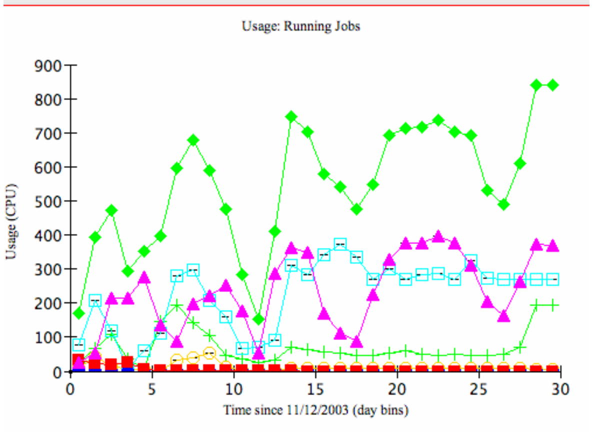

Figure 4 CMS daily use of Grid2003 since the beginning of SC2003.

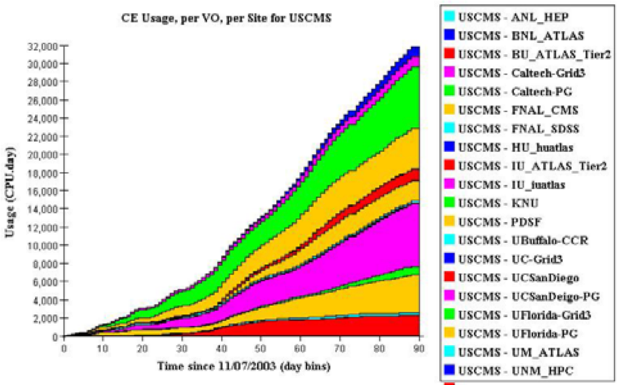

Figure 5 CMS cumulative use of Grid2003. The chart plots the distribution of CPU usage by site in Grid2003 over a three month period beginning November 2003.

5.3 LIGO Results

Grid2003 has proved a useful grid environment for LIGO applications. The search codes to perform wide-area, wide-frequency blind searches were designed so that the computation load can be distributed among different and very loosely coupled computers -- the results of the calculations performed on one machine are completely independent of what is happening on any other machine. Limitations from overloaded head nodes caused by our application were overcome by use of the Condor GridMonitor.

5.4 GridFTP Data Transfer Demonstrator

A goal of demonstrating 2 TB data transfer across Grid2003 per day was established at the beginning of the project and proved to be realistic. The Grid and the sites proved robust to long running data transfer demonstrations. Issues of account privileges, ports and firewalls caused the main problems in deployment and configuration.

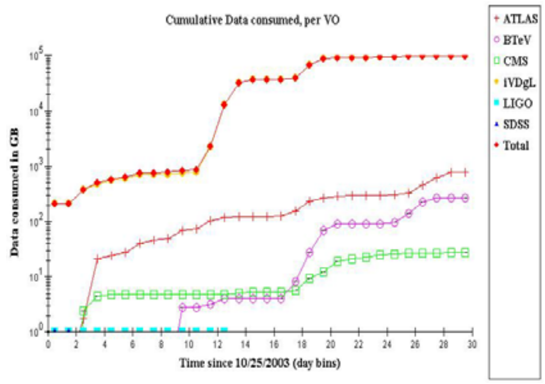

Figure 6 Data consumed by Grid3 sites, by Virtual Organization, showing nearly 100 TB transferred during the SC2003 season. The GridFTP demo accounted for the vast majority of data transfers.

6 Milestones and Metrics

The Grid2003 project met the final milestones as documented in the plan. Here we summarize some of them:

1. **Number of CPUs (target = 400, actual = 2163).** The actual number varies with time as sites bring resources into and out of Grid2003. A peak of over 2800 processors occurred during SC2003. Note that more than 60% of available CPU resources are non-dedicated facilities. Grid3 effectively shares resources not directly owned by the participating experiments.
2. **Number of users (target = 10, actual = 102).** About 10% of the users are application administrators who do the majority of the job submissions. However, more than 102 users are authorized to use the resources through their respective VOMS services.
3. **Number of applications (target > 4, actual = 10).** Seven scientific applications including at least one from each of the five GriPhyN-iVDGL-PPDG participating experiments were, and continue to run on Grid3. In addition, the three computer science demonstrators are run periodically.
4. **Number of sites running concurrent applications (target > 10, actual = 17).** This number is related to the number of sites classified as “computational service” sites defined on the Site Catalog page varies with application.
5. **Data transferred per day (target = 2-3 TB, actual = 4 TB).** This metric was met with the aid of the GridFTP-demo which runs concurrently with the scientific applications. Plots of statistics collected may be found at the project website [29]. **Percentage of resources used (target = 90%, actual = 40-70%).** The maximum number of CPUs on Grid3 exceeds 2500 most of the time. On November 20, 2003 there were sustained periods when over 1300 jobs ran simultaneously (the metrics plots are averages over specific time bins, which can report less that the peak depending on chosen bin size).
6. **Efficiency of job completion (target = 75%, actual: varies).** The value of this metric varies depending on the application and on the definition of failure. Generally speaking, for well-run Grid3 sites and stable applications this figure exceeds 90%. Work is under way to collect more detailed statistics on job failure.
7. **Peak number of concurrent jobs (target = 1000, actual = 1300).** Achieved on 11/20/03.
8. **Rate of faults/crashes: (target < 1/hour, status: varies).** We have not started to measure this metric in quantitatively, but have begun to collect summaries from the application groups.
9. **Operations support load: (target < 2 FTEs, status: typically 10 part-time)**. We were continuously adding applications and sites throughout the SC2003 conference, and this process continues today. Once a site becomes stable, it usually remains so except for hardware problems. Several sites replaced disks

and/or nodes without perturbation to the operation of the overall system.

7 Project Lessons

We list here some recommendations for changes and/or future work as a result of the experiences of Grid3 to date. These are presently being used as input for upgrades to Grid3.

1. **Automated configuration, testing, and tuning, scripts** give immediate payback and are worth the effort to develop them for a project the scale of Grid2003.
2. **API for Troubleshooting and Accounting information.** Specifically GRAM and GridFTP, the job submission and file transfer systems, respectively, should provide *direct* information without having to parse log files.
3. **Contact and Support Model**: It is recommended that the contact, operations and support model be revisited. Factorization of responsibilities, perhaps at the service level, should help and be explored.
4. **Efficiency Metrics:** The efficiency targets for Grid2003 were not met. Understanding why will require increased effort in analysis of the end-to-end applications.
5. **Job Execution Policies**: Tools should be deployed and analyses done to check that the current Grid3 job policies are actually working.
6. **Job Resource Requirements:** Sites should publish more information about their policies for job execution and resource usage, e.g. maximum CPU time allowed.
7. **Storage Services and Data Management:** Grid3 currently has little or no infrastructure support for these services. These issues need to be discussed and a first deployment prototyped and tested.
8. **Troubleshooting:** Additional tools are necessary for troubleshooting, specifically tools for analyzing and querying log files, the ability to link a job ID on the execution side with a job ID at the submit (VO) side.

8 Summary

We have discussed the deployment and use of a persistent, shared, multi-virtual organization (VO), multi-application grid laboratory, the first of its kind. The infrastructure remains in place and is currently undergoing upgrades for future application demonstrators. As well as serving as a valuable proving ground for grid operation techniques, Grid3 continues to deliver new scientific results for its application projects and, in addition, to attract new users from a range of disciplines, including computer science.

9 Acknowledgements

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