3RD EGEE USER FORUM

CLERMONT-FERRAND, FRANCE

BOOK OF ABSTRACTS

2008



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Overview of the 3rd EGEE User Forum

The 3rd EGEE User Forum[1], held from 11-14 February in Clermont-Ferrand (France), attracted more than 300 participants with more than 100 presentations, 19 demos and 36 posters. The User Forum has become a key annual event for the project, allowing the users of the EGEE infrastructure and services to present their work and plans, and to discuss experiences and planned developments with other users and the service providers. It took place towards the end of the second phase of the EGEE project, co-funded by the European Commission, and just before the start of its third phase which starts on 1 May 2008 for two years.

The Programme Committee, led by Vangelis Floros (GRNET, Athens), put together a rich programme, with parallel sessions covering major application areas and key areas in Grid technology such as workflow, data management and Grid access. Business applications and industrial developments were present across all the sessions, and many collaborating projects presented their work during the User Forum, adding greatly to the depth and impact of the event.

There were several keynote talks in plenary sessions, with external invited speakers notably overviewing research in the French Grid'5000 project, and the key role of Grids in the Large Hadron Collider (LHC) experiments. EGEE speakers also highlighted the support of the more than 200 Virtual organizations (VOs), the porting of applications, and the status and planning for the European Grid Initiative Design Study (EGI-DS) project working on the transition from the EGEE project to a federated, sustainable European model. There was also a presentation on the adoption and deployment of Grid technology for Health in Europe via the SHARE project.

An essential, and very successful part of the Forum, was the practical demonstrations and posters included in an overall exhibition organized by the Local Organising Committee, led by Nathanael Verhaeghe (Clermont Ferrand, HealthGrid). The 19 live demonstrations of Grid applications ranged from mathematical models of living cells to bioinformatics portals, as well as tools to make using Grids simpler and easier to control.

The Health-e-Child project, represented by Jerome Revillard and David Manset, won the prize for the best demonstration with their Gateway and Case Reasoner, a concrete implementation and use-case of a gLite-based healthgrid for European paediatrics. "EGEE plays an active and invaluable role by supporting the HeC community in better understanding how best to use gLite, how to Gridify biomedical applications and stay up to speed with ongoing developments," said demo-winner David Manset, director of biomedical applications at maat Gknowledge.[2] Emmanuel Medernach of LPC,

[1] http://egee-uf3.healthGrid.org/

[2] http://www.g-knowledge.com/

France, won the poster prize for his project "Fair Grid Scheduling," which looked at ways of efficiently sharing Grid resources.

Looking back over the three annual EGEE user forums, the basic question has changed from 'if' Grids can be used to produce scientific results to 'how best' to use Grids for these ends, as well as the development of new business models. There are now some 10,000 users registered in more than 200 VOs, and in 2007 there was 25 Petabytes (PB) of data stored at sites used by EGEE users, and more than 11 PB of data were involved in mass data transfers. The total processing within the Grid infrastructure consumed some 114 million CPU-hours.

EGEE will hold its next conference, EGEE'08[3], in Istanbul (Turkey), from 22 to 26 September 2008. The 4th User Forum will take place in spring 2009, held in Europe in conjunction with The Open Grid Forum (OGF). We look forward to reporting on more major developments, and on the key move towards Grid support by National Grid Initiatives (NGIs), coordinated within Europe.

In addition to thanking the Programme and Local Organising Committees, we would like to thank the sponsors of the 3rd EGEE User Forum, the EGEE Advisory Committee (EAC) for invaluable support, the Editorial team for this Book of Abstracts, and the European Commission for its continued support.

Bob Jones, EGEE Project Director



[3] http://www.eu-egee.org/egee08

EGEE services for users

The services provided by EGEE to its user communities fall into four broad categories: Grid infrastructure, support, communication, and middleware.

Infrastructure: The use of the EGEE production infrastructure has increased steadily with the number of VOs and applications doubling during the lifetime of the EGEE-II project. There are currently more than 200 registered virtual organizations that contain more than 7500 individuals. Collectively, these people now use roughly the equivalent of 20000 single CPUs continuously on the EGEE infrastructure. The virtual organization managers estimate that roughly 14000 scientists are directly affected by the results of these calculations. Both the scientific and geographic distributions of users show broad adoption of Grid technology. The collected statistics indicate that the bulk of the user community has passed through the application prototyping stage and now uses the Grid infrastructure heavily in production.

Support: The project provides a broad spectrum of user support services: "help-desk" support, documentation, training, and application porting.

The project provides "help-desk" support through the Global Grid User Support (GGUS) system. Behind the scenes, GGUS routes tickets to teams with specialized expertise, such as middleware support, VO-specific support or operations support. To the users, it gives a unique entry point into the EGEE support infrastructure. The published GGUS user support metrics show that there are on average around 1000 tickets in the system each month and around 75% of them are solved.

Two teams within the applications support activity provide application porting support—GILDA and GASuC. The GILDA team focuses on porting applications using a t-infrastructure and sits on the boundary between the training and applications support. This team has ported around 30 applications to the Grid infrastructure, most of which are now using the EGEE production infrastructure. The GASuC (Grid Application Support Centre) is a new group focusing on porting applications directly to the production infrastructure. A detailed procedure for porting has been defined and contacts with a first set of applications have been made.

In addition to the generic support activities specific support is given to a few scientific areas, which are important both for their scientific merit and as a proving ground for the development of Grid technology, ensuring it satisfies real user needs. These areas are Astronomy and Astrophysics, Computational Chemistry, Earth Sciences, Fusion, High Energy Physics and Life Sciences.

Communication: The primary means of forging strong, self-reliant user communities is through the EGEE conferences and EGEE User Forums. Both of these events are well-attended and well-rated by the EGEE user community. The future User Forums will maintain the same focus and concentrate on bringing the full EGEE user community together.

In addition to these major annual events specific user communities organise events throughout the year, and the applications support activity in EGEE ensures efficient communication between the

different communities and the rest of the project. Consequently there is natural synergy between communities, which results in a sharing of tools and procedures.

Middleware: The efforts of the High Energy Physics and Life Sciences communities have greatly contributed to the current level of stability and reliability achieved by the core gLite middleware. The core middleware is heavily used and generally satisfactory for the users. However, the core middleware is only a small part of the software stack needed by real applications. Third-party software, internal developments, and commercial software complement the functionality provided by the core gLite middleware. Consequently the project has established the RESPECT (Recommended External Software for EGEE Communities) programme, to "commercialize" and generalize internal developments (such as the security features of the medical data management tools, HEP experiment Dashboard, or the AMGA metadata catalog), and to integrate higher-level services that have proved useful as well as popular commercial software.

Overall, the expanding use of the infrastructure and increasing number of disciplines using it indicate that the EGEE services are satisfying the user community. As always, more can be done to improve the utility of the infrastructure and effectiveness of the provided support; specific areas for improvement have been identified and will be addressed in the remaining part of EGEE-II and in EGEE-III.

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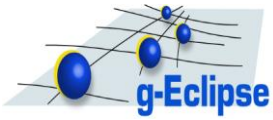
































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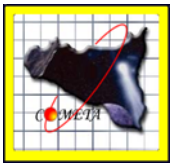












Organization of the book of abstracts

We have organized this book in a sequence of chapters, each chapter associated with an application or technical theme introduced by an overview of the contents, and a summary of the main conclusions coming from the Forum for the chapter topic.

The first chapter gathers all the plenary session keynote addresses, and following this there is a sequence of chapters covering the application flavoured sessions, namely:

- Astronomy and Astrophysics
- Computational Chemistry and Materials Science
- Earth Sciences
- Finance and Multimedia
- Fusion
- Life Sciences

These are followed by chapters with the flavour of Computer Science and Grid Technology, namely:

- Data Management
- Interaction with the French Grid'5000 initiative
- Grid Access
- Interoperability and Resource Utilisation
- Monitoring, Accounting and Support
- Workflow and Parallelism

The final chapter covers the important number of practical demonstrations and posters exhibited at the Forum.

Much of the work presented has a direct link to specific areas of Science, and so we have created a Science Index, presented below. In addition, at the end of this book, we provide a complete list of the institutes and countries involved in the User Forum.

Access to slides of User Forum presentations

The slides of the oral plenary and parallel session presentations may be downloaded from http://indico.cern.ch/conferenceTimeTable.py?confId=22351. Please note that the authors should be contacted if you wish to re-use any of this material.

Editorial acknowledgements

The Editorial team would like to acknowledge the support of many people in producing this document. The source of the 146 abstracts themselves has been the users who actively contributed to the User Forum with oral presentations, demonstrations and posters. The conveners of these sessions, drawn from the Programme Committee, have been invaluable in providing text and graphics to introduce the chapters. We have particularly valued the advice and support of Massimo Lamanna, the organiser of the first two User Forums in 2006 and 2007, and the final proofreading made by Anna Cook.

The Editorial team

Science index

Figure 1 below shows number of abstracts in different scientific fields. It is followed by an index for the abstracts in each field, which gives the abstract and page numbers.

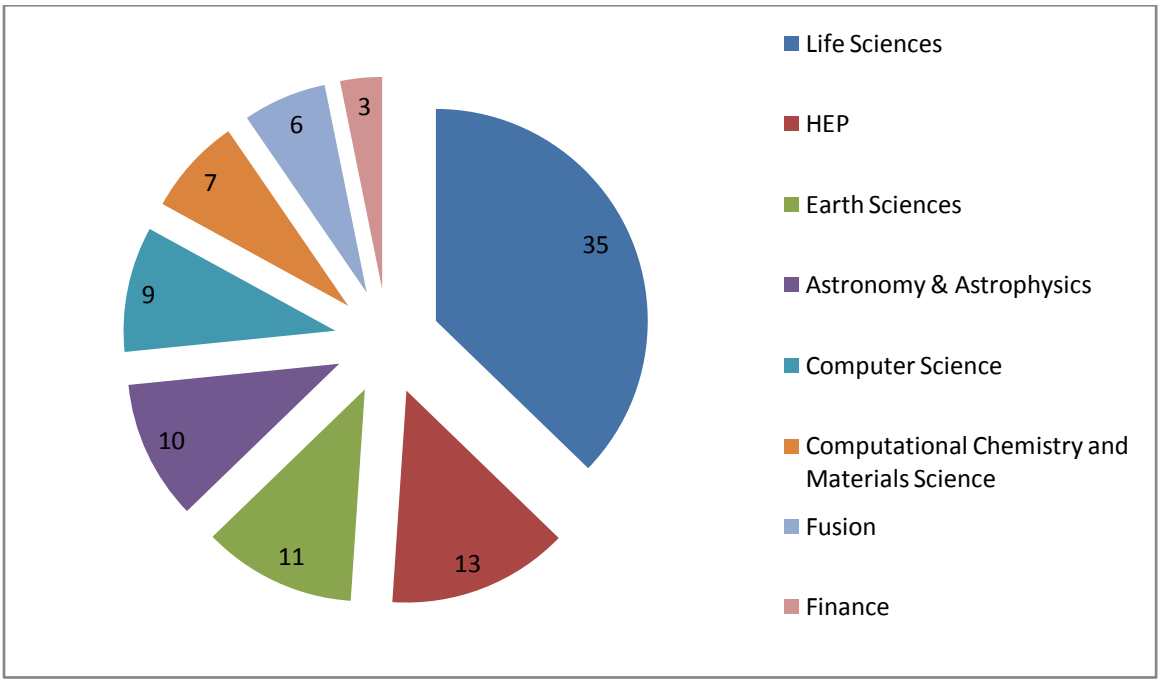


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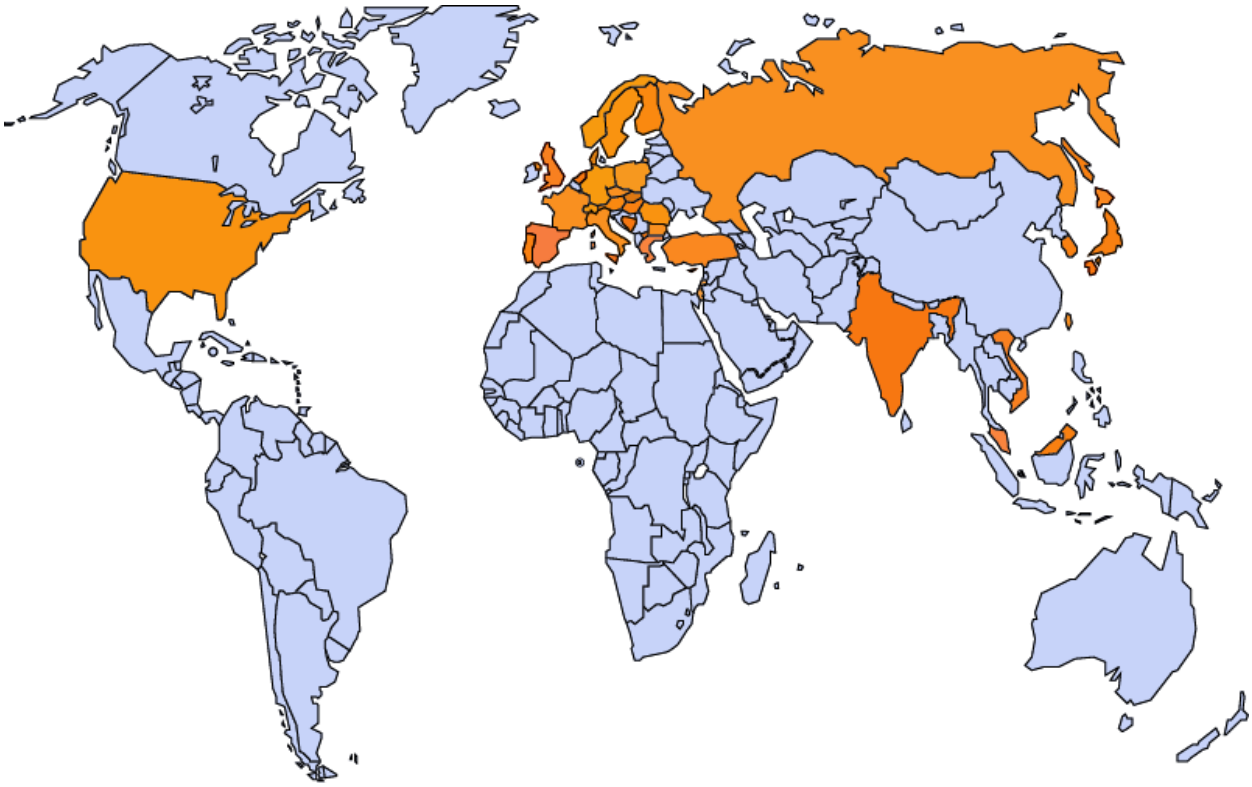
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- Israel
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- Russia
- Slovakia
- South Korea
- Spain
- Sweden
- Switzerland
- Taiwan
- Turkey
- United Kingdom
- United States of America
- Vietnam

PLENARY KEYNOTE PRESENTATIONS



1. European Grid Initiative Design Study (EGI_DS)

Author: D. Kranzlmüller, (GUP, Un.Linz, Austria)

Dieter Kranzlmuller is Professor of Computer Science at the Johannes Kepler University, Linz, Austria, with a special focus on parallel programming and debugging, and cluster and Grid computing. He is Project Director of EGI-DS, and national representative of Austria in the e-Infrastructures Reflection Group (eIRG).

Short Overview: The European Grid Initiative (EGI) Design Study started in Sept 2007 with funding from the EC's 7th FP. It represents an effort to establish a sustainable Grid infrastructure in Europe. The National Grid Initiatives (NGIs) are the main foundations of EGI. The aim of EGI_DS is to study the appropriate requirements, design the functionality, and to implement a prototype structure of the EGI organization, which will take up the coordination and operation of the pan-European Grid infrastructure.

Analysis: To successfully complete the set objectives of the EGI vision (http://www.eu-egi.org/vision.pdf), EGI_DS has committed to coordinate and support the following actions: 1).Consolidate the requirements for an EGI organisation from the NGIs and other important stakeholders such as application communities, infrastructure operators, related projects, NRENs. 2).Define the functional role of the EGI organisation with respect to the NGIs at the start of this organisation, and plan for the evolution of its functions as it matures. 3).Establish a legal, financial and organisational basis (supported by the member states) for the EGI organisation to undertake these functions. 4).Establish the EGI organisation and manage the transition from the existing project-based Grid support to a sustainable production service. 5).Ensure that all stakeholders within the member states, international standards bodies, research Grid services in other countries are aware of the EGI and have relationships.

Impact: The future EGI organization will constitute a key element in the European Research Area (ERA) by providing a sustainable Grid infrastructure required by the whole European research community. The current leading Grid infrastructures in Europe, EGEE and related infrastructure projects (such as e.g. BalticGrid and SEEGRID-2), represent a key source of the experience and ideas. EGI_DS works closely with these infrastructure projects to permit a transition into an EGI-like structure before the end of the next phase of those projects. In addition, EGI_DS is linking the European Grid infrastructure with similar infrastructures elsewhere. The project provides the focus for international collaborations and together raises global attention for EGI. This facilitates the international cooperation in the future.

Conclusions: The EGI Design Study started in September 2007 and continues until the end of 2009. The EGI Blueprint Proposal is planned be finished by September 2008, as the deadline of the EGI Proposal for the EU is expected to be sometimes in September 2009. The EGI Organization entity should be in place and operational at the beginning of 2010.

Keywords: Sustainability, National Grid Infrastructures, European Grid Initiative

Further Information: http://www.eu-egi.org

2. HealthGrid and SHARE: retrospect and prospects for Grids in health

Author: Tony Solomonides, Bristol Institute of Technology, UWE, Bristol, UK and HealthGrid, France (tony.solomonides@uwe.ac.uk.)

Overview

The concept of Grids for health crystallized in Europe in 2002 in the wake of several EU-funded projects and a wave of enthusiasm for social applications of the new technology. It has since been carried forward through HealthGrid, a joint initiative among a number of projects and individuals which has resulted in the incorporation of a non-profit organization in France, based in Clermont-Ferrand. This European collaboration has organized five HealthGrid conferences and published a visionary White Paper [1] setting out, mainly for senior decision makers, the concept, benefits and opportunities offered by the newly emerging Grid technologies in a number of different healthcare and biomedical research domains.

Starting from the conclusions of the White Paper, the EU funded SHARE project aims to identify the most important steps and significant milestones towards wide deployment and adoption of healthGrids in Europe. The project has defined a strategy to address the issues identified in the action plan for a European e-Health [2] and has devised a roadmap for the major technological and ethical and legal developments and social and economic investments needed for successful take up of healthGrids in the next 10 years. The final road map is now in beta version, having undergone a full review by a panel of over 25 prominent European experts at a workshop in December 2007.

A sister organization, HealthGrid.US has now been set up in the United States and is organizing the next conference, HealthGrid 2008, in Chicago, on 2nd to 4th June 2008.

[1] V. Breton, K. Dean and T. Solomonides (eds), The HealthGrid White Paper, Proceedings of Third HealthGrid

Conference, IOS Press, Vol 112 (2005) pp 249–321

[2] Action plan for a European e-Health Area, COM(2004) 356, European Commission, http://europa.eu.int/information_society/doc/qualif/health/COM_2004_0356_F_EN_ACTE.pdf.

Further Information: http://www.eu-share.org, http://www.healthGrid.org

3. Computer science Grids and research in Grid computing

Author: F.Capello, Senior Researcher at INRIA. He was director of the French Grid5000 project, and is currently Scientific Director of ALADDIN, a computer science platform for research in Grid and P2P computing.

Overview

The Computer Science discipline, especially in large scale distributed systems like Grids and P2P systems and in high performance computing areas, tends to address issues related to increasingly complex systems, gathering thousands to millions of non trivial components. Theoretical analysis, simulation and even emulation are reaching their limits. Like in other scientific disciplines such as physics, chemistry and life sciences, there is a need to develop, run and maintain generations of scientific instruments for the observation and the experimentation of complex distributed systems running at real scale and under reproducible experimental conditions.

Grid'5000 is a large scale system designed as scientific instruments for researchers in the domains of Grid, P2P and networking. More than a a testbed, Grid'5000 has been designed as a "Computer Science Fully Reconfigurable Large Scale Distributed and Parallel System". It allows researchers to share experimental resources spanning over large geographical distances, to allocate resources, to configure them, to run their experiments, to realize precise measurements and to replay the same experiments with the same experimental conditions.

Computer scientists use this platform to address issues in the different software layers between the hardware and the users: networking protocols, OS, middleware, parallel application runtimes, applications. In this talk, we will present: 1) the motivations, design and current status of Grid'5000, 2) some key results at different level of the software stack, 3) the impact of this system as research tools, 4) ALADDIN, the INRIA initiative to make Grid'5000 a sustainable research platform

Further Information: https://www.Grid5000.fr/mediawiki/index.php/Grid5000:Home

4. Application porting in EGEE

Author: Gergely Sipos is a researcher in Computer Science at MTA SZTAKI, Hungarian Academy of Science. He has been very active in EGEE training events, and is currently deputy leader of this activity in EGEE-II. He will have specific responsibility for the application porting and user support task in EGEE-III.

Overview

In addition to the broad, high-level support provided to new virtual organisations, detailed, technical aid to Grid application developers is critical for broadening the EGEE Grid user community. Several members of the EGEE project already provide support for new and experienced Grid users who wish to port legacy applications to the EGEE Grid infrastructure. Grid experts from these porting teams work closely with application owners in order to understand their requirements and to identify the most suitable methods, approaches and tools for the porting process.

The talk introduces the different application porting groups and discusses how this support action will evolve in the third phase of EGEE. The most relevant applications that the porting groups work on will be also introduced alongside typical scenarios and methods that are applied during the porting process.

The generic support process in EGEE-III will be distributed over several groups in Europe, and led by MTA/SZTAKI. According to the needs of the user there will be processes involving interviews, training and practical demonstrations of the use of porting technology. For example much use will be made, as appropriate, of existing general portals such as GRIDWAY, GENIUS, P-GRADE and GANGA. The emphasis will be to make user communities self sufficient with the actual porting being done by expertise within the VO being guided by the generic support.

Further information:

MTA SZTAKI Porting group, Grid Application Support Centre http://www.lpds.sztaki.hu/gasuc
P-GRADE Portal http://www.portal.p-grade.hu/

UCM Porting group http://www.dsa-research.org/

GridWay http://www.Gridway.org/

CERN Porting group GANGA and DIANE ganga.web.cern.ch

GILDA Porting group https://gilda.ct.infn.it/

5. Challenges and successes of the HEP Grid

Author: Fairouz Malek is a senior researcher in particle physics at LPSC, CNRS/IN2P3, Grenoble (France). She has been active in the LHC/ATLAS experiment since 1999, and is LCG-France project leader since 2004. As such she has major responsibilities for the use of Grid technology by the ATLAS experiment.

Overview: High Energy Physics(HEP) has been heavily involved in the planning and execution of Grid projects since 1999 starting with the findings of the LHC/MONARC project and the Hoffman report, which planned computing support for the LHC(Large Hadron Collider) experiments now due to start running in Autumn 2008 producing huge quantities of data. While waiting for the start very heavy use has been made of Grids for accomplishing the high volume simulations necessary for preparing the physics detectors and the physics analyses. In addition to the use of LHC experiments large scale data has been processed for current experiments running in US and European colliders, at Fermilab in the US and DESY in Germany.

The LHC machine will generate particle collision at 40 MHz, and the 4 experiments will record data at an integrated rate of ~1 GB/sec. In a typical years running some 15 Petabytes of new data will be stored, and the data processing involved will involve the equivalent of ~60,000 of todays fastest CPUs. This scale, combine with the natural distributed nature of the community, has led HEP to be main users of Grid technology serving the experiment Virtual Organisations.

Each experiment has a version of a multi-tier computing model with the central node being at CERN, and so-called Tier-1 centres typically being national centres and hundreds of so-called Tier-2 centres being distributed in the regions. There is a necessity for distributing data to all these tiers with appropriate processing functions being provided, for example at Tier-2s for individual user physics analyses. There is a very important requirement for keeping track of the location and status of all the physics data in the experiments, involving the skilled use of metadata tools for vast distributed databases.

There are some 40 counties involved in the WLCG (Worldwide LHC Computing Grid) with the main Grids involved being EGEE (250 sites) and the US OSG (15 sites). There are tools available permitting interoperability between the participating Grids. There is an increasing emphasis on individual user analyses using Grid interfacing portals such as GANGA and CRAB, each of which have 100s of users, and run thousands of jobs a day. Globally HEP experiments were running ~100,000 jobs/day in 2007, the majority being involved in large scale production simulations.

With the LHC starting in autumn 2008 there are ongoing 'data challenges' involving large scale data transfers between participating sites, running at rates in excess of 1GB/s. Currently a very high premium is being placed on the scalability, sustainability and reliability of operation, since Grids are an integral, and essential, part of LHC computing processing.

Further Information: http://lcg.web.cern.ch/LCG/ Worldwide LHC computing Grid

6. VO-level application support in EGEE

Author: Andrea Sciaba is a particle physicist who has extensive experience both in data analysis for physics, and in the use of Grid technology. Since the beginning of DataGrid in 2001 he worked within INFN on interfacing CMS experiment applications to the Grid, and since 2002 he has worked at CERN in supporting users in porting and running applications. This experience has extended outside particle physics, and notably to biomedical applications.

Overview: The EGEE Grid infrastructure provides computing and storage resources to dozens of scientific communities from several domains. The applications run on the Grid have different requirements on functionality, processing power and storage space. High energy physics experiments in particular provide a serious challenge for any Grid infrastructure, due to the sheer amount of the data produced and the complexity of the workflows. A very close relationship between the Grid and its users is therefore vital, and it involves several aspects: middleware development, deployment strategies, resource planning, and user training and documentation.

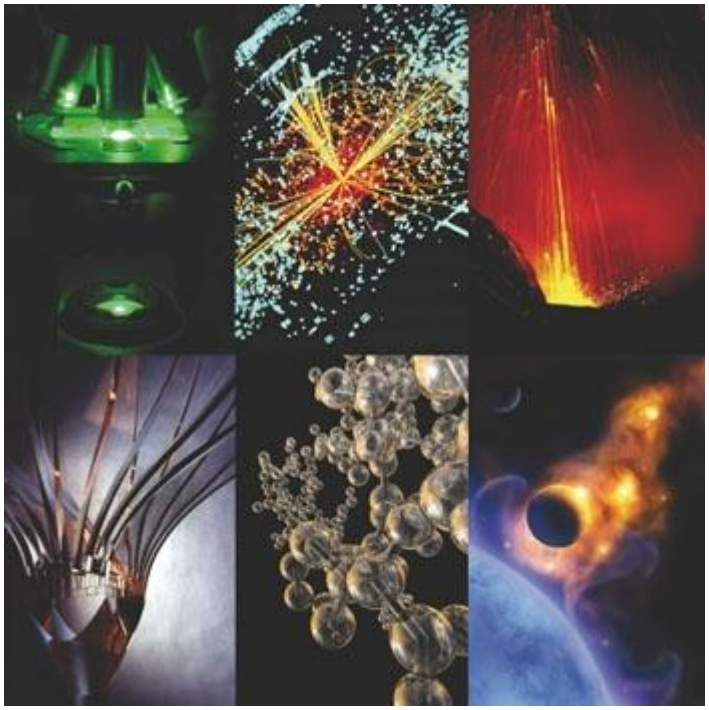
This contribution gives an overview on how Grid support at the Virtual Organisation level works in EGEE, and focuses on real-world examples, coming mainly (but not only) from the experience developed at CERN in supporting the LHC collaborations. From this experience general lessons useful for the project and for other user communities have been drawn.

The EIS (Experiment Integration Service) group at CERN worked intimately with all the experiments, and also with other key applications in EGEE. They have shown that it is essential in supporting a VO running on the VO to have dedicated effort coming from the VO itself. Essential components of the support service for VOs have been the GGUS system for servicing user 'tickets' generated when problems are encountered, and a variety of monitoring tools, notably the vary successful Dashboard monitoring system, which has been extended and generalized to support VOs outside the field of HEP.

Further Information

https://twiki.cern.ch/twiki/bin/view/LCG/LCGExperimentIntergrationandSupport

http://dashboard.cern.ch/



SCIENTIFIC APPLICATIONS



Astronomy & Astrophysics

Astronomy & Astrophysics

Convener: C.Vuerli (INAF-OA, Trieste, Italy)

The purpose of the A&A session was to consolidate the presence of the Astrophysical Community in EGEE. The first A&A session was organized in Budapest in the framework of the 2007 EGEE Conference. Applications that this community can bring to the EGEE Grid infrastructure are potentially very interesting as they are rather challenging in terms of requested resources and capabilities and are therefore an excellent test-bed for the Grid infrastructure. Astronomers in turn can take great advantage of the Grid as it offers an environment where typical A&A applications runs can be successfully carried out.

The agenda of the A&A session included six presentations concerning the most relevant astrophysics projects that already approached the Grid to run their applications, and one presentation illustrating the activities in progress to make the Grid and the Virtual Observatory mutually interoperable. Each presentation described the scientific aspects of the project, the effort spent so far to use the Grid technology within the project and future plans concerning this activity. Time was reserved at the end of the session for a general discussion on the following points: a) presented projects and applications; b) typical problems that it is necessary to tackle when porting A&A applications in Grid; c) future plans and activities aimed at consolidating the A&A component in EGEE.

The results coming from the Forum were:

- A&A and EGEE
  - A&A groups having big project-related applications are interested to port them to EGEE
  - Very often this process is pushed (and driven) by local/regional Grid strategies with respect to EGEE

- And what about A&A individuals and small groups that want to approach the Grid for the first time?
  - An EGEE A&A cluster now exists and a generic A&A VO has been created
    - astro.vo.eu-egee.org
  - The VO is now operative. Users can register to it and use the available resources

- But…the VO needs to grow in terms of
  - Both users and resources
    - New resources will be shortly contributed to it by Grid sites like INAF (Italy), Cometa (Italy), IFCA (Spain) and others
  - Training and dissemination play a key role

7. High performance computing on the Grid infrastructure of COMETA

Author: ORLANDO, Salvatore (INAF - Osservatorio Astronomico di Palermo)
Co-authors: Sacco, Germano (COMETA consortium, INAF - Osservatorio Astronomico di Palermo); COMETA, team (COMETA consortium); Peres, Giovanni (Dip.S.F.A. - University of Palermo); Reale, Fabio (Dip.S.F.A. - University of Palermo); BOCCHINO, Fabrizio (INAF - Osservatorio Astronomico di Palermo)

Short overview:
We report about our experience regarding the porting of High Performance Computing (HPC) applications to the Grid. In particular, we ported FLASH, a multi-dimensional, adaptive-mesh, parallel code capable of handling general flow problems in astrophysical environments. The HPC simulations performed using FLASH require a substantial amount of computational resources made available through the Grid infrastructure of the COMETA consortium.

Analysis:
FLASH is a parallel MHD code based on Message-Passing Interface (MPI) library and designed to be executed on HPC systems. The simulations performed required a substantial amount of distributed computational resources made available through the Grid infrastructure of COMETA.

Impact:
FLASH is a modular multi-D parallel code designed to allow users to configure initial and boundary conditions, change algorithms, and add new physics modules. Since the code is based on the MPI library, MPI and MPI2 libraries are distributed on the Grid infrastructure. Also, each cluster of the infrastructure is equipped with a fast interconnection network with low communication latency to allow the best performance of HPC applications. The execution of our application is particularly time-consuming and requires many processors (> 32); to check the produced files and/or to estimate the status of the job, we use a watchdog utility that checks for changes in logfiles and production files, reporting their content to the storage element, and registering their names into the file catalog (LFC).

Conclusions:
Grid infrastructures can be used to execute HPC applications if the following requirements are satisfied: distribution of MPI and MPI2 libraries on the infrastructure; clusters equipped with a fast interconnection network with low communication latency; queue dedicated to HPC applications with preemption capability on the other queues; use of watchdog utility for job monitoring during execution; long term proxy to allow the running of jobs whose execution is particularly timeconsuming.

Keywords: High Performance Computing, Astrophysics, Hydrodynamics, Magnetohydrodynamics

Further information: http://flash.uchicago.edu, http://www.astropa.unipa.it/FLASH/

8. The ZEN project

Author: Tilquin, André (CPPM/IN2P3)

Short overview:
The ZEN project, on the Universe expansion, is to provide a consistent and complete phenomenological framework bringing together theoreticians, phenomenologists and experimentalists. This framework handles theories, observed data, and statistical tools based on a phenomenological approach in order to allow a consistent interpretation of the free parameters, and the inclusion of experimental systematic errors. A new method, based on a frequentist approach, has been developed and ported on EGEE.

Analysis:
Evidence for the accelerated expansion of the Universe has been observed in the last decade with the many cosmological observations. The origin of accelerated expansion remains one of the most challenging research activities today. Progress in this field requires both theoretical innovations and many accurate observational probes with controlled systematic error estimates. The difficulty in performing combinations of different observations is to manage in a global analysis a large number of cosmological and astrophysical parameters (14 or more). As correlations are large and cannot be ignored at the percent accuracy level, the statistical method and the construction of an efficient numerical tool represent an important step of the ZEN project. We promote a frequentist approach which is commonly used by the High Energy Physics community and well under control. Our results are in agreement with complementary methods (mainly Baesian using MonteCarlo Markoff chain).

Impact:
The framework has already been developed and we adapt it within the Grid facility. This tool allows us to analyse new data in a coherent way very rapidly and intensely and is very useful for the design of future projects and the optimization of their strategies. The expected new data from various probes will be added into this framework, which will probably give us new interesting results for the cosmology. First attempts to introduce cosmological analysis based on frequentist statistical method on Grid have been successfully performed. Future experimental results will probably help us to understand better the nature of dark energy.

Conclusions:
ZEN needs a large number of CPUs, more than 1500 each run, but few storage. ZEN is running actually in the ESR VO, in parallel we are invited by INFN to install ZEN in the EUchina VO, in collaboration with Peking University and IHEP in Beijing. All major technical problems have been solved but still more developments are needed. Our first scientific results clearly show the power of EGEE in such analysis.

Keywords: Cosmology, Dark energy, EGEE, Euchina

9. Experiences of porting the astrophysical simulation "The unified theory of Kuiper-belt and Oort-cloud formation to EGEE Grid''

Author: Astalos, Jan (Institute of Informatics, Slovak Academy of Sciences)
Co-authors: Hluchy, Ladislav (Institute of Informatics, Slovak Academy of Sciences); Dobrucky, Miroslav (Institute of Informatics, Slovak Academy of Sciences)

Short overview:
Main goal of the simulation was to work out a unified theory of the formation of all: Jovian planets, Kuiper belt, Scattered Disc (populations of small bodies beyond the Neptune's orbit) and Oort cloud. The simulation was based on the dynamical evolution of a large number (~10000) planetesimals treated as test particles in the proto-planetary disc. The main reason for using the Grid was the need for about 40 CPU-years of computing time.

Analysis:
The experiment was performed in the scope of collaboration between Astronomical Institute of Slovak Academy of Sciences, Catania Observatory and Adam Mickiewitz University in Poznan. The simulation was ported to EGEE by Institute of Informatics Slovak Academy of Sciences and it ran in EGEE and TriGrid from February to October 2007. The simulation consists of a sequence of sub-simulations with many independent tasks within each sub-simulation. The necessary requirement is to finish all the tasks of a given sub-simulation before starting the next sub-simulation. The main problem when running the large number of jobs in Grid was the reliability of Grid infrastructure. Job management was rather time consuming due to the time spent on the analysis of the failed jobs and their resubmission. Moreover, the jobs that were waiting at some sites in a queue for a long time were blocking whole simulation.

Impact:
To overcome these problems we developed an easy-to-use framework based on "pilot jobs" concept that uses only services and technologies available in EGEE. It consists of pilot jobs ("workers") and automatic job management script. Workers are running the application code in cycle with input datasets downloaded from Storage Element using RFIO access. Output datasets are stored in output folder. To check the progress, the user only needs to list the contents of the output folder. To identify hanging jobs or the jobs that performs too slowly, the workers are periodically sending monitoring information to SE ("heart beat"). To avoid ermination of workers by queuing system, the workers are running only for limited time. The main goal of the job management script is to maintain the defined number of active workers with detection of failed submissions, finished and waiting workers. It uses job collections to speedup the startup and automatic blacklisting of full and erroneous sites.

Conclusions:
One of the expectations of Grid users is that they just put their application code and input data into the Grid, configure and start the processing and after the processing (with occasional checking the progress) they download the output data. In our approach we tried to get as close as possible to this expectation. The users of the astrophysical application were satisfied with our framework and we plan to use it for porting of similar applications to EGEE.

Keywords: astrophysical simulation, parameter study

10. Making the Grid and the virtual observatory mutually interoperable

Author: Taffoni, Giuliano (INAF-OA Trieste)
Co-authors: Pasian, Fabio (INAF-OA Trieste); Vuerli, Claudio (INAF-OA Trieste)

Short overview:
The Virtual Observatory (VObs) is rapidly evolving as a fundamental tool for the astronomical community. It may be seen as a Grid of federated astronomical databases. To process the huge amount of data residing in the VObs it is necessary to provide an adequate amount of resources. The combination of the VObs and of the Grid technology is the right answer to this issue offering at the same time a complete and integrated working environment to the astrophysical community.

Analysis:
Astrophysical applications handle simulated, theoretical and observed data and the amount of data requested by a single application is not negligible. Astronomical data are usually kept in databases most of them are now federated in the VObs. Users accessing these data usually expect some key capabilities like: a) find data by specifying their characteristics; b) retrieve them whatever is their physical location; c) generate them on-the-fly if not found; d) permanently store them in some place for the benefit of future users; e) apply further processing to them; f) save the results somewhere to be subsequently exploited by the whole community. The Grid allows the sharing of resources of different nature (hardware, software, data, and so on) so its tight synergy with the VObs is of strategic importance. A set of standards, tools and services are currently in preparation to make possible the necessary interoperability of these two technologies.

Impact:
To build the bridge between the Grid and the VObs it is necessary to make interoperable the suite of standards and web services of the VObs with tools and services of the Grid. The work in progress impacts some key aspects like: a) authentication and authorization mechanisms to gain access to VObs resources (data) and Grid resources through a single authentication transaction (single sign-on); b) access to both VObs resources and Grid resources simultaneously, in a transparent way to the final user and in both directions (from the VObs to the Grid and from the Grid to the VObs); the two approaches foresee the ability to provide “wrapped” science applications, either legacy code or new, as services in an application server (from the VObs to the Grid) or the ability to federate VObs components (astronomical databases) as embedded resources of the Grid. A standard working environment making easier the integration of applications with VObs and the Grid is in both cases mandatory.

Conclusions:
Current plans for what concerns the deployment depend on the adopted solution. Databases federated in Grid require to be integrated in the Grid middleware properly enriched of new tools and services. The execution of “wrapped” applications in Grid do have less impact on the Grid although some integration work for what concerns the authentication mechanism and the application working environment is still necessary. It is currently foreseen to go on with both the solutions.

Keywords: Virtual Observatory, Databases, Integrated Working Environment, Astronomical Applications.

Further information: http://www.ivoa.net/, http://www.euro-vo.org/pub/

11. LOFAR@EGEE

Author: Belikov, Andrey (Kapteyn Astronomical Institute)

Short overview:
The LOw Frequency ARray (LOFAR) is a key international project in radioastronomy. The challenging data storage and data processing of LOFAR will require an intensive use of both computing and data storage Grids. The LOFAR information system will be created to store data and to provide an access to the data of the LOFAR project to wide astronomical community as well as to manage the data reprocessing during the project. The EGEE nodes will become a part of this data storage.

Analysis:
The data volume produced by LOFAR will reach 4 PB per year. Data processing of Lofar requires an online access to the most of this data volume. We will need to implement a distributed data storage in a multicomponent environment, and the multicomponent environment (from the point of view of hardware, software and Grid concepts) will become a key feature of the project. We will need to integrate EGEE storage elements as a part of storage space for LOFAR information system.

Impact:
EGEE storage elements will become a part of the LOFAR storage space. The main issue in the realisation of this project is a data exchange between EGEE and non-EGEE storage elements, consistency of the data stored in non-uniform storage environment (based on different Grid technologies) and an access to the data from non-homogeneous computing elements.

Conclusions:
Dutch national astronomical data center OmegaCEN is in charge of the development of LOFAR information system in cooperation with LOFAR Consortium. OmegaCEN has already successfully developed an information system for astronomy Astro-Wise (http://www.astro-wise.org) which will serve as a prototype for Lofar information system. The developing and implementation of information system will start at the beginning of the next year and will be completed to the end of 2008.

Keywords: interoperability, applications, information system, radioastronomy

Further information: http://www.lofar.org http://www.lofar.nl http://www.astro-wise.org

12. Cosmological application in the Grid environment: detection of SZ clusters of galaxies in data from the ESA Planck satellite mission

Author: Lopez-Caniego, Marcos (Instituto de Fisica de Cantabria, CSIC-UC, Santander, Spain)
Co-authors: Herranz, Diego; Martinez-Gonzalez, Enrique (Instituto de Fisica de Cantabria, CSIC-UC, Santander, Spain)

Short overview:
In 2008 ESA's Planck satellite will be launch. The main objective of this mission is to produce a map of the anisotropies of the Cosmic Microwave Background radiation (CMB), a relic radiation from the Big Bang. To study this map, the compact source emission from distant galaxies and clusters of galaxies must be detected and extracted. We report on the work done detecting SZ clusters in realistic simulations of Planck.

Analysis:
Several techniques have been proposed to detect the SZ clusters. Most of them are based on linear filters that try to take into account the frequency dependence of the SZ effect to combine information from different channels to produce a single map where the clusters can be detected with a higher SNR than in the individual frequency maps (Planck will image the microwave sky in nine frequencies ranging from 30 GHz to 857 GHz). Within the Planck Collaboration an exercise to detect SZ clusters using realistic simulations has been proposed. The purpose of this exercise is to compare the performance of different algorithms to detect the SZ clusters, give an estimation of their integrated flux (and error) and an estimation of their size (and error). We have tested our implementation of the Matched Multifilter (MMF) developed by Herranz et al. 2002. We have analyzed nine full resolution Planck sky maps and detected aprox. 1100 clusters above the 5 sigma level.

Impact:
To do this kind of analysis we have to analyze 9 all-sky maps at full Planck resolution (aprox. 200 MB each). Then, we have to divide each one of these maps into 373 projected patches (512x512 pixels in size), this makes a total of 3357 patches (it would take 18 hours to run in a single CPU). Once we have the patches written to disk, we apply the MMF algorithm to the data. The analysis of each set of nine patches centered in the same region of the sky takes between 3 to 35 minutes, depending on the number of iterations. In our case, we want to estimate the size of the clusters properly, and, therefore, the analysis lasts aprox. 35 minutes per region. Since there are 373 regions to be analyzed, it would take about 266 hours to do this analysis (approximately 10 days in single CPU). We have done this analysis in 13 hours using 20 working nodes.

Conclusions:
This analysis using multifrequency maps required 13 hours of CPU time in each of the 20 planck vo working nodes and aprox. 20GB of space at IFCA, 18 GB of which were the input patches to be analysed. The output of the analysis is a list of detected clusters (just a few KB's) and 373 combined maps, one per region, where the detection is performed (2 GB). In the future a version of the Planck Sky Model introducing the satellite systematics will be released and this analysis will be repeated.

Keywords: Astronomy. Cosmology, Planck. Detection of SZ Clusters Galaxies.

Further information: http://www.rssd.esa.int/index.php?project=Planck

13. VO AUGER large scale Monte Carlo simulations using the EGEE Grid environment

Author: Schovancova, Jaroslava (CESNET)
Co-authors : Chudova, Jiri (CESNET and Institute of Physics, ASCR, Prague); Sitera, Jiri (CESNET); Sustr, Zdenek (CESNET); Dr. Travnicek, Petr (Institute of Physics, ASCR, Prague); Dvorak, Frantisek (CESNET); Filipovic, Jiri (CESNET); Kmunicek, Jan (CESNET); Krenek, Ales (CESNET); Matyska, Ludek (CESNET); Mulac, Milos (CESNET); Ruda, Miroslav (CESNET); Salvet, Zdenek (CESNET)

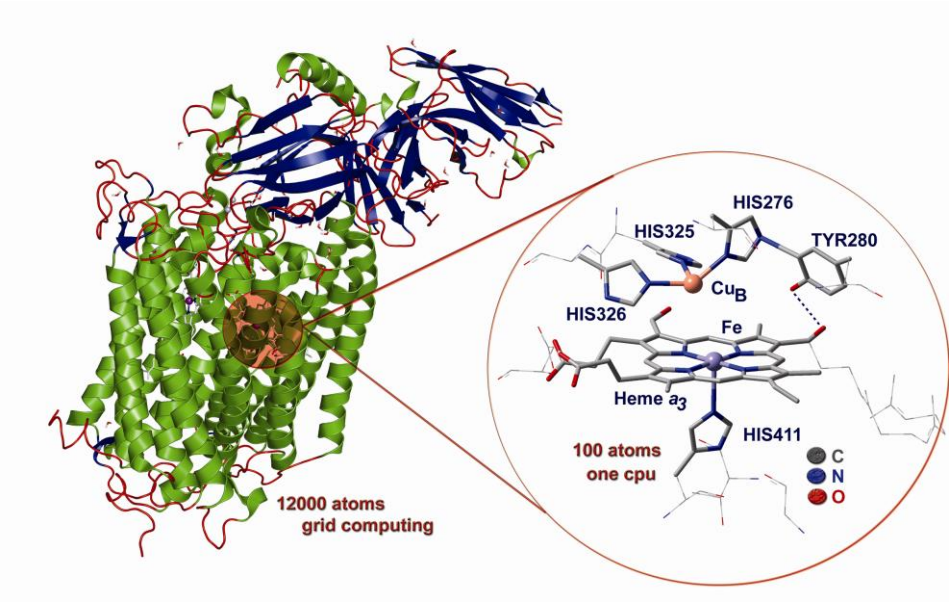
Short overview:
The Pierre Auger Cosmic Ray Observatory is studying ultra-high energy cosmic rays showering down on Earth. CPU intensive Monte Carlo simulations are needed to compare predictions of different models with observed data. We share our experience with usage of EGEE Grid resources to run these simulations. Also our experience with Job Provenance will be presented.

Analysis:
VO AUGER simulations made use of many CPUs connected in the EGEE Grid, which enabled us to simulate events with higher precision. The results of simulations were uploaded and stored on Storage Elements and registered in LFC Catalogue, therefore they can be accessed globally by all the VO AUGER members.

Impact:
We developed a framework for submission of many simulation jobs with different input parameters. This framework uses standard gLite job handling commands and it effectively and easily handles Large Scale simulations with a limited manpower, thus VO AUGER members can use the Grid to simulate their own ``private'' offline productions and share results of performed simulations with the whole AUGER collaboration. We established a VO naming scheme policy in order to manage the resulting data on various storages. We also use Logging and Bookkeeping and Job Provenance as a generic gLite service designed for long-term archiving of information on executed jobs focusing on scalability, extensibility, uniform data view, and configurability, which allows more specialized catalogues to be easily built.

Conclusions:
In conclusion, the Grid turned out to be very useful infrastructure for Large Scale simulations for the AUGER collaboration. The VO AUGER members can submit their computations to several Computing Elements and the AUGER collaboration members can access the simulations results worldwide.

Keywords: Pierre Auger Observatory, High Energy Physics, Large Scale MC offline production, Job Provenance



Computational Chemistry and Materials Science

Computational Chemistry and Materials Science

Convener: M. Sterzel (ACC Cyfronet/AGH, Cracow, Poland)

Computational chemistry and materials science are very rapidly adopting the Grid as a new computational platform, becoming the third consumer of computational power in EGEE after HEP and Life Sciences. Simulations cover many different areas from very accurate computations of chemical reactions between small molecules up to large molecular systems such as zeolite catalysts, semiconductors, polymers or even proteins helping to design new materials and understand the properties of existing ones.

The program of the session covered such topics as modeling of enzyme reactions (cytochrome C oxidase) as well as several aspects of materials science studies. Materials science talks included studies of the properties of nano-CMOS transistors, Quantum Dots and metal clusters (novel nanostructures with applications in semiconductor electronics, organic dyes and catalysis) and the memory and quantum effects during relaxation process of electron-phonon interaction in semiconductors. In addition to the computational data obtained on ScotGrid, EGEE and SEE-GRID2 Grids the contributions presented data analysis algorithms used for the Grid platform in particular.

The majority of topics allowed attendees to have an overview not only of scientific achievements of computational chemistry and materials science communities but also of computational challenges and difficulties faced by them. Complementary to this session, demos and posters highlighted other applications in materials science and computational chemistry areas and showed how the achievements of these communities can be beneficial to others.

The main messages coming from this session were:

- **Scientific results are being produced**
- **Special difficulties**
  - Job submission and handling a huge number of short time jobs
  - Data management (e.g. tracking 2 files per semi-conductor device quickly becomes problematic for huge ensembles)
- **Work on other Grid projects**
  - For example SALUTE is one of SEE-GRID2's supported applications.
  - SALUTE stresses the availability and scalability of the various Grid services and resources on the SEE-GRID2 infrastructure
- **Benefits from Grid usage**
  - Sharing of expertise and experiences made using the large computational resources available through Compchem and SEE VOs
  - Sharing of techniques for managing a large amount of submitted jobs
  - The use of the Grid provides not only CPU power but also a platform for sharing the achieved results among scientists and avoiding of duplication of efforts
- **This community has a strong interest in the deployment of MPI**

14. SALUTE: new results for the inhomogeneous case

Authors: Karaivanova, Aneta (IPP-BAS); Atanassov, Emanouil (IPP-BAS); Gurov, Todor (IPP-BAS)

Short overview:
SALUTE (Stochastic ALgorithms for Ultra-fast Transport in sEmiconductors) is a Grid application developed to study the memory and quantum effects during relaxation process of electron-phonon interaction in semiconductors. These effects are important for better understanding of the behavior of some types of nano-devices and optimizing their design. Using SALUTE new results for the inhomogeneous case, when the electron evolution depends on the energy and space coordinates, were obtained.

Analysis:
SALUTE integrates a set of advanced Monte Carlo and quasi-Monte Carlo algorithms developed by the application team. In our recent work we studied the inhomogeneous case in the presence of electric field. We obtained new results for the distribution density, energy distribution and Wigner function, which give insight into the quantum effects that occur in this case. The understanding of the physics of the inhomogeneous case give more realistic picture of the intra-colisional field effect and are important for improving the simulation process for new semiconductor devices.

Impact:
SALUTE is a computationally intensive application which needs vast amount of CPU power, good data storage and transfer capabilities in order to achieve the desired accuracy and spatial resolution of all graphs. It is well known that when temporal or spatial scales become short, the evolution of the semiconductor carriers cannot be described in terms of the Boltzmann transport and a quantum description is needed. As a rule quantum problems are very computationally intensive. The use of the Grid provides not only CPU power but also a platform for sharing the achieved results among scientists and avoiding of duplication of efforts. The results that we obtained using the SEE-GRID infrastructure in one day could be achieved on a single cluster for several days, which would slow down the analysis process significantly or decrease the resolution.

Conclusions:
SALUTE is a flagship SEE-GRID2 application and currently runs on SEE-GRID2 infrastructure which uses EGEE gLite middleware. This application exercises the availability and scalability of the various Grid services and resources on the SEE-GRID2 infrastructure. The accounting data shows that a total of more than 100 000 CPU hours were used, with a peak utilization of more than 300 CPUs running simultaneously, making use of more than 24 Grid clusters. Up to 3 GB of data were produced in one run.

Keywords: Grid Computing, Electron Quantum Transport, Monte Carlo Methods

15. Supporting statistical semiconductor device analysis using EGEE and OMII-UK middleware

Author: Reid, Dave (University of Glasgow)
Co-authors: Roy, Scott; Millar, Campbell; Roy, Gareth; Stewart, Graeme; Asenov, Asen - (University of Glasgow); Sinnott, Richard (NeSC)

Short overview:
Progressive scaling of CMOS devices has driven the phenomenal success of the semiconductor industry. Silicon technology has now entered the nanoCMOS era with 40nm gate length transistors in production. However the semiconductor industry faces many fundamental challenges which will affect the design of future integrated circuits. The NanoCMOS project aims to apply eScience technologies to this problem. We describe our experiences (good and bad) with EGEE and OMII-UK technologies for this purpose.

Analysis:
The only method by which variability in nano-CMOS transistor characteristics (and thus the variability and yield of the circuits making use of them) can be predicted, understood and designed around is through large scale numerical simulation. To capture in detail the statistical parameter distributions in real device architectures requires vast computational resources generating extensive device ensembles. Using resources such as ScotGrid (www.scotGrid.ac.uk), it has been possible, for the first time, to generate an ensemble of more than 100,000 microscopically different 35nm gate length devices – comparable with state-of-art production devices. Early results indicate that designers must assume much larger parameter variations than are currently considered. It is also clear that some of the assumptions underlying present design techniques are no longer valid, due to significant, non-analytic deviations at the extremes of the statistical distribution.

Impact:
Previously, the sheer number of different device simulations required to properly analyze the statistics of device variability have made solutions impractical with conventional computing resources. However, the availability of HPC resources such as ScotGrid have made such simulations viable. Computation on this scale, however, is not without problems, and whilst using GANGA as a submission interface alleviated difficulties associated with large scale job submission to Globus other difficulties arose resulting in a considerable proportion of rogue jobs. This complicated data management, as it is important to avoid the generation of duplicate devices in order to preserve correct ensemble statistics. In consultation with ScotGrid admins, we have managed to overcome some of these difficulties to produce the first device ensemble of this scale. Work is also on-going exploiting OMII-UK middleware and in particular the use of technologies such as GridSAM for job submission and management.

Conclusions:
Simulation of a 100,000 device ensemble has consumed a considerable amount of computing power - over 11 years of CPU time over the course of approximately 6 weeks. In order to fully understand device variability we must now consider additional physical effects, and simulation of smaller devices. Currently we plan to proceed with the generation of large statistical ensembles for 25, 18, 13 and 9nm devices in order to examine variability at extreme levels of scaling.

Keywords: NanoCMOS transistors, device variability, numerical simulation, OMII-UK, GANGA

Further information: http://www.nanocmos.ac.uk/

16. Exploiting Grid for condensed matter applications: quantum dots and building clusters atom-by-atom

Authors: Kanhere, Dilip (Pune University); Pujari, Bhalchandra (Pune University); Zorriasatein, Shahab (Pune University); Ghazi, Mohammad (Pune University); Kaware, Vaibhav (Pune University); Joshi, Kavita (Pune University)

Short overview:
Quantum Dots (QD) and clusters represent novel nanostructures with applications in semiconductor electronics, organic dyes, catalysis etc. Their electronic structure is crucial for tailoring desired properties. We use Grid to calculate their properties (band gaps, bonding, stability, magnetics state, quantum states) using self consistent field (SCF), density functional theory (DFT). We also investigate evolution of properties as a function of size. The work is done under EU-India Grid Project.

Analysis:
QUANTUM DOTS: A fully self consistent real space DFT approach has been implemented. We calculate the ground state charge and spin density, magnetic state, eigenvalue spectrum and investigate effects of impurity over a wide range of sizes of quantum dots (50-300 nm with 2-20 electrons). The results reveal Wigner localized state (Wigner molecule). The impurity induces the novel magnetic states ans anti ferromagnetic spin distribution and enhances the localization. CLUSTERS: We have obtained equilibrium geometries (~100) of clusters of Sodium (Sizes 20-150) by a combination of simulated annealing and local minimization. We calculate stability, binding energies, HOMO-LUMO gap etc. We also investigate growth patterns and fine that the growth shows order- disorder cycles. The shape analysis of the ground states is shown to be correlated with the shapes of heat capacities. Thus nature of the ground states and the isomers spectrum dictates the behavior of clusters at finite temperature.

Impact:
For both the problems the possible SCF solution need several hundred independent runs which can be executed asynchronously. In the first problem, for a fixed value of dot size ~100 SCF runs are needed (for fixed number of electrons). A exhaustive study of up to 20 electron QD, needs in the few hundreds of thousands of runs. Although the single run of this calculation is not CPU extensive, the mare number itself is too heavy for a small cluster to perform the calculations in reasonable amount of time. Similarly for the finding isomers of a single cluster typically 400 minimization are executed.The number of jobs to be executed turns out to be number of clusters*400*charge state. For a thorough understanding of evolutionary characteristic we undertake 3 types of clusters: Na_n (Jellium, n=20-147), Ga_n (covalent n=20-70) and Al_n (n=20-70). The magnitude of the computational intensity can be guessed from the fact that the total no of runs required is ~100,000 (~5 Hrs per run).

Conclusions:
For a class of problems discussed here the Grid computing turns out to be extremely efficient. (Resources: EGEE, Garuda, Local machines) The number of runs required is ~100000 and each can be executed on P4, Xeon machines. We have obtained the results ~50 clusters of Na (with shoot-and-forget strategy). Future plans involve Na_n (n=20-147) and Ga_n(n=20-70). The resulting detailed comparison of the growth pattern is expected to answer a fundamental question: "how do clusters grow, atom by atom?" keywords : Quantum dots, Impurities, Wigner, Atomic Clusters, Electronic Structure, Density Functional Theory

Further information: http://physics.unipune.ernet.in/~cmg/Grid.html

17. The study of cytochrome C oxidase on the EGEE Grid

Authors: Gervasi, Osvaldo (Dept. of Mathematics and Computer Science, University of Perugia); Prof. Farantos, Stavros C. (Department of Chemistry, University of Crete, Iraklion 711 10 and Institute of Electronic Structure and Lasers, Foundation for Research and Technology-Hellas); Daskalakis, Vangelis (Institute of Structure and Lasers, Foundation for Research and Technology-Hellas); Giatromanolakis, Manos (Institute of Structure and Lasers, Foundation for Research and Technology-Hellas)

Short overview:
Our Grid experience carrying out Molecular Dynamics calculations on the enzyme cytochrome c oxidase (CcO) on EGEE through Compchem VO will be presented and discussed. The biomolecule (CcO) consists of approximately 10000 atoms and the calculations would require years of our local CPU time. Performances and drawbacks of the current status of the Grid will be discussed.

Analysis:
The current project involves Molecular Dynamics calculations on cytochrome c oxidase. CcO is the terminal enzyme of respiratory chains found in the inner mitochondrial membranes or in many bacteria and the last acceptor of electrons from oxidizing processes involving nutrient molecules. The biophysical interest of this project stems on long standing problems which concern the assignment of difference spectra of isotopically substituted ferryl oxygen.

Impact:
The Molecular Dynamics calculations on cytochrome c oxidase is a heavily demanding application in terms of the CPU time required. Furthermore, it is demonstrated that the study of the vibrational spectra and dynamics for pumping water molecules from the active site, it presents a perfect example for a Grid application. We performed the domain decomposition of the initial conditions and a large number of sequential jobs have been launched on the Grid. To this end, the computer codes running on our local clusters were Gridified and some scripts were written to make the Grid calculations feasible, automating the management of the large number of jobs. Some errors occurred in the scheduling of the jobs have been managed esubmitting the failed ones automatically. The large number of CPUs available on HellasGrid and on Compchem and SEEGrid VOs made it possible to perform the preliminary production runs, while the project is still in progress.

Conclusions:
The paper reports our experience in studying the spectroscopy and reaction dynamics of enzymes with classical dynamics on the production EGEE Grid environment using the HellasGrid and CompChem and SEEGrid VOs.

Keywords: Computational Chemistry, Dynamics and Spectroscopy of Proteins, Classical Molecular Dynamics

Further information: http://tccc.iesl.forth.gr http://compchem.unipg.it



Earth Sciences

Earth Sciences

Convener: M. Petitdidier (IPSL/CNRS, France)

Earth Sciences (ES) is an all-embracing term for sciences related to planet Earth, covering a large and diverse user community, academic as well as industrial. The phenomena under study are dependent on geographical coordinates, altitude and time. This community has set up active collaboration with teams on a worldwide basis and is accustomed to work in a distributed manner. Since several years the ES applications show an increasing need for access to intensive computing facilities and to large and heterogeneous sets of data. The community has two major computing problem areas: (1) modeling, which requires vast amounts of computational resources, and (2) the exploration and production of large, shared data sets. This community has investigated Grid and developed web services since the emergence of this technology.

Different presentations showed applications ported on EGEE in atmospheric chemistry, climate, hydrology, seismology, cloud and precipitation domains. These demonstrated that the Grid provides more computing resources to the user but is also a way of sharing data, algorithm and of developing common tools and can be considered as an e-collaboration platform. Even if EGEE is suitable for intensive data processing and production, statistical approach, job on alert, simulation and modeling, the interface between ES environment and Grid middleware is not simple for many applications and developments. There persists a significant gap due to complex computing protocols in ES. The unsatisfied needs in terms of data management, workflow and portals were pointed out and a roadmap proposed and discussed.

The main points from the Forum were:

- **Spectrum of applications presented**
  - New applications with important challenges (scenarios for soil pollution by pesticides, new processing of the whole seismology dataset of the Geoscope network)
  - Mainly for the Research community with a few for companies and civil protection
- **Key ES requirements are not satisfied, barriers for porting applications**
  - Analyzed by DEGREE (collaborating European Commission-funded project)
- **In EGEE-III seek improvement and/or implementation of functionalities more adapted to Earth Sciences**
  - "Generic " solutions
- **New tools needed to use the whole Grid potential**
  - Need for exploration of huge data sets
  - Creation of a platform integrating web services, computing power, information systems etc.

18. Earth science application overview in EGEE infrastructure

Author: Petitdidier, Monique (IPSL)
Co-author: Weissenbach, David (IPSL)

Short overview:
Earth Science (ES) is an all-embracing term for sciences related to the planet earth covering a large and diverse user community, Academy, organisation and industry. Since 2000 within DataGrid and CrossGrid ES applications from various domains (seismology, hydrology, geosciences, geology, pollution, atmospheric chemistry…) have been ported on a Grid infrastructure in order to get more computing resources, to share data and algorithms and to explore or produce large data sets. Some applications a

Analysis:
Due to the large variety of ES applications it is not possible to describe all the results obtained. However some ES applications, already ported, provide scientific results published in international journal and conference proceedings, and included in PhD report. Those results are a mean to convince the ES community of the potentiality of the Grid infrastructure like EGEE. The ES applications that already obtained results could be used to point out the kind of problems very well suited to Grid infrastructure like statistical approaches (monte Carlo method, ensemble of jobs..), sharing data or algorithm, performing a very large number of independent jobs that permits to have a rapid solution.

Impact:
The role of Grid technology to get scientific results depends on the motivation to use Grid. As for the need of more computing resources like for the earthquake application, without Grid the results will be obtained too lately to have an impact on the community. As for sharing algorithms like Geocluster, Grid avoids to implement locally the software that is never a straightforward task or to adapt the code; also the resources allotted via the Grid permit to use the software at full scale. As for sharing data Grid avoids to duplicate large sets of data that is not always possible and permits to develop common tools.

Conclusions:
All the applications have been ported on EGEE. There are no average conditions. In seismology some jobs uses MPI, others need to use simultaneously 200-400CPUs, or to access the geoscope data centre to process systematically on Grid all the data, or to carry out simulation. In atmospheric chemistry one application processed and handled 70000 files, the other application is a long run simulation and the output data are transferred to local storage in the laboratory. In hydrology, one application

Keywords: Earth Science, data management, workflow

19. Long range air pollution transport over Europe, studied on the Grid

Author: Ostromsky, Tzvetan (IPP - BAS, Sofia, Bulgaria)
Co-authors: Dimov, Ivan (IPP - BAS, Sofia, Bulgaria); Zlatev, Zahari (NERI, Roskilde, Denmark)

Short overview:
Large-scale environmental models are powerful tools, designed to meet the increasing demand in various environmental studies. The pollutants and other chemical species actively interact with each other and can be moved in a very long distance. All relevant processes should be taken into account. This makes the air pollution modeling a difficult computational task. The huge demand of computational resources has always been a limitation factor in the development and practical use of such models.

Analysis:
The Danish Eulerian Model (DEM) is a powerful air pollution model, designed to calculate the concentrations of various dangerous species over a large geographical region (e.g. Europe). This is a huge computational task and requires significant resources of storage and CPU time. Parallel computing is essential for the efficient practical use of the model. However, it is not sufficient when a large number of experiments have to be done. A number of experiments for one year period were necessary to carry out in order to detect the set of the most important parameters, which have influence on certain specific pollutant (e.g. the ozone). The computational Grid was used for this purpose. Promising results have been obtained within a reasonable time by using EGEE infrastructure. Overview of these results will be presented in this talk.

Impact:
The most powerful supercomputers have been used in the past decade for the development and test runs of DEM. Both MPI and OpenMP standard tools have been used in order to achieve highest parallel efficiency without loosing portability. Parallel computing was the only possible technique in order to get real data results in real time, even for the simplest 35-species chemical scheme. With the development of the more sophisticated chemistry submodels (with 56 and 168 different chemical species respectively), it was no longer possible to obtain sufficient affordable parallel resources for all our experiments. That is why we have to use Grid technology as well. It allows us running several long experiments (for one year period) simultaneously on several EGEE cites. Parallelism via MPI was also used in these experiments.

Conclusions:
The Grid technology set up new horizons for use and further development of the Danish Eulerian Model. We consider it as very attractive and affordable, especially for the countries from Eastern Europe. Results show that parallel computing on the Grid is one of the most promising computing techniques that could deal efficiently with such tasks.

Keywords: Environmental Model, Air Pollution, DEM, EGEE, Parallel Computing, MPI

20. Dissemination and exploitation of Grids in Earth science

Author: Hluchy, Ladislav (Institute of Informatics, Slovakia)
Co-authors: Tran, Viet (Institute of Informatics, Slovakia); Petitdidier, Monique (Institut Pierre Simon Laplace); Som de Cerff, Wim (Koninklijk Nederlands Meteorologisch Instituut); Schwichtenberg, Horst (Fraunhofer Institute for Algorithms and Scientific Computing); Linford, Julian (European Space Agency); Fusco, Luigi (European Space Agency)

Short overview:
Earth Science (ES) is an all-encompassing term for sciences related to the planet Earth like seismology, geology, hydrology, and meteorology. DEGREE is a Specific Support Action (SSA) project that aims to promote Grid technologies throughout the large and diverse Earth Science community as a platform for e-collaboration in academic and industrial organizations.

Analysis:
The key requirements of ES applications on data management, job management and portal technology have been identified and analyzed in five ways: (1) A panel of representative ES applications have been analysed; (2) Existing data management tools and policies that are being used in ES applications are surveyed in order to find common required features of ES community; (3) The existing Grid data management technologies have been analyzed in order to provide the solutions for the requirements; (4) The available Grid middleware and tools for job submission and workflow management have been analyzed and several missing features required by ES applications are identified; (5) Existing Grid portals for ES applications are surveyed for creating common Grid based portal and service oriented architectures for ES applications.

Impact:
The aim of DEGREE project is to create a bridge between ES and Grid communities in order to influence the next generation of Grid technologies with accordance to ES needs. The requirements of ES applications and identified missing technologies are delivered as feedback to developers of Grid middleware. To better understand the requirements, test suites have been created with typical ES applications and test cases for realistic illustration of the requirements. Grid developers can use the test suites for testing and validating their middleware and tools. Roadmaps for building and promoting Grid technologies in ES communities are being created for new ES applications.

Conclusions:
The work in DEGREE project will increase the collaboration and close the gaps between ES and Grid communities. It delivers feedback from ES communities to Grid developers and will promote and widen the use of Grid technologies in ES applications. This will help to shape the next generation of common Grid platforms for ES applications.

Keywords: Earth science, data management, workflow, portal, roadmap

Further information: http://eu-degree.eu

21. Grid computing for wildfire danger assessment: porting RISICO on gLite

Authors: D'Andrea, Mirko (CIMA Foundation); Dal Pra, Stefano (INFN)
Co-authors: Verlato, Marco (INFN); Fiorucci, Paolo (CIMA Foundation); Gaetani, Francesco (CIMA Foundation); Angelini, Valerio (CNR-IMAA)

Short overview:
The RISICO application, use-case selected by the CYCLOPS project estimates distribution of wildland fire risk over the Italian territory helping civil protection agencies to plan the firefighting system. A short description of RISICO is presented, along with motivation for the Grid porting of the application. A submission strategy for both application input data and output retrieval is considered. A mechanism to ensure automatic resubmission of eventually failed jobs is also described.

Analysis:
RISICO works on a set partitioned on identical and algorithmically independent squared cells.Computing a cell requires "cell status" and meteo data and produces a "next status" as also the wanted output of the simulation. A RISICO run on the Italian territory with cells of 1 km^2 requires approximatively the computing of 330.000 cells and 150Mb of input data, producing 1Gb of output data in a 20 min of time on a common workstation. Finer simulations using 0.01 km^2 sized cells, leads to quadratically increased input and output data size as also needed computation time. We can afford these higher needs through Grid. We divide a run into a few tens of jobs, each using Storage Elements for input and output data, and the requirement that every job succesfully ends in a given maximum time. This gets achieved thanks to a "job status monitor" program running at UI level which polls about jobs termination retrieve outputs and resubmits failed or late to finish jobs.

Impact:
The RISICO application running at WN level is a quite straightforfward rebuild of the original C++ source code, with no need for particular libraries. A GRisico wrapper script takes care of launching the executable after downloading three needed input compressed archives: the list of cells to compute, their status, meteo data for the given cell-set. The actual Logical File Names are provided through the InputSandbox. End of job execution gets recognized from our job status monitor program by polling LFC catalog for output file existence. This permits to retrieve it earlier than the OutputSandbox, whose readiness needs official LB answer. After execution ends it uploads the new computed status and the output as compressed archived. Time statistics for every step are taken by the wrapper script and returned through the OutputSandbox. They'll be eventually useful when verifying the submission strategy.

Conclusions:
Tests on a production Grid environment with data from a real case scenario (VO cyclops) lead to satisfying results. Attention must be paid however to an effective ranking requirements choice in jdl. Up to now failed or unfinished jobs get resubmitted on provenly fast queues. Plans are to refine the resubmission strategy in an attempte to ensure a maximum completion time. A further goal is to integrate RISICO with geospatial services for input and output data sharing.

Keywords: Forest fires, Risk Assessment, Civil Protection, Disaster Management

Further information: http://www.cyclops-project.eu/



Finance and Multimedia

Finance and Multimedia

Convener: S.Holsinger (Trust-IT Services Ltd., Italy)

The Finance sector is one of the driving forces for the use of distributed or Grid computing for business purposes. Science is a great source of practical inspiration for the sort of computer intensive tasks that banks and financial institutions need to do on a regular basis, such as large-scale Monte Carlo simulations of market behavior to predict investment risks or stock market analysis. Cluster and Grid computing offers the same solutions here as it does in the scientific world and there is a great deal of synergy between the two fields. In this session there was an interesting application covering the areas of stock analysis application that automatically manages the analysis of a large mass of financial data.

The Grid also offers a unique solution to multimedia users, allowing seamless data dissemination and performance scalability, as illustrated by the GridVideo application. gLite and the Grid projects supported by the EU are now approaching a degree of maturity where they can provide practical solutions to demanding commercial-sector problems. Government agencies will also soon reap the benefits of Grid developments with the potential of altering taxation policies or asset allocation strategies. The main points emerging from this session were:

Porting business applications

- Porting applications to Grid environments requires an important effort
- Reliability is a great issue
- A Grid is composed of heterogeneous systems that change over time and the porting efforts need to takethis into account.
- Non-trivial multi job applications need some standardized way to communicate

Continue to market user case studies to attract business

- Meet with businesses and inform them of Grid and EGEE, and benefits
- Present them with User Case Studies
- Currently gLite business case studies are being collected for use in marketing and meetings

22. GridVideo: a Grid-based multimedia application

Authors: Iellamo, Giuseppe (Università di Messina); Minutoli, Giuseppe (Università di Messina); Bruneo, Dario (Università di Messina); Puliafito, Antonio Università di Messina)

Short overview:
In this paper we describe GridVideo, an implementation of a multimedia application based on the Grid computing paradigm. In GridVideo media files are stored across the Grid into chunks; then, when a user requests for a streaming; all the chunks are tailored in order to match the client device characteristics. Grid is used in order to share computational resources (given that tailoring operations are computational intensive) and to access to distributed data.

Analysis:
The application is divided into two different activities: - the Multimedia Upload activity during which service providers make multimedia objects available to their customers by uploading them to the Grid Storage Elements - the Multimedia Streaming activity where the media are requested by end-users through a GUI. Upon these requests the media chunks are recovered, tailored and finally streamed towards user device. This activity calls for stringent time requirements between different jobs. Using the Grid allows for both seamless data dissemination during the Upload activity(through the use of Storage Elements and file catalogs) and performance scalability during the Streaming activity(by adapting the amount of resource used to the number of users).

Impact:
GridVideo features different modules in order to carry out the two activities explained before. The module for upload is quite straightforward: a simple GUI that uses the data management APIs to upload files on the SEs, and job management APIs in order to split the input file. The modules (running either on UIs and WNs) devoted to the Streaming activity are much more complex because of the time requirements. In particular in order to offer a gap-free reproduction we have to ensure that all the needed jobs start together. Moreover a messaging system is needed between the jobs and the UI application. In order to solve these problems we relied on what we call 'idle_jobs' (a sort of job agent, submitted in a proactive way to the Grid) to ensure time requirement satisfaction and we used the JMS technology in publish/subscribe mode so as to enable communications between the involved entities.

Conclusions:
Porting a complex, non-trivial multi job interactive application to the Grid is not an easy task. In particular it is difficult to choose the right way to segment the application into jobs without incurring into excessive penalties for the network communications. Some standardized communication mechanism between jobs is needed. Last but not least reliability is a big issue: there are many point of failure so in order to ensure reliability the application has to be carefully designed.

Keywords: Distributed multimedia streaming, Job coordination, Jms

23. Stock analysis application

Authors: Michalareas, Giorgios (Department of Electronics and Computer Science, University of Southampton, UK); Corso, Ezio (ICTP / EU-IndiaGrid team); Skouras, Spyros (Athens University of Economics and Business)
Co-authors: Cozzini, Stefano (ICTP / EU-IndiaGrid team)

Short overview:
The primary objective is of analysing massive financial databases on an instrumentby- instrument basis (one instrument's data analysed at each node) but may have many other application domains. It may be a valuable tool for the Grid community at large: mtransfers and unzips large quantities of data from secure storage to each node, performs identical computationally intensive statistical analysis of the data at each node and then zips and securely stores the voluminous results of this analysis.

Analysis:
The proposed application will automatically manage the analysis of a large mass of financial data. For each financial instrument there is a zip file: its content is one text file per trading day containing high frequency time-series information for that instrument. Overall there are 4 TB of unzipped data: compression reduces it to roughly 100 GB. One analysis run consists in launching one job for each stock; for each instrument about 150 time-series are constructed and analysed; about 700 instruments will be analysed in each run. Many runs are expected, as both the analysis and the time intervals of interest will change during open-ended research on the properties of the data. For a reasonably exhaustive analysis on all the data, about 200 GB of zipped output files are expected.

Impact:
The application is organised in two tiers: the first one handles the Grid infrastructure, while the second one is exclusively concerned with the analysis of the data. The analysis is run in the Worker Node; it expects to have locally available a set of data files for processing, and it will produce a predefined set of local output files. The Grid infrastructure code in turn consists of two parts: one to launch and monitor the analysis, and one to prepare the local environment in the WNs for the analysis. The launching and monitoring part is installed in a UI host; it accepts: a file containing the list of data to process, the analysis code to execute, and the Grid output directory in a predefined secure SE. The code that prepares the WN local environment: fetches data files from the secure SE, pre-processes them, launches the analysis, clears any local temporary files, and saves them back in the SE.

Conclusions:
Currently the application facilitates processes that could also be achieved by Gridscripting. This is only a starting point towards a fully fledged distributed Gridapplication architecture WSx-compliant, integrated in the Information System and ready for QoS as an application-level Grid service for financial research. The "second tier" of the application described in (3) can be viewed as a general purpose tool that is useful to any researcher wishing to perform similarly intensive analysis.
Keywords: WSx-architecture QoS Finance general data-intensive analysis

Further information: https://euindia.ictp.it/stock-analysis-application

24. Using Grid technologies for the mapping out of taxation policy

Authors: Ploskas, Nikolaos (University of Macedonia); Glavelis, Themistoklis (University of Macedonia); Margaritis, Konstantinos (University of Macedonia); Samaras, Nikolaos (University of Macedonia)

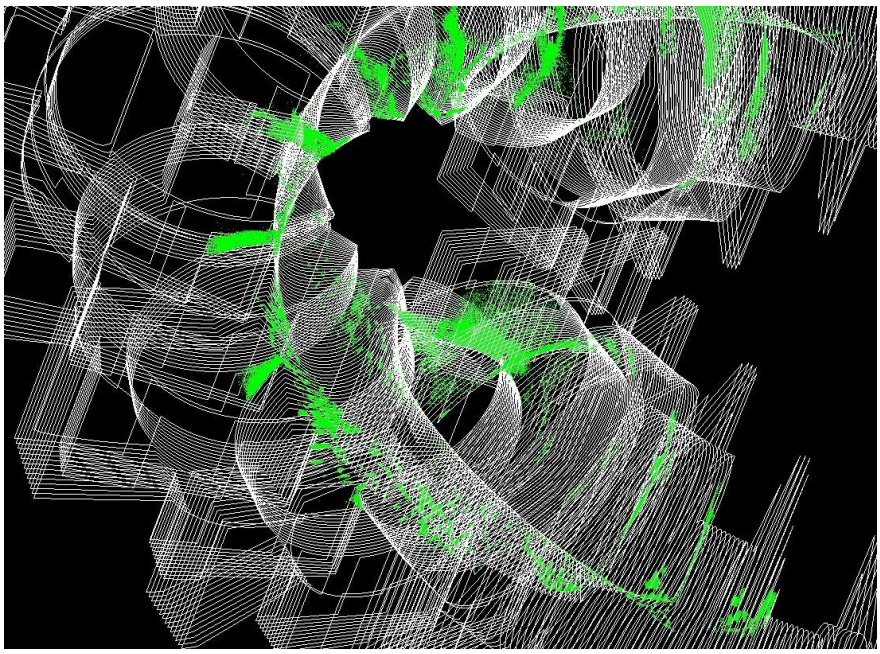
Short overview:
It is a fact that the impact of taxes in the economy is significant. Consequently, it is very important for the Public Administration to have reliable elements and alternative scripts that are related with the effective application of tax policy. This paper presents an application which is a powerful tool for the tracing of taxation policy. The scope of this tool is to present the ongoing opportunities that Grid technologies provide to many sectors, such as the sector of Public Administration.

Analysis:
The regression that we used to appreciate the tax policy of Greek government is the following: Sgovt = a0 + a1*T +a2*TR +a3*INT +a4*G where ai, i=1, …, 4 are the coefficients of the regression and a0 is the constant term, Sgovt the Government budget deficit/surplus, TR is the Transfer Payments, INT is the Net Interest Payments and G is the Government Purchases. Due to the lack of real elements of many years, the application creates a lot of instances of data. Sample of elements for the past fifteen years were taken from the databases of OASA, Eurostat and National Statistical Service of Greece. The application exports a report that includes all the statistic and econometric results of the model with the most adequate data. Using such a kind of report the government could forecast its budget deficit or surplus setting up various scripts. Obviously, this is only a tool for examining different solutions of the taxation policy and cannot substitute the theoretical approach of the problem.

Impact:
Having a vast list of historical elements relative with interaction of various factors in the tax policy, we can seek models that can be used for formulation of forecasts with regard to the future development of important tax sizes. According to these models, we can advance in control of various affairs, altering either the prices of entries or the prices of parameters of models. Because of application's demands for memory and computational resources, it is infeasible to be executed locally in a typical computer, so a Grid should be used in order to accomplish this operation. The infrastructure of Hellas Grid and Eumed Grid gives the possibility for processing big volume of data and having substantially simultaneous control of different approaches, models or scripts.

Conclusions:
The application was developed with the high-level open source language Gnu Octave (edition 2.9.12). With the help of the infrastructure of Hellas Grid we were able to execute our application. The size of the produced data set was about twenty gigabytes and the execution time of the application was usually, since the availability of the Grid differs each moment, little above one hour.

Keywords: Grid, Taxation Policy, Public Administration, Econometrics, Octave



Fusion

Fusion

Convener: F. Castejon (Ciemat, Madrid, Spain)

Numerical modeling has always been important in Fusion research, but lately it has become a key activity. The Fusion community is preparing itself for the exploitation of the next generation of magnetic confinement devices, especially of ITER, a large international project with seven partners (EU, Russia, USA, Japan, China, Korea and India) and the large Wendelstain 7-X stellarator, which will be built in Germany with the European Commission's support.

Numerical tools are being developed to extract the maximum scientific performance of these devices, whose plasmas are a challenge for the present computing facilities. Grid technologies have an important role to play in this plasma theory and modeling activities. We have identified a number of problems in magnetic confinement fusion for which Grid computing is a key tool. Some applications have been ported to the Grid and are running presently in EGEE infrastructure. These applications have already produced relevant scientific results for both stellarators and tokamaks, and have been useful to open new ways to solve physical problems in those devices. Examples are the Ion Kinetic Transport simulation, that enables the study of collisional confinement without the common and doubtful approximations that are customary in fusion community; the stellarator optimization application, that enables the Grid to explore the best stellarator geometry for confinement; the Massive Ray tracing code for simulating the microwave heating; plus a number of applications that are being used to simulate diagnostics, ion dynamics in the Neutral Beam heating system for ITER, etc. As a result, several new projects have started from the EGEE deployment experience as int.eu.Grid and EUFORIA.

The Fusion session of EGEE'07 showed several examples of fusion application results and demonstrated the added value that Grid technologies have given to numerical fusion research. The main points coming from this session were:

- **Fusion VO in EGEE used for scientific production in Fusion Research.**
  - http://Grid.bifi.unizar.es/egee/fusion-vo/
  - http://www-fusion.ciemat.es/collaboration/egee/
  - 14 Partners ~ 4500 CPUs - 45 TFlops
- **New relevant scientific results obtained with Grid capabilities.**
- **Complex workflows are being established.**
  - Kepler workflow orchestration is a promising tool. Workflows between Grid-HPC based on Kepler
- **New Project EUFORIA: Opportunity for bringing more partners of Fusion Community to Grid Computing.**
  - workflow orchestration is the final goal of EUFORIA

25. Interfacing gLite services with the Kepler scientific workflow

Author: Metery, Rene (CS)
Co-author: Guillerminet, Bernard (CEA)

Short overview:
End users want to use services hiding the complexity of the Grid as well as easing the integration of their application into this environment. If they can also have a workflow service to build the chaining of jobs with pre and post-processing for their applications the benefit would be even higher. The aim of the integration of gLite services in Kepler fits perfectly the need for users to have a simple and powerful tool to build a workflow submitting jobs on Grid infrastructure.

Analysis:
The interfacing process has been realized with the different operations made by an end-user in mind, when he wants to authenticate and submit a job on the Grid. First the creation of an actor making the voms-proxy-init operation was needed to create a temporary proxy as well as returning informations concerning his role in his Virtual Organization. Then the creation of several separate actors making all the operations of the job lifecycle was mandatory to build a complete and modular workflow. After having validated all the actors on the Pre Production Service infrastructure, the creation of a workflow representing the complete job lifecycle has been possible.

Impact:
This work will be used to build complex workflows simulating the plasma and the whole fusion device. These simulations are highly computation demanding and require to launch many tasks on the Grid environment. The gLite-based middleware and the actors which have been developed and implemented in Kepler will allow the end-users to easily build scientific workflows and submit jobs on the EGEE Grid infrastructure. As soon as they have their application integrated into Kepler, they can chain pre and post-processing to Grid submission without the need to create an interface directly with their application.

Conclusions:
The deployment of Kepler could be done on any UI or computer with the gLite librairies embedded. While interfacing the tool to the middleware we learnt that gLite has several well-designed APIs but also a lack of documentation for others like the VOMS services. In the future, Several other gLite services like the data managment ones are planned to be interfaced with Kepler as well as other middleware to improve the interoperability.

Keywords: Workflow, Kepler, Job Submission, Fusion

26. Optimisation of applications support in RDIG fusion VO

Authors: Voznesensky, Vladimir (Inst. of Information Systems, RRC "Kurchatov Inst.")
Co-authors: Semenov, Igor (Nuclear Fusion Inst., RRC "Kurchatov Inst."); Dobretsov, Vladimir (Inst. of Information Systems, RRC "Kurchatov Inst."); Ryabinkin, Eugene (Inst. of Information Systems, RRC "Kurchatov Inst."); Larionov, Andrey (Inst. of Information Systems, RRC "Kurchatov Inst."); Mikhailov, Mikhail (Nuclear Fusion Inst., RRC "Kurchatov Inst.")

Short overview:
Grid alternatives are more expensive and, hence are less available, but usually seem more appropriate for numerical optimisation computations. A stellarator optimisation application has demonstrated the efficiency and the ability of the EGEE Grid to meet the demands of such computations. A reflectometry signal optimisation application, currently being developed, has similar functional requirements but needs the computational power obtainable only in a Grid.

Analysis:
Two examples of CPU-intensive numerical optimisation applications were found in Russian nuclear fusion and plasma science: optimisation of stellarator magnetic field configuration and optimisation of the reflectometry radiowave shape in ITER plasma. The first application has been successfully ported from a supercomputer to the EGEE infrastructure. This porting has revealed two issues. First, the Grid dictates use of mathematical methods that allow asynchronous completion of parallel jobs without loss of efficiency. For optimisation, that means shifting from iterative (gradient-based) methods to results-based spool-driven (genetic, stochastic interpolation) ones. Second, tools for such application-specific jobs and data management are required. The second application is in its development phase. The functional requirements are the same, but it requires orders of magnitude more CPU than the first one. Supercomputers cannot fulfill it's demands.

Impact:
A novel Grid portal prototype, Grid InterFace (GIF), is presented. GIF is designed to be a complete solution for the optimisation applications. It consists of a web interface, script-driven job management engine, object database, HTTPS sandbox I/O service, WMProxy and LB clients. An application developer uses the portal to describe all aspects of a Gridapplication. An authorized end-user can define the parameters and spawn a calculation for the application. In case of the genetic optimisation application, an initial developerdefined Python script generates several Grid jobs. Each job calculates a target function value at a random point. Then, the system submits the jobs and waits for their completion. Another script is spawned after every job completion. It adds the calculated function value and it's point to the persistent genome pool, gives the current best genome to the user, selects the parents from the pool to breed and generates a new job to spawn.

Conclusions:
Existing and prospective optimisation applications found, for instance, in fusion science, need a special application-driven non-predictable workflow manager not fullfilled by existing middleware. The authors present a prototype of such system that serves as an interface and a driver environment for such applications. About two man-years will be required to make the portal production-grade and run the reflectometry signal optimisation application on the Grid.

Keywords: Non-predictable workflow, Grid portal, fusion, genetic, optimisation, script-driven.

Further information: http://vo.nfi.kiae.ru/pmwiki/pmwiki.php?n=Main.StellaratorOptimization

27. Distributed task scheduling for physics fusion applications

Author: Herrera, Jose (UCM, Spain)
Co-authors: Dr. Montero, Ruben Santiago; Prof. Llorente, Ignacio Martín; Dr. Huedo, Eduardo (UCM, Spain)

Short overview:
A new scheduling algorithm to distribute tasks on Grid environments will be described. The algorithm is an enhancement of the distributed dynamic self-scheduler algorithm used in loop parallelization. The algorithm will be applied to the efficient distribution of tasks in physics fusion simulation codes.

Analysis:
There are two kinds of parallel loop schedulers to distribute program loops among the processors of a parallel architecture: static and dynamic scheduling. In this work, we will focus on dynamic schedulers because they are more suitable for heterogeneous environments such as a Grid. In general, in these algorithms a central node dynamically distributes a fraction of the computational workload (chunk) to the rest of the worker nodes. Depending on how the chunks are calculated, different simple self-scheduling schemes can be devised. An alternative to these schemes is the distributed self-schedulers. In this case, the scheduler takes into account the characteristics of the different components of the system (e.g. the cpu speed or the system load) to optimize the chunk assigned to each node. This work presents a new distributed self-scheduler scheme that takes into account all Grid characteristics: a high degree of heterogeneity, high fault rate, dynamic resource availability, etc.

Impact:
The effects of this new distributed algorithm will be proved in the MARATRA (Massive RAy TRAcing in Fusion Plasmas) system. MARATRA aids those community members who are working on the optimization of plasma heating by electron Bernstein waves (EBW). This new algorithm allows the execution of tasks in the MARATRA system using loop parallelization methods. This approach presents important advantages over the traditional task schedulers, for example, a better workload balancing between all Grid resources or a decrease of the scheduling overhead. Furthermore, the estimated execution time of each Grid node during the tasks distribution process allows the dynamically adaptation of the whole application. Hence, the workload of each task will be dynamically distributed depending on the behaviour of each node. The goal of this distribution scheme is to adapt the MARATRA system to the Grid environment.

Conclusions:
The high degree of heterogeneity and high fault rate of existing Grid infrastructures require the implementation of new self-scheduling algorithms to calculate the task chunk size of parameter sweep and high throughput computing applications. The presentation will describe a new algorithm inspired in the distributed selfschedulers schemes used for loop distribution on parallel architectures. Its advantages are demonstrated for the execution of a Physics Fusion application.

Keywords: SelfSchedulers, Grid, Dynamic, Distributed, Fusion, Algorithm

28. Fusion results within EGEE

Author: Castejon, Francisco (CIEMAT)
Co-authors: Velasco, José Luis (BIFI); Tarancon, Alfonso (BIFI); Vazquez-Poleti, José Luis (Universidad Complutense); Voznesensky, Vladimir (Kurchatov Institute); Tereshchenko, Max (General Physics Institut, Russian Academy of Sciences); Cappa, Álvaro (CIEMAT)

Short overview:
Modeling is becoming a key activity in fusion research. Several applications have been chosen as demonstrative examples of the Grid capabilities: Ion Kinetic Transport; study of ion trajectories in tokamak and stellarator plasmas; MaRaTra: Massive Ray Tracing; Plasma heating modelling within WKB theory implies the use of large number of rays; Stellarator optimization allows the searching of optimal magnetic configurations; Plasma reflectometry optimisation; Application in development phase.

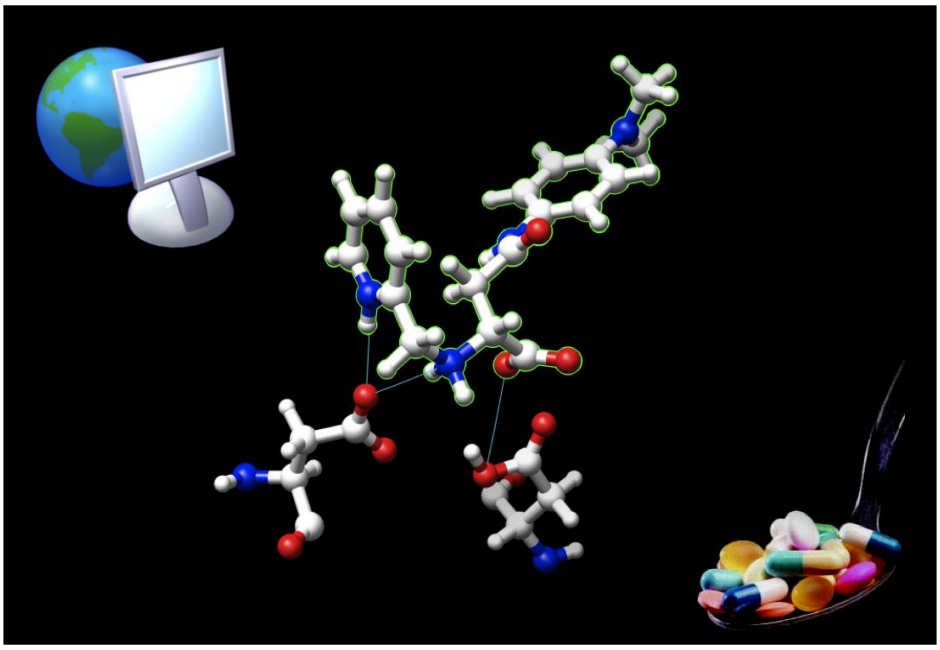
Analysis:
Ion kinetic transport application allowed the estimation of ion collisional transport both in tokamaks and stellarators, showing properties that could not be found by the customary methods: transport is not diffusive and that there exist important asymmetries, oppositely to what was thought. Further improvements of the applications are ongoing. MaRaTra calculations have allowed to estimate the heating of plasmas confined in complex geometries, like that of TJ-II stellarator, by quasielectrostatic waves. This is especially challenging, since it is necessary to consider a huge number of rays. The optimization of wave launching requires a large number of runs with 10^4 - 10^5 rays. The heating system for TJ-II stellarator has been designed using these results. Gridway metascheduler is used in MaRaTra Stellarator Optimization. The application is running and several stellarator configurations are explored. Future activities will involve the optimization of TJ-II stellarator. Kepler

Impact:
Ion Kinetic Transport: Grid computing has allowed to remove the doubtful approximations that are used in the customary modelling tools, i.e., we do not assume that transport is diffusive, we do not perform any average on magnetic surfaces and we can perform estimates for arbitrary mean free paths, being therefore a method valid for low collisonality plasmas, as the ones that will be present in a fusion reactor. These achievements could be done by following a huge number of independent particles during all their life in the plasma. MaRaTra: A huge number of independent calculations are needed for optimizing the launcher and the receiver. This problem structure is perfect for Grid computing: a bunch of rays is running in every node of the Grid. Stellarator Optimization. Different stellarator configurations can be studied in separated nodes of the Grid. A genetic algorithm chooses the best one regarding a target function. Different target function can be implemented within the algorithm.

Conclusions:
The Fusion VO was used for MaRaTra and Ion Kinetic Transport. The Stell. Opt. and the Relfletometry applications run in the Russian Grid. The CPU time for a single case is about 2 years. The future plans involve the enhancement of Ion Kinetic Transport and MaRaTra applications with new equations and the exploitation of Stell. Opt. The experience in using the Grid and the middleware will be exploited in Euforia Project. New applications will be ported and Kepler will be used for complex workflows

Keywords: Fusion. Workflow

Further information: http://www.fusion.ciemat.es



Life Sciences

Life Sciences

Conveners V. Breton (CNRS/IN2P3-LPC), C. Blanchet (CNRS/IBCP)

Life Sciences is a very active field of research on the EGEE infrastructure. Several EGEE related projects are also exploring the use of gLite middleware for bioinformatics and healthcare. In many different fields of Life sciences, the research communities are increasingly using the Grid resources for applications. As a consequence, the Biomed Virtual Organization is now standing as the leading non LHC-Virtual Organization with an average of 7000 jobs submitted every day to the Grid and more than 4 million hours of CPU consumed in the last 12 months.

The User Forum was a wonderful opportunity to obtain an overview of the present adoption of Grids in the Life Sciences communities through the oral sessions but also through the posters and demos exhibition and the satellite workshops and tutorials.

The Life Sciences session program reflected the variety of topics currently addressed in EGEE and its related projects. The first two oral sessions were devoted to applications in the field of molecular biology covering genomics, transcriptomics and proteomics while the third session was focused on drug discovery and medical imaging. The contributions ranged from describing the Gridification of a given application to presenting scientific results obtained on the Grid. Complementing the session program, demonstrations and posters from EGEE partners and related projects highlighted other life sciences applications during the Forum with emerging fields such as system biology.

The following were the main messages coming from the Forum:

- **The Grid is now used to produce scientific results for the Life Sciences**
  - 11 abstracts on scientific results
  - 18 abstracts on application porting and deployment
- **Compute-intensive applications are routinely operated on the Grid**
  - Typical size: a few to 10-20 CPU years
  - As with the LHC experiments efforts required for improving robustness of services
  - Special approaches are used to reduce latency and improve efficiency
    - Pull model with agents (WISDOM)
    - BOINC on EGEE (Superlink)
- **Significant progress towards the federation of databases**
  - See the Health-e-child demo (winning demo for the Forum)
  - Several groups reported the use of AMGA (Health-e-child, HOPE, WISDOM)
  - There is an issue on the future evolution and maintenance of AMGA and secured storage service
- **Limitations identified in deployment and performance**
  - MPI deployment: only 1000 out of 17000 CPUs on Biomed VO are running MPI
  - >1GB RAM needed for some applications
  - Data bandwidth sometimes insufficient for applications
- **Prepare for transition after EGEE-III**
  - Stronger involvement of National Grid Initiatives (NGIs) and collaborating projects
  - Prepare migration from EGEE-III to EGI

29. Genome wide association studies of human complex diseases with EGEE

Author: Munteanu, Alexandru Ionut (INSERM, UMR S 525, Faculté de Médicine Pitié-Salpêtrière, Paris, France)
Co-authors: Cambien, François (INSERM, UMR S 525, Faculté de Médicine Pitié-Salpêtrière, Paris, France); Tregouet, David (INSERM, UMR S 525, Faculté de Médicine Pitié-Salpêtrière, Paris, France)

Short overview:
Until now, association analyses between gene polymorphisms and diseases was limited to a few number of polymorphisms because those analyses require much computational power. The EGEE Grid provides enough computation power for analysing the whole human genome. The following describes the THESIAS program created for this research, but also how we have used EGEE with this software.

Analysis:
As part of the research conducted at the INSERM U525 laboratory, the THESIAS software was created in order to analyze statistically, associations between gene polymorphisms and diseases. Given a data set containing the genotypes of case and control individuals, THESIAS measures haplotype frequencies combining several polymorphisms and associations with the disease. Until now this kind of analysis was restricted to single genes and a few polymorphisms (<25). The recent availability of DNA chips allowing to genotype hundreds of thousands of polymorphisms across the genome implies a change in scale in the necessary computations. For whole genome haplotype analysis we decided to use the EGEE Grid.

Impact:
Identifying which DNA sequences variations(SNPs) are associated to a disease on the entire human genome has a complexity which increases exponentially with the number of SNPs. Frequencies of combinations of multiple SNPs must be estimated and ideally all the possibilities would be analyzed. However, there are at least 10 millions SNPs on the human genome and calculating all the combinations is hardly imaginable. Fortunately, SNPs located close to each other (for example within a gene) are frequently tightly correlated, they are said to be in linkage disequilibrium (LD) and they define haplotype blocks that can be tagged by a limited number of marker-SNPs. The most recent genotyping arrays contain 1 million marker-SNPs and are highly informative. Computational burden may be further reduced by investigating haplotypes (sets of closely linked SNPs) in a sliding window. This research can lead to the identification of new causes and mechanisms of disease of potential therapeutic interest.

Conclusions:
As a proof of principle, we have analyzed thousands of SNPs for their association with cardiovascular disease in thousands of individuals. Easy-gLite, a UI on top of the gLite UI has been created to simplify batch job submissions, monitoring and automatic resubmission of failed jobs. We will soon use EGEE on analysing the whole genome, with about 500,000 SNPs, which is at least 50 times more important than our last analyses.

30. BioinfoGrid: bioinformatics Grid applications for life sciences

Author: Milanesi, Luciano (National Research Council - Institute of Biomedical Technologies)

Short overview:
The project aims to promote Bioinformatics Grid applications for life science, in order to carry out Bioinformatics research exploiting Grid networking technology. BioinfoGrid combines Bioinformatics services and applications for molecular biology users with the Grid. A summary of the main results achieved in the frame of the BioinfoGrid project to better exploit the potentiality of the Grid will be presented.

Analysis:
The BioinfoGrid adopt high-level user interfaces, common to all the different BioinfoGrid applications, in order to exploit the Grid services provided within European Grid Infrastructures using a more user-friendly approach. One of the activities within the project was to develop a Bioinformatics Portal, to simplify the services request and the jobs submission to the Grid, including the automation of Workflows in order to dynamically establish complex genetics analysis. The project supports studies on applications for distributed systems for Microarray technology, for Gene expression studies, for Gene Data Mining, analysis of cDNA data, Phylogenetic analysis, Protein functional analysis and system biology simulations in Grid.

Impact:
The BioinfoGrid project exploits the use of Grid technology on a global network between several research laboratories, allowing the shared use of computational power, data storage and complex data analysis. The Bioinformatics complex calculations involving huge amounts of data by the implementation of a dedicated workflow to distribute the jobs on thousands of computers spread on a wide geographical area in order to greatly reduce calculation times. The adoption of the use portal certificate (robot certificate) is planned and it will be very useful in increasing the medical and biology user communities to use the Bioinformatics applications in Grid. BioinfoGrid project contribute to expand Grid awareness inside the bioinformatics community through numerous dissemination activities, summer schools, practical workshops and international conferences.

BioinfoGrid was able to establish large collaboration between the European Grid Infrastructure EGEE and the Bioinformatics research user community in various fields of Bioinformatics applications. In the case of the Avian Flow data Challenges, the BioinfoGrid project contributes in deploying molecular docking pipeline analysis for the in silico drug discovery. Finally the BioinfoGrid project developed a BioinfoGrid portal able to run several bioinformatics applications.

Keywords: Bioinformatics, Workflow, Genomics, Proteomics, Transcriptomics, Portal.

Further information: http://www.bioinfoGrid.eu

31. TriAnnotPipelineGrid, a tool for the automated annotation of wheat BAC sequences

Authors: Leroy (INRA Clermont-Ferrand); Mr. Reichstadt (AuverGrid)

Co-authors: Giacomoni and Charpentier (INRA Clermont-Ferand); Alaux and Reboux (INRA URGI); Claude, and Liauzu, (LifeGrid); Tanaka, and Itoh (National Institut of Agrobiological Sciences)

Short overview:
The main goal of the TriAnnorPipelineGrid project is to provide to the scientific wheat community, and especially to the IWGSC), new resources for efficient BAC sequence analysis, as well as a platform for the re- annotation of BAC sequences as knowledge of the wheat genome sequence is increasing and new genes, transposable elements and new biological targets are continually identified.

Analysis:
A long term project of the IWGSC is to sequence the wheat genome to decipher the chromosomal location and biological function of all genes. This knowledge should enhance the understanding of the biology of the wheat plant and create a new paradigm for the improvement of this major crop. Because of the genetic and metabolic conservation among species in the grass family,efforts to decipher gene function in wheat and its close relatives will work synergistically with similar efforts in maize,rice,sorghum,barley and other grasses,for a global understanding of the function,structure,and evolution of the grass genomes. The aim of the project is to provide a wheat automated annotation system to annotate new BAC sequences and regularly updating previous BAC annotations. It also provides a GBrowse graphical viewer. The pipeline integrates programs for prediction and analysis of protein-coding gene structure, as well as the identification of transposable elements and repeats in BAC sequences.

Impact:
The project aims are: 1. Improving time calculation through the use of the Grid technology. BLAST, RepeatMasker, HMMPFAM, est2genome, Gmap have been already adapted to the Grid (AUVERGRID), 2. Store all the output within a CHADO data base for improving Gbrowse graphical display. 3. Adding new modules such as a gene modelling and new prediction tools The project is performed through a strong collaboration between the INRA URGI bioinformatics platform at Evry, France; the NIAS at Tsukuba, Japan; The Broad Institut, US ; and Iowa State University This program also benefits from a Genoplante project (GNPannot 2008-2010 WP5) to allow an on line BAC annotation curation using Apollo; A FP7 European project (TriticeaeGenome 2008-2010 WP5) to add the REPET pipeline for Transposable Element annotation; and a Generation Challenge Programme (2008-2009) for developing a web service on GreenPhyl (CIRAD).

Conclusions:
The main goal of the TriAnnotPipelineGrid project is to provide to the scientific wheat community, and especially to the IWGSC, new resources for efficient BAC sequence analysis, as well as a platform for the re- annotation of BAC sequences as knowledge of the wheat genome sequence is increasing and new genes, transposable elements and new biological targets are continually identified.

Keywords: wheat, genome sequencing, bac sequence analysis, Grid, IWGSC, LifeGrid

Further information: http://urgi.versailles.inra.fr/projects/TriAnnot/pipeline.php

32. High-throughput Grid application for life sciences: the gene analogue finder

Author: De Sario, Giulia (Istituto di Tecnologie Biomediche, CNR)
Co-authors: Donvito, Giacinto (INFN Bari) ; Tulipano, Angelica (INFN Bari) ; Maggi, Giorgio (INFN Bari); Gisel, Andreas (Istituto di Tecnologie Biomediche, CNR)

Short overview:
Up to now, researchers have compared genes looking at their sequence similarity. However the correlation "sequence – function" is only partially applicable. Descriptive annotations, such the one provided by the Gene Ontology (GO) and its associations with the gene products (GOA), offer information for a way of comparing genes according to their functional description. The application consists of an algorithm that uses the data of GO and GOA to find functional analogous gene products, i.e. gene

Analysis:
The algorithm is a very high data and data-access intensive application. The results of the functional analogous search demonstrate that the information contained by the GO is adequate to run such analysis using the gene production description. For example most of the homologous gene products of most of the model organisms were assigned as functional analogues, although the annotations were done independently. This result also proofs that the algorithm assigns functional analogues in the right way. More important, the algorithm finds significant functional analogous gene products within the same or within different organisms, also non-model organisms, which have such a low sequence similarity so that with conventional methods those assignments would not have been found. Functional analogous associations represent very important information for scientists in the laboratory which are able to find new information and hints about the functionality of the gene product they are working on.

Impact:
The GO and GOA repositories are updated in a monthly frequency improving the annotation quality but also increasing the number of annotated gene products. The results show that most of the gene products from non-model organisms are poorly annotated and therefore were not considered within this search or produced low level informatin. For that reason the algorithm is highly dependent on new releases of the GO and GOA and the functional analogous search needs to be updated as frequent as possible. Only by using the Grid technology we are able to fulfill this need and are able to offer the best results to the scientific community by recalculating the whole search results using each new monthly release of GO and GOA.

Conclusions:
The algorithm is a very high data and data-access intensive application. To avoid the problem of concurrent accesses to the data, the system temporally distributes both the analysis tool and the data on WNs where the tool has to operate. The jobs were distributed over the EGEE Grid infrastructure within the VO biomed using about 300 WNs. The input data is in the size of 600MB and the results in the order of 2GB. The process was terminated within a day instead of about 60 days using one CPU.

Keywords: bioinformatics, life science, temporal data distribution

33. Grid solving a bioinformatics challenge: a first step to anchoring the nucleosome

Author: Blanchet, Christophe (CNRS IBCP)
Co-authors: Michon, Alexis (CNRS IBCP); Zakrzewska, Krystyna (CNRS IBCP); Lavery, Richard (CNRS IBCP)

Short overview:
How proteins find their targets amongst millions (or more) of competing sites is still largely an unsolved problem. Understanding this process in detail is however central to understanding the mechanisms underlying gene expression. A better understanding of site-specific targeting is also a vital step towards rational reengineering of proteins for therapeutic purposes.The problem becomes even harder when a complex of several proteins binds to DNA, as in the case of the nucleosome core particle.

Analysis:
The nucleosome involves a complex of eight proteins (histones) binding to 147 basepairs of DNA. Simulating a nucleosome core bound to a single DNA sequence would require treatment of roughly 250,000 atoms and many months of computer time. To understand selective binding we need to compare many potential binding sequences and hence perform many such simulations. Given that any of the four nucleic acid bases can occupy each position within the bound DNA, there are roughly 10^86 potential sequences to test. We have been able to reduce this task by dividing the DNA into overlapping fragments containing four nucleotide pairs (4^4=256 sequences for each pair). By minimizing each sequence in turn for each fragment, and then moving one step along the nucleosome-bound DNA, we can reconstruct the binding energies of all possible sequences with approximately 36,000 optimizations using the JUMNA program (developed in our team). The whole task would take roughly four years on a single processor.

Impact:
We have used the production Grid set up by the EGEE-II project. We have submitted 35,840 energy minimizations as individual jobs on the Grid. This means that each job had gone through the submission processes, and thus paid the overhead inherent to the Grid architecture and internal processes: from the submission through the user interface (UI), via the scheduling step on the resource broker (RB) to the execution on the computing element (CE), a cluster with several worker nodes (WN). The whole computing task was launched through 12 RBs, which have scheduled all the jobs on 23 CEs. The total cumulated computing time was about 1,275 days, with a job duration of 51 minutes on average. The full calculation was completed after 4 days and 16 hours, running up to 1039 jobs simultaneously. This was 271 times faster than using a single machine.

Conclusions:
Using the EGEE Grid to obtain a first indication of the binding specificity of the nucleosome turned out to be rather efficient. The results have demonstrated the sustainable status of the EGEE Grid for large-scale experiments with a real laboratory workflow. We are planning to continue our study with an improved model that will require 140,000 energy minimizations, corresponding to roughly 16 years of sequential CPU time.

Keywords: Bioinformatics, Molecular simulation, Large scale experiment

Further information: http://gbio-pbil.ibcp.fr

34. Performance analysis and optimization of AMGA for the WISDOM environment

Author: Ahn, Sunil (KISTI)
Co-authors: Kim, Namgyu (KISTI); Lee, Seehoon (KISTI); Hwang, Soonwook (KISTI); Dr. Koblitz, Birger (CERN); Breton, Vincent (CNRS)

Short overview:
AMGA is a gLite-metadata catalogue service designed to offer access to metadata for files stored on the Grid. We evaluated AMGA to analyze whether it is suitable for the WISDOM environment, where thousands of jobs access it simultaneously to get metadata describing docking results and the status of jobs. In this work, we address performance issues on AMGA and propose new techniques to improve AMGA performance in the WISDOM environment.

Analysis:
In the WISDOM environment, thousands of job agents distributed on the Grid may have access to an AMGA server simultaneously (1) to take docking tasks out of the AMGA server to execute on the machine that they are sitting, (2) to get the related ligand and target information, and (3) to store the docking results. The docking tasks take about 10 to 30 minutes to finish depending on the machine that they run and the docking configuration. We have carried out some performance analysis on the current AMGA implementation. Due to the overhead required to handle GSI/SSL connection on the Grid, it showed about 350% poorer throughput compared with a direct DB access. In the current version of WISDOM, AMGA is used as a placeholder for a task distribution table where docking tasks are stored and maintained. We have found a serious performance degrade due to the overhead caused by the need to lock the whole table to prevent different agents from taking the same task.

Impact:
First, in order to address the SSL/GSI-related performance issue, we have proposed a load-balanced multiple server and a DB connection pool technique in AMGA, Our preliminary test results demonstrate a linear performance improvement in proportion to the number of AMGA servers. Secondly, to deal with the performance degrading problem associated with the locking of the whole table, we modified the AMGA source code and added a new API that allows the two separate AMGA APIs, SELECT and UPDATE needed to take a task, to be invoked at once. Our preliminary tests show that the new API allows about 50 tasks to be retrieved per second in contrast with one task per second being retrieved using the two separate SELECT and UPDATE API calls.

Conclusions:
We addressed performance issues on the use of AMGA in the WISDOM environment and presented some new techniques to drastically improve the performance of AMGA. The techniques are expected to be integrated in the new release of WISDOM environment, being deployed in the EGEE biomed VO infrastructure for the next WISDOM data challenge.

Keywords: WISDOM, AMGA, metadata catalog, performance measurement

35. Analysis of metagenomes on the EGEE Grid

Authors: Aparicio, Gabriel (UPV); Blanquer, Ignacio (UPV); Hernandez, Vicente (UPV)

Short overview:
A Metagenome is a sample of several complete genomes of several living beings. The analysis of metagenomes is a key issue in biological research, but it is a computationally intensive task. An environment has been developed and deployed on top of EGEE and has been successfully used for the analysis of four metagenomes from digestive track, soil and sea bacteria consortia. The environment has enabled to complete a study which would have taken 1.5 CPU years in optimal conditions in 10 days.

Analysis:
Metagenomic analysis requires several iterations of alignment and phylogenic classification steps. Source samples reach several millions of sequences. These sequences are compared to the eukaryotic species of the "Non-redundant" database. The deployment process involves three stages: First, public databases are copied in relevant SEs to reduce the access time by increase the geographic replication of the data. Second, the available resources are tested through short test jobs that check the different operations. Finally, the experiment is performed. The sequences of the source sample are split into different jobs. Each job is submitted through the RBs to the CEs that have been selected in the test phase. Jobs copy all the relevant databases from close SEs to the local storage, install locally the BLAST and clustalW software and execute the scripts. After the completion of the job, results are copied back through the SEs and GridFTP as a backup solution.

Impact:
Metagenomic analysis is needed in the cases in which it is impossible to grow significant samples of isolated specimens. Many bacteria cannot survive alone, and require the interaction with other organisms. In such cases, the information of the DNA available belongs to different kinds of organisms. Four experiments have been executed with up to 800K sequences. The environment has enabled to reach performances of more than 8.000 sequences per hour. The complete experiment was performed in 10 days. A standard PC would have taken 1.5 CPU years in optimal conditions and would not reach more than 66 seqs/hour). However, the failure ratios of the jobs are high. In the largest case, 55% of the jobs were resubmitted. From the failing jobs, 49% end in the aborted state, 26% had problems accessing the catalogue, 7% fail using the wget command, 4% could not install the BLAST tool due to problems in the configuration of the compiler and 14% were cancelled due to its long duration.

Conclusions:
An environment has been developed to fragment, automate and check the operations of Metagenomic analysis. It has been tuned-up considering the most efficient and reliable resources, the optimal job size, and the data transference and database reindexation overhead. The environment re-submits faulty jobs, detect endless tasks and ensure that the results are correctly retrieved. New metagenomic studies are being completed, and the full processing chain is being enriched with more steps.

Keywords: biomed, biocomputation, metagenomics, service challenges

Further information: www.grycap.upv.es/bio

36. WISDOM: Grid enabled identification of active molecules against targets implicated in malaria

Authors: Da Costa, Ana Lucia (CNRS-IN2P3, LPC Clermont-Ferrand)
Co-authors: Kasam, Vinod (Fraunhofer-SCAI)

Short overview:
Malaria is a deadly tropical disease affecting and killing millions of people every year. Malaria is traditionally ignored by the pharmaceutical industries as it is restricted to mainly poor and developing countries and also due to the heavy costs (~$800 million) involved in the drug discovery activities. Novel and cost effective tools are needed for finding potential new drugs for malaria.

Analysis:
The in silico workflow which we employed starts with docking to evaluate the bindingenergy between a target and a ligand, then selected compounds are refined by Molecular Dynamics (MD). In 2005, against Plasmepsin target, the WISDOM initiative achieved 41 million dockings, using FlexX, in 45 days on 1700 computers which is equivalent to 80 CPU years on one machine. The best 5000 compounds identified were reranked by MD with Amber9 in 7 days equivalent to 124 CPU days on one machine. In 2006, this success led to a second assault against 4 other malaria targets. During 90 days, ~140 million dockings were achieved which is equivalent to 413 CPU years, representing an average throughput of 80,000 dockings per hour. MD simulations were performed on 15000 docking poses against wild type Dihydrofolate reductase target and 5000 docking conformations against Glutathione-S-transferase target respectively. The total 25 000 simulations lasted for 25 days equivalent to 347 CPU days in one machine.

Impact:
In silico datas have been valitated experimentally in wet laboratory. 30 compounds coming from MD step were selected manually, based on key interactions, and tested against recombinant aspartic protease Plasmepsin II expressed from the encoding gene. 6 compounds out of 30 showed similar or better inhibitions compared to Pepstatin A, a general inhibitor of aspartic proteases. All tested 30 compounds demonstrated plasmepsin II inhibition activity at nanomolar concentrations. In the meanwhile, 10 compounds out of this 30 were tested in vivo to figure out the impact on Plasmodium falciparum growth as well as the potential toxicity on human cells model. Premilinary results are very promising to go further in drug discovery process. Biological tests will be performed in near future for other targets as well.

Conclusions:
Grids have significantly reduced the overall time required for database screening against a particular target. Computing resources from Biomed virtual organization were used exclusively. The molecular docking was deployed on the EGEE Grid infrastructure, refinement by Molecular Dynamics on the French regional Grid AuverGrid, both using the WISDOM production environment. The successful experimental results reveal the suitable combination of EGEE infrastructure and in silico drug discovery.

Keywords: Malaria, Plasmepsin, virtual screening, docking, molecular dynamics, in vitro, EGEE, AuverGrid, Wisdom

Further information: http://wisdom.healthGrid.org/

37. Molecular dynamics refinement and rescoring in WISDOM virtual screenings

Authors: Rastelli, Giulio (Università di Modena e Reggio Emilia); Dr. Degliesposti, Gianluca (Università di Modena e Reggio Emilia)

Short overview:
The Wide In Silico Docking On Malaria (WISDOM) project is focussed on virtual screening of large databases of small molecule compounds through in silico methods deployed on the EGEE Grid computing infrastructure. One of the biological targets chosen for these screenings is Plasmodium falciparum Dihydrofolate reductase (PfDHFR), a well validated target for antimalarial drug discovery.

Analysis:
After the docking screening of compounds contained in the ZINC database into the crystal structure, the docking results have been refined using molecular dynamics (MD) in order to validate and optimize the ligand orientation into the binding site of the target. Subsequently, the candidates have been rescored using more accurate scoring functions based on molecular mechanics Poisson Boltzman Surface Analysis (MMPBSA) and molecular mechanics Generalized Born Surface Analysis (MM-GBSA) approaches. Such procedure was designed and validated on aldose reductase [1] and it is fully automated and able to prepare input files, efficiently refine the structures with MD, and rescore the compounds before the final selection of the best hits. [1] Ferrari A. Degliesposti G. Sgobba M. Rastelli G. Bioorganic & Medicinal Chemistry 15 (2007) 7865-7877

Impact:
In the PfDHFR application, the molecular interactions with the most important amino acids in the active site were evaluated as an important criterion for estimating the likeliness of binding, in addition to docking scores. The interaction frequencies with key residues showed an enrichment of interacting compounds on the top of the list, allowing the selection of a subset of 15.000 focused compounds to be processed with MD refinement. After rescoring, two new lists of ordered compounds were obtained and ranked according to MM-PBSA and MM-GBSA free energies of binding. For comparison, known nanomolar inhibitors of PfDHFR were included in the analysis. Interestingly the known inhibitors were on the top of the list, confirming the reliability and the predictive power of the refinement method applied. At the same time, the top-scoring list contained a number of different (not related to already known drugs) compounds which will be very interesting to evaluate for their PfDHFR inhibition.

Conclusions:
Based on the MD results, a subset of best-scoring compounds will be tested for their in vitro inhibition of P. falciparum DHFR. Further investigation on molecular interactions and binding free energy predictions will be performed on the PfDHFR resistant mutant enzyme.

Keywords: molecular dynamics, virtual screening, Grid, drug design

38. Grid distribution supporting chaotic map clustering on large mixed microarray data sets

Author: Tulipano, Angelica (INFN Bari)
Co-authors: Angelini, Leonardo (INFN Bari); De Sario, Giulia (Istituto di Tecnologie Biomediche, CNR); Donvito, Giacinto (INFN Bari); Maggi, Giorgio (INFN Bari); Marangi, Carmela (Istituto per le Applicazioni del Calcolo, CNR); Gisel, Andreas (Istituto di Tecnologie Biomediche, CNR)

Short overview:
Microarray data are a rich source of information because they contain the expression values of thousands of genes and in addition, especially in public repositories, hundreds of experiments with the same array design are available. Comparing expression levels over a wide range of experiments can reveal new and valuable information about behaviours of genes. Furthermore, because of the vast amount of experiments available, technical errors can be filtered out.

Analysis:
To find correlation between genes within different experiments, clustering is a good and challenging analysis method for data sets of such size and complexity. We have chosen an unsupervised hierarchical clustering algorithm based on the cooperative behaviour of an inhomogeneous lattice of coupled chaotic maps, the Chaotic Map Clustering. Analyzing data sets of 587 samples we were able to retrieve stable groups of genes. Using the biological knowledge of the gene ontology, we could show, applying a Fisher exact test, that each of the clusters have a set of over-represented functionalities and in most of the cases also clearly different functionalities from cluster to cluster. In order to evaluate the vast number of clusters found by this process we use a cluster validation method based on resampling subsets of the data under investigation are constructed randomly, and the cluster algorithm is applied to each subset. Measures of sensitivity and of positive predictive value are pro

Impact:
The clustering of each resampled subset is a very time-consuming process and it is not possible to retrieve the results within a reasonable time using one CPU. To validate the clusters by resampling, only a distribution of the task over several processing units will solve the problem of processing time. Since the task can be easily splitted into several smaller, independent sub-task we chose the Grid infrastructure to distribute the calculation. After performing the initial clustering and calculating of the resampled matrices on a single machine, each resampled matrix was clustered on a different WN. The clustering of one matrix takes about 2 hours and therefore a resampling validation with 100 matrices about 200 hours, or 8days. Using the Grid, the whole set of the 100 resampled matrices were clustered in 4 hours instead of about 8 days. The improvement in processing time allows the user to increase the number of resampled matrices and therefore improve the precision of the positiv

Conclusions:
The whole set of the 100 resampled matrices were distributed over 100 WN of the EGEE infrastructure within the VO biomed and processed totally in parallel, clustering those matrices in a time slightly longer than a clustering of one matrix. The process used mainly CPU since the output data files are small. The only problem we were confronted with is the size of the RAM usage. The clustering process occupies about 1.5 GB of the WN's RAM which in certain cases leads to the failure of the job which in certain cases leads to the failure of the job.

Keywords: bioinformatics, life science, clustering, cluster validation

39. ThIS on the Grid

Authors: Camarasu, Sorina (CNRS - CREATIS LRMN); Guigues, Laurent (CNRS - CREATIS LRMN); Benoit-Cattin, Hugues (CNRS - CREATIS LRMN); SARRUT, David (CNRS - CREATIS LRMN, Léon Bérard Cancer Center)

Short overview:
We present ongoing developments and first results on porting ThIS (a Therapeutic Irradiation Simulator) on the EGEE Grid. ThIS is a Geant4-based software dedicated to the Monte-Carlo simulation of irradiations of living tissues with photons, protons or light ions beams for cancer therapy. The large number (~100000000) of simulated particles needed for only one simulation requires a very high computation time that can be considerably diminished if the application runs on the Grid.

Analysis:
Our main requirements concern computing resources and data management. The simulation is split into sub-jobs. Each sub-job uses a different random seed number, allowing to be statistically independent and to be run concurrently. By dividing one simulation into hundreds of different sub-jobs, computation time can be reduced from more than one day to less than 1 hour if computing resources on the Grid are rapidly available. Data requirements are also important. ThIS needs about 50Mo of input data and can produce between 15 to 150Mo of output data per each sub-job. hIS is based on the Geant4 toolkit and consequently uses Geant4 and CLHEP libraries. In order to keep our application independent on the installed software on the Grid, we decided to compile it statically. Thus, each time a complete simulation is run, we provide the executable and all the needed input files as a tar ball stored on a storage element (SE) of the Grid. Once completed, output data are retrieved and merge on a SE.

Impact:
Porting ThIS on the Grid is making use of a large number of Grid services, from basic ones like the file catalogue to more evolved services proposed by the Workload Management System (WMS). Among the latter, we can cite the submission of parametric jobs, as well as the possibility to specify input data stored on the SE of the Grid. A parametric job causes a set of very similar jobs to be generated from one JDL file. This is exactly the case for our multiple sub-jobs. They are all the same except for the random sequence that must be different from one sub-job to another and a few other parameters. Our application needs large input data files that cannot be passed in the input sandbox of a job. Therefore, we exploited the possibility to specify input data stored on the storage elements of the Grid. Moreover, this functionality ensures that the WMS will schedule the job to a computing element close to one of the storage elements where the data is.

Conclusions:
The process of porting ThIS on the EGEE Grid is currently in progress. Our first results show that the Grid can bring an important amelioration in computation time. However, work still needs to be done in order to cope with delayed and failed jobs among the jobs belonging to the same simulation. As a second stage in the porting and deployment of ThIS we consider implementing a web-based Grid portal that would make ThIS available for physicians and researchers who could benefit from it.

Keywords: Therapeutic Irradiation Simulator, Grid, application porting, parametric jobs, data management

Further information: http://www.creatis.insa-lyon.fr/rio/ThIS/

40. Distributed system for genetic linkage analysis using EGEE and BOINC

Author: Silberstein, Mark (Technion - Israel Institute of Technology)
Co-authors: Sharov, Schuste, Geiger, - (Technion - Israel Institute of Technology)

Short overview:
Genetic linkage analysis is a statistical tool used to seek for disease-provoking genes. However many analyses are infeasible due to the high computational demands. Superlink-online web portal enables such demanding analysis tasks through their automated parallelization, submission, and execution on thousands of BIOMED VO CPUs. We designed a system which efficiently and reliably executes millions of jobs, overcoming high scheduling overheads, unbounded queuing times and job failures.

Analysis:
Tasks are submitted via web and parallelized into thousands or even millions of CPUbound jobs ranging from a few seconds to a few minutes long. Efficient and reliable execution is complicated due to unbounded queuing times, high execution and scheduling overheads, high job failure rates and insufficient scalability of the EGEE middleware. Our solution is to first submit lightweight clients which, when started on remote resources, fetch the actual jobs from the central job server and execute them. For this purpose we adopt open-source BOINC platform, used in the last few years for large-scale cycle-stealing such as SETI@HOME and many others. Built for volatile desktop environments, BOINC is capable of efficiently managing billions of jobs and millions of unreliable clients, yielding high performance through sophisticated scheduling mechanisms to overcome network, hardware and software faults. Furthermore, BOINC is firewall friendly and has a built-in accounting functionality.

Impact:
Our system decouples the application logic from the job submission and management mechanisms, essentially building on demand a virtual dedicated cluster from EGEE resources. The system has two main components. One application-independent part maintains the required amount of active BOINC clients in EGEE (i.e. the number of resources in the virtual cluster) by monitoring and actively rescheduling stuck, failed or evicted BOINC clients back into the Grid. A thin wrapper over publicly-available BOINC clients is used to enable their execution in EGEE. Another part, based on BOINC server, maintains the queue of the actual application jobs and accommodates the partial results. The jobs and results are communicated in a secure way, the integrity and validity are checked and user-specified routines are invoked to produce the final result. The system can efficiently execute even seconds-long jobs, as BOINC clients run them back-to-back, caching the executable and constant data remotely.

Conclusions:
Execution of over million jobs, each ranging from a few seconds to minutes, completed within 30 days on BIOMED VO CPUs, consuming about 2 TFLOPs on 300 (average) concurrently executing clients (from 100 to 700). The run was fully-automated and completed despite the failures of the BOINC server hardware, UI and broker nodes. The system is generic and will facilitate porting other applications. The use of BOINC allows us to effortlessly integrate the clusters and desktop Grids outside of EGEE.

Keywords: Bioinformatics, Job management, short jobs, BOINC, pilots

Further information: http://bioinfo.cs.technion.ac.il/superlink-online

41. Grid based telemedicine application for GATE Monte Carlo dosimetric studies

Author: L. Maigne (CNRS/IN2P3, LPC Clermont-Ferrand)
Co-authors: M. Diarena, S. Nowak, C. Thiam, V. Breton - (CNRS/IN2P3, LPC Clermont-Ferrand); D. Donnarieix (Centre Jean Perrin)

Short overview:
GATE is a pilot application dedicated to medical physics in the biomedical area of the EGEEII project. It has benefited of fundings from the French regional LifeGrid project and is tested on the regional Grid infrastructure in Auvergne AuverGrid. For a usage of GATE in clinic, the goal is to share and store medical images with their metadata from hospital (PACS systems) to use them in GATE calculations on the Grid infrastructure. Those functionalities are developed under a secured web portal.

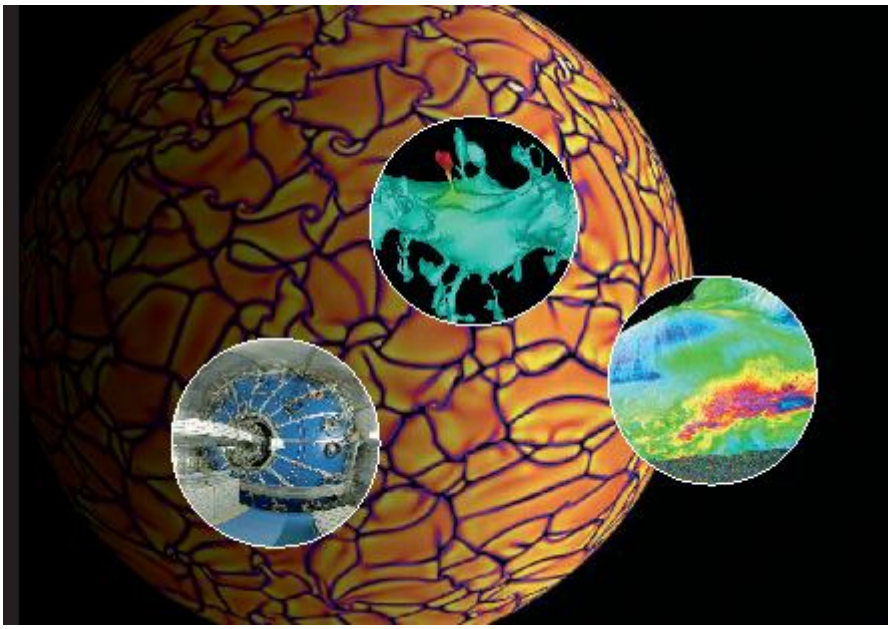
Analysis:
The secured web portal has been designed to be used by physicians and medical physicists to perform Monte Carlo calculations: to optimize the acquisition and data processing protocols of medical scans, to ensure accurate treatment plannings for some specific radiotherapy applications. In that way, developments focus on the creation of a secured web platform to access Grid computing to split the GATE simulations. Functionalities of this platform enable: a secure authentication to assess Grid computing; the retrieving of medical data from a PACS server - this service contains the anonymization of data, encryption and extraction of metadata stored in a base on the Grid; the secured and parallelized computing using medical images on the Grid; the monitoring and re-submission of calculations in case of failure; and the visualization of results (dosimetry map, sonograms, etc.) as images, directly from the client machine in use.

Impact:
The architecture of the platform is made of a secured web server, a plug machine at hospital and an efficient and reliable network for the transfer of confidential medical data. The platform uses web services technology and Grid services provided by the EGEE Grid infrastructure. Physicians access the platform using a web portal developed on GridSphere portlet container that present a user friendly interface to access several distributed medical services to manage medical images and information. Medical information is stored locally in user's hospital using AMGA metadata catalogue and information between services are exchanged using SOAP messaging protocol. Medical images are stored, anonymized and encrypted on the Grid while their corresponding metadata are stored in the AMGA server. The platform allows physicians to submit monitor, and manage GATE simulations for which the limiting issue right now is its time consuming on a single CPU.

Conclusions:
A secured web portal prototype has been installed at hospital in order to be used by medical staff. The web portal offers the user a transparent and secured way to create, submit and manage GATE simulations using realistic scans in a Grid environment. The gain in computing time obtained by splitting the simulations is very encouraging. The convivial web portal and the Grid performances could enable, in a near future, the usage of GATE simulations to treat patients for specific treatments.

Keywords: Medical Data Management, Monte Carlo, PACS, Web Services, GridSphere
Further information: www.lifeGrid.fr

GRID TECHNOLOGY





Data Management

Data Management

Conveners: P.Mendez-Lorenzo (CERN), P.Pagano (CNR/ISTI)

All aspects of data management are important for Grid applications. These encompass the storage, sharing, access and transfer of vast quantities of distributed information. For example the data needed by a modern HEP experiment is of the order of several petabytes per year of activity, and is distributed and replicated over a worldwide infrastructure. This data is organized in many millions of files, and accessed via metadata access systems.

The first session included three talks with the common topic of organising easy access to large datasets via the use of metadata descriptions and user interfaces using these descriptions. It was very interesting to compare these developments, and to discuss commonalities and key differences.

The second session's main theme was interoperability with the provision of tools for the sharing of information between Grids using different tools for storing information, with the particular example of the SRM and SRB models usage by LCG and TeraGrid. It was important to summarise the messages coming from three papers on this theme. Another presentation evaluated the use of four different relational databases within EGEE.

The last session had the flavour of the practical use of data management services by medical and physics applications which all have the same problem of storing and accessing data distributed across many sites with different storage systems and access protocols.

The main points emerging were:

- **There are developments towards data access described by multiple and heterogeneous metadata with high level application dependent descriptions**
  - Different application areas use different metadata tools such as AMGA(HEP and Biomedicine), and GDSE (Astrophysics)
- **Tools and frameworks are ready to be exploited and new ones are coming - need ongoing discussion and cooperation to avoid duplication of effort**
  - gCube Metadata Framework
  - Service Oriented Framework for Earth System Science (coming)
  - AMGA WS-DAIR (work still in progress)
- **Test suites and environments exist for comparative evaluations of metadata systems. This work should continue.**
  - AMGA
  - GRelC: Grid Relational Catalog
  - G-DSE (INAF + INFN)
  - OGSA-DAI
- **Different security requirements in applications**
  - While HEP data are worldwide read accessible, privacy is a fundamental key in some other communities such as Biomedicine and business. The provision of secure data storage remains an issue, though progress is being made.
- **Reliability , scalability and interoperability**
  - Inaccessible storage is more damaging than inaccessible CPU.
  - Important work is ongoing for the interoperability of SRM and SRB. This is promising since it involves the use of existing software components. But there remains an issue of long term maintenance of these components.

42. Medical data manager: an interface between PACS and the gLite data management system

Authors: Montagnat, Johan (CNRS); Frohner, Akos (CERN); Texier, Romain (CNRS); Nienartowicz, Krzysztof (CERN); Baud, Jean-Philippe (CERN)

Short overview:
The medical imaging community uses the DICOM image format and protocol to store and exchange data. The Medical Data Manager (MDM) is an interface between DICOM compliant systems such as PACS and the EGEE Data Management System. It opens hospital imaging networks to the world scale Grid while protecting sensitive medical data. It can be accessed transparently from any gLite service. It is an important milestone towards adoption of Grid technologies in the medical imaging community.

Analysis:
Hospitals continuously produce tremendous amounts of image data that is managed by local PACS (Picture Archiving and Communication Systems). These systems are often limited to a local network access although the community experiences a growing interest for data sharing and remote processing. Indeed, patient data is often spread out different medical data acquisition centers. Furthermore, researchers in the area often need to analyze large populations whose data can be gathered through federations of PACS. Opening PACS to the outer Internet is challenging though, due to the stringent security requirements applying to medical data manipulation. The gLite Data Management System provides the distribution, user identification, data access control and secured transportation core services needed to envisage wide scale deployment of the medical imaging applications. The MDM provides an upper layer to interface to PACS and manipulate medical data with the required level of security.

Impact:
The MDM core is a DICOM-SRM interface that converts file access queries into DICOM GET operations. An internal database is used to register medical images and to map Grid file identifiers into DICOM identifiers. Image files are therefore be visible from the gLite file catalog for future use by services invoking the data management system. Patient privacy is preserved through data anonymization and encryption. DICOM image headers are whipped out prior to image transfer. All data is encrypted prior to exposure to the Grid network in order to avoid any data leakage. The encryption / decryption phases are transparently handled by the data management system through calls to the Hydra service. Data access is controlled through user DN-based ACLs. An AMGA metadata server is used to store the medical records of the patient independently from the image. It ensures secured and controlled access to the metadata that is isolated from the images.

Conclusions:
The MDM was originally designed using gLite 1.5 components and was recently ported to the production data management system. It is packaged with an installation script and freely available for download. The next step will be the deployment of a significant number of MDM service interfaced to pre-clinical PACS in order to demonstrate a wide area medical imaging network supported by the Grid infrastructure. Future plans also include distribution of the medical metadata collected.

Keywords: Medical Data Management, Secured Files Storage, DICOM

Further information: http://rainbow.essi.fr/wiki/dokuwiki/doku.php?id=public_namespace:mdm

43. OpenSAML extension library and API to support SAML2.0 - XACML protocol for interoperable authorisation infrastructure in distributed-Grid applications

Authors: H. Sagehaug (BCCS/UIB, Norway); Y. Demchenko (UvA, Netherlands); V. Venturi and A. Forti (CNAF/INFN, Italy)

Short overview:
The proposed OpenSAML extension library and API implements SAML2.0 profile of XACML may provide a basis for interoperability between different AuthZ services. It supports communication between two major components of the generic AuthZ service architecture: Policy Enforcement Point (PEP) and Policy Decision Point (PDP). The library and API are implemented as pluggable modules that can be used with different Java based AuthZ services e.g. gLite Java AuthZ Framework (gJAF), GT- AuthZ, G-PBox.

Analysis:
Authorisation is an important component of the Grid security infrastructure. AuthZ decision is typically based on the AuthZ policy that contains a set of access control ules depending on user credentials or attributes. In many cases AuthZ service is a part of the application platform and uses a policy specific to application. Consistency of the access control enforcement can be achieved by introducing the Site Central AuthZ Service (SCAS) that will allow applying common policies centrally and leave a possibility for applying local policies and enforcement mechanisms. The proposed SAML-XACML library and API provide all necessary functionality for the PEP (bound to the Grid resource or application) to call out to external SCAS. The API provides the helper classes to create and parse SAML-XACML messages and also extendible functionality for policy Obligations handling. The proposed functionality is specifically targeted to support pool account management when submitting Grid job to WNs

Impact:
The library is being tested with the G-PBox as one of the suggested SCAS implementations. G-PBox is a XACML based Policy Decision Point (PDP) that provides also reach functionality for hierarchical policy management what is considered as an important component of cross and inter-organisational access control management. C-based implementation of the SAML-XACML protocol provided by Globus will allow also using LCAS/LCMAPS service as a SCAS. AuthZ decision made by SCAS can be conveyed to the gLexec at WNs in a form of SAML assertions and enforced there. Additional benefits of using OpenSAML as a platform for implementing SAML-XACML protocol is that this will allow future easy integration of the EGEE/Grid AuthZ infrastructure with the primary Shibboleth/SAML based universities and NREN Authentication and Authorisation Infrastructure (AAI). In this case users can use their general purpose credentials issued by their home organisations to access Grid services and applications.

Conclusions:
This development has been done in the framework of the gJAF development and EGEE-OSG AuthZ interoperability initiative, and may be one of the modules in achieving interoperability in the Grid. SAML-XACML protocol is recommended as a protocol to access Grid AuthZ service. The library and API have being contributed to the Internet2 OpenSAML project. Further development includes formal definition of the SAML-XACML AuthZ profile for Grid applications, attributes in use and Obligations handling API.

Keywords: Authorization, SCAS, gJAF, G-PBox

44. New results on a comparative evaluation of software providing access to different relational databases interfaced to the Grid

Authors: Donvito, Giacinto (INFN-Bari); Maggi, Giorgio (INFN-Politecnico)
Co-authors: Taffoni, Giuliano; Vuerli, Claudio; Barisani, Andrea; Pasian, Fabio; Manna, F. - (INAF); Gisel, Andreas (CNR-ITB); Calandrucci, Tony and Aiftimiei Cristina (INFN); Atul, Jain (INFN+Politecnico Bari); Barbera, Roberto (INFN+Università Catania); Carota, Luciana (INFN); FIORE, Sandro; Aloisio, Giovanni; Cafaro, Massimo; Vadacca, Salvatore; Negro, Alessandro (Università Lecce)

Short overview:
The problem of managing and accessing huge datasets distributed across multiple sites and stored interfaced into heterogeneous databases is common to several research areas. We report on the comparative evaluation of four tools to access different types of data resources exposed onto Grids: G-DSE[4], GRelC, OGSA-DAI[5] and AMGA.

Analysis:
A way to access widespread databases within a computational Grid environment, through a set of secure, interoperable and efficient data Grid services is very common in eScience projects. Use cases in the bioinformatics and astrophysical communities span from very simple queries up to really stressing ones. A stress test has been set up exploiting the EGEE Grid infrastructure by submitting jobs and monitoring them by means of the Job Submission Tool. In this configuration it is possible to easily reach the server software and hardware limits and to test the software in a real environment, taking into account the different latency between the server and all the clients, to put in evidence the efficiency of each software tool in delivering the output.

Impact:
The evaluation test, reported here, addresses the needs of the bioinformaticscommunity engaged, in the BioinfoGrid (www.bioinfoGrid.eu/) and the LIBI (www.libi.it/) projects, in the adoption of a Grid infrastructure layer at the base of their research activities and of the Astrophysical community of the INAF (Istituto Nazionale di Astrofisica) (www.inaf.it/) interested to access data in astronomical databases from the Grid, The access to data from the Grid is also a crucial problem for the adoption of the Grid technology to provide services in public administration (EGG project). This software could be integrated on the gLite Grid infrastructure in order to add the possibility to access Relational Databases

Conclusions:
Each of the four tested software, shows some specific strength that can be helpful in some particular application environment. We will show these characteristics for each software and the final results obtained running the client in a widely distributed environment. We will highlight also the capability of each software to be integrated on the gLite infrastructure and on the work on-going in this field

Keywords: Data Management, Astrophysics, Bioinformatic, Relational Databases

[4] wwwas.oats.inaf.it/Grid/index.php?option=com_frontpage=1

[5] www.ogsadai.org.uk/

45. Evaluating metadata access strategies through implementing the GOME test suite

Author: Gemuend, Andre (FhG/SCAI)
Co-author: Schwichtenberg, Horst (FhG/SCAI)

Short overview:
The aim of the DEGREE test suite activity was to generate test specifications that can be used to identify key requirements that Grid middlewares should meet for operating earth science applications. The GOME validation test suite is one of these specifications and focusses mainly on metadata management. We implemented the test specification using gLite and three different meta data backends, the Grid Relational Catalogue (GRelC), the ARDA meta data catalogue (AMGA) and OGSA-DAI.

Analysis:
With the realisation of the GOME validation test suite we tested the capabilities of the three underlying data access services as well as their integration into the gLite middleware. For the validation process data from a satellite and data from ground measuring stations have to be assigned by their spatial coordinates. For this we used GIS features available in modern databases when applicable and the services allowed it, e.g. with OGSA-DAI using the PostGIS extension for the PostgreSQL database. We additionally reviewed some of the advanced features of the underlying services.

Impact:
The GOME validation test suite consists of distributed jobs with two different purposes. The first is to assemble the metadata repository with meta data extracted from the real datasets and the second is to use this repository to collocate related data sets. This collocation is done using a containment test on the spatial coordinates of the measurements. Thus the meta data is in this environment used to reflect and index relationship of data so the application can quickly identify data belonging to the specified sample. This is a typical application of meta data in the evaluation of experimental data or data obtained from simulations where you isolate a criterion and analyse its influence.

Conclusions:
For the final review of the services we considered the following criteria: Deployment – setup and integration of the service Integration – use of Grid authorization / authentication, collaboration with other services, reusability of data repository Access – data retrieval mechanism (e.g. query language and data transport) Features – features needed (or helpful) to realize the test suite, possible extensions Development – available APIs or client libraries, complexity of model.

Keywords: data management, metadata, database integration, ogsa-dai, amga, grelc

46. A service oriented framework to create, manage and update metadata for earth system science

Authors: Ronneberger, Kerstin (DKRZ); KINDERMANN, Stephan (DKRZ)
Co-author: Biercamp, Joachim (DKRZ)

Short overview:
A precondition to effectively share and exchange data is a proper description of its content, properties and quality in a standardized metadata format. Yet, a metadata format, complex enough to describe diverse data for a broad community, needs tools to comfortably view, create, parse and update these metadata automatically as well as manually. We develop a system of such tools, based on XML standards, for metadata in the ISO19115/19139 format, describing earth system science data.

Analysis:
The system is built modular and service oriented to be expandable and easily maintainable. All Xml metadata instances, as well as the service layer composed of XSL stylesheets, XQuery/XUpdate modules and XML templates and property files are stored in a native XML database (eXist) and are accessible via different interfaces, depending on the interest in the metadata. For users of the data, described by the metadata, a detailed view on the information contained, is offered; users of the metadata can explore the structure and content of the metadata format via HTML pages; additional interfaces to manually (for existing data) and automatically (during processing) create, update and parse metadata files are offered to potential providers of data and metadata. For the automatic update, a request file can be submitted to the eXist database via a java interface, which sets on OGSADAI. Manual update is realized via an interactive GUI based on XForm technology.

Impact:
The interfaces of the presented system offer a convenient way to explore and use the XML implementation ISO19139 of the ISO19115 format. They thus help to describe existing or emerging data in order to share them. The ISO19115 format has proven useful to describe GIS and earth system science data and is already in use by several academic and business actors (e.g. ANZLIC, ESRI, con terra GmbH). The German C3Grid (part of the D-Grid initiative), adapted this format for the Grid field to offer a common view and access to data of the large German climate and earth system data providers. This C3Grid framework is set up to be expandable by further data providers. The EGEE infrastructure e.g. has been integrated as both, a data provider and processor. The presented system is intended to attract further EGEE users or earth system science data providers to share their data via this framework with the traditional earth system science community.

Conclusions:
The described system is currently under development and could thus not prove its feasibility yet. It is developed in collaboration with the C3Grid project and is set up to offer each current and potential data provider the opportunity to expand the system to include specific requirements needed for their data by means of stylesheets or XML templates. Once the system is in place, it might prove useful to establish a direct connection between the eXist database and the C3Grid portal.

Keywords: Metadata management, earth system science, GIS, SOA, ISO19115/19139, XML, XSLT, XQUERY, OGSADAI

47. The gCube metadata framework: integrated environment for managing metadata objects and relationships on top of Grid-enabled storage systems

Author: Simi, Manuele (CNR-ISTI)
Co-authors: Kakaletris, George (University of Athens); Pagano, Pasquale (CNR-ISTI)

Short overview:
A metadata object is any kind of data about other data. Any system aiming at managing content has to deal with them. Typically, systems are targeted on a limited set of metadata formats and they built their own semantics for such formats. The gCube Metadata Framework provides an efficient and generic API, exploitable by domain-specific services, that does not care about the format or semantics of the metadata. It rather focuses on management along with efficient storage and retrieval facilities.

Analysis:
The framework allows to: i) store, update, validate, manipulate, and retrieve metadata through the Metadata Catalog; ii) arbitrarily transform metadata through the Metadata Broker; iii) index metadata through the XML Indexer and discover them through XQuery and XPath expressions; iv) manage annotations through the Annotation Management stack. The granularity of each operation varies from a single metadata entity, to bulk, passed by–reference, entities that allow managing entire collections. The outputs of the operations can be a static or dynamic, continuingly updated products of their inputs. Each component is a well defined Web Service. The framework itself has been factored to support inclusion of new services at any (even run-) time. Moreover, apart the service that manages the upload and the relationships among the metadata items and the objects they describe, the rest of the services can be omitted, if the provided functionalities are not desired.

Impact:
The gCube Metadata Framework has been successfully adopted within the DILIGENT infrastructure, where, hundreds of thousands of metadata objects, potentially outsourced onto the gLite Data Management System through the gCube Data Management API, have been stored and manipulated along the project's lifetime. It proved to be scalable and efficient, well capable of serving the needs of heterogeneous communities. The XML Indexer has been exploited in the query workflows by gCube's native Search Engine, satisfying complex queries in acceptable response times, thanks to the transparent partitioning mechanism implemented. Alongside this, several transformation programs have been employed by the Metadata Broker, in order to generate new metadata collections, in different formats, towards facing interoperability and presentation challenges. On top of these, semi-structured annotations, over diverse types of content, add new potential to the exploitation of annotations in Information Retrieval.

Conclusions:
The design and the implementation of the framework will evolve to simplify the plugability of different storage systems as backend support. Eventually storing metadata directly on the gLite Data Management System, overcoming the gCube Data Management layer, will become feasible.
Furthermore new services dedicated to the management of specialized object-to-object relationships will be analysed and integrated in the framework to serve application specific needs.

Keywords: Metadata Management, gCube, DILIGENT, D4Science, XML

Further information: http://www.gcube-system.org/

48. The development of SRM interface for SRB

Authors: Tsai, Fu-Ming (Academia Sinica Grid Computing); Wei-Long, Ueng (Academia Sinica Grid Computing)
Co-authors: Shun-Che, Hsiung (Academia Sinica Grid Computing); Tsung-Hsien, Lin (Academia Sinica Grid Computing); Eric, Yen (Academia Sinica Grid Computing); Simon C., Lin (Academia Sinica Grid Computing)

Short overview:
Storage Resource Manager (SRM) is a widely adopted interface to the storage management system of production Grids currently. With the heterogeneity of Grid, the best way to share data is to integrate data sources through SRM, a uniform interface with dynamic space and file management. In this project, the SRM for SRB is developed, to make the popular SRB data Grid system interoperable with the EGEE infrastructure and support the SRM services for SRB, such as space reservation and VO support etc,

Analysis:
The standard SRM services for SRB were developed to make the popular SRB data Grid system interoperable with the gLite e-infrastructure. AMGA is used to implement the File catalog and to provide uniform interface for replication and to the backend database. Currently the development is under standard SRM functional testing and validation, and establishment of full SRM 2.2 functionalities will be finished by early 2008. In the first phase, targeted use cases are to: 1) Make SRB an archival system of gLite-based e-Infrastructure, 2) Support Lifetime policy for files - volatile, durable, and permanent, and 3) Impose the same VO and security control to SRB as the Grid infrastructure. Other than the basic directory, permission and data access functions, user authorization, web service interface, Gridftp deployment, and SRB-DSI had been supplemented and demonstrated at the SC07 in November 2007 as well, followed by the interoperation between SRB and DPM, dCache, Castor, etc.

Impact:
File exchange between gLite and SRB is enabled. The core middleware position of gLite is enforced by the uniform SRM interfaces to major mass storage systems and even a data Grid system like SRB. The specification of SRM is further endorsed and outreached. Dynamic space reservation and VO support capabilities are imposed onto SRB to furnish standard storage services to it. On the other hand, the gLite is able to take advantage of SRB federation among different administrative zones.

Conclusions:
SRM services of SRB were established by this work, and made the interoperation among Grid systems that benefit from and is made of SRB. In the future, SRM client could access to any of the storage systems with SRM services and the search and brokering among those SRM-enabled storage would be possible.

Keywords: data Grid, data management, storage resource management, SRM, SRB, storage resource broker

49. Distributed data management on the petascale using heterogeneous Grid infrastructures with DQ2

Authors: M.Branco, V.Garonne, and P.Salgado (CERN); M.Lassnig, (CERN & University of Innsbruck)

Short overview:
We describe Don Quijote 2 (DQ2), a new approach to the management of large scientific datasets by a dedicated middleware. This middleware is designed to handle the data organisation and data movement on the petascale for the High-Energy Physics Experiment ATLAS at CERN. DQ2 is able to maintain a well-defined quality of service in a scalable way, guarantees data consistency for the collaboration and bridges the gap between EGEE, OSG and NorduGrid infrastructures to enable true interoperability.

Analysis:
DQ2 is specifically designed to support the access and management of large scientific datasets produced by the ATLAS experiment using heterogeneous Grid infrastructures. The DQ2 middleware manages those datasets with global services, local site services and enduser interfaces. The global services, or central catalogues, are responsible for the mapping of individual files onto DQ2 datasets. The local site services are responsible for tracking files available on-site, managing data movement and guaranteeing consistency of available data. The end-user interfaces provide users with the ability to query, manipulate and monitor datasets and its transfers. The distinction between global and local services is a core design decision as it clearly separates site-specific information, e.g. local site storage management, from global information. With this separation, any change within site infrastructures does not affect global reliability of the system and QoS requirements can be guaranteed.

Impact:
Data movement is driven from the destination site using a unique pull-based subscription methodology. A user subscribes a dataset to a site and the system keeps track of all changes. The site services then fulfill the subscription by enacting the data movement in an intelligent and optimised way. The enacting layer relies on the EGEE gLite-FTS, glite-LFC, gLite-BDII, NorduGrid-RLS and OSG-LRC to interconnect the EGEE, NorduGrid and OSG infrastructures transparently. This allows scientists to work with all three Grid infrastructures without specialised knowledge and eases the way they can store and access their data. The integration of all three Grid infrastructures and the support for multiple Grid storage systems (CASTOR, dCache, StoRM, DPM) is therefore one of the key points of the systems. The other key points are the systems proven scalability to the petascale, its non-invasiveness to existing services and its fault-tolerance to support heavily data-dependent sciences on the Grid.

Conclusions:
DQ2 is used within ATLAS, handling bookkeeping and data placement requests across large, medium and small computing centres worldwide. Large-scale dedicated tests are routinely run in preparation of live data-taking and DQ2 already manages millions of files with storage requirements in the petascale. Data movement peaked at stable 1.2 GB/sec for multiple days already and thus proved the systems scalability. Future plans involve optimising data placement, performance and enduser experience.

Keywords: Data Management, Petascale, Distributed Computing

Further information: https://twiki.cern.ch/twiki//bin/view/Atlas/DistributedDataManagement

50. Grid storage interoperability now!

Author: Jensen, Jens (STFC-RAL)
Co-authors: Ross, Derek (STFC-RAL); Downing, Roger (STFC-DL); Hodges, Matt (STFC-RAL)

Short overview:
Using gLite data management tools, we demonstrate data transfers between a Storage Element with a Storage Resource Manager (SRM) interface and a Storage Resource Broker.

Analysis:
SRM and SRB are traditionally the two "islands" in Grid data, achieving interoperability only amongst themselves. We now show data being transferred between SRMs and SRBs, effectively making SRBs available (with some restrictions) as a Storage Element to gLite-based Grids. The main use case is to enable data sharing between such Grids - files are copied from one to the other and can be registered in transfer catalogues. Rather than using simple tools, the use case calls for using gLite's advanced data management tools. This work has been done as a contribution to the OGF GIN (Grid Interoperability Now) activities, and as it builds heavily on gLite, it is a suitable activity for the EGEE user forum.

Impact:
SRM is used by gLite-based Grids as an interface to Storage Elements - indeed gLite has its own implementation, the Disk Pool Manager, DPM. SRMs in the WLCG collaboration together manage tens of petabytes of data (according to the information systems). SRB are used by many "data Grids" by, for example TeraGrid and many national Grids. Being able to transfer data between these two worlds opens up the possibility of analysing existing SRB data on gLite resources. Conversely, we can also make SRM data available to the Globus-based Grids that traditionally analyse data held in SRB, but that is already less difficult. The important aspect of this work is that it builds on existing tools and requires no development effort. It is Grid Interoperability Now!

Conclusions:
We show how gLite advanced data management tools can be used to manage data not only in SRM, but also from SRBs which are made available as Storage Elements to gLite based Grids. Interoperability is achieved now, with no additional development efforts.

Keywords: Data management, SRM, SRB, interoperability, GIN.

Further information: http://www.Gridpp.ac.uk/wiki/SRM_SRB_interoperability

51. gLibrary/DRI: a Grid-based platform to host multiple repositories for digital content

Authors: Calanducci, Antonio (INFN Catania); Ramos Pollan, Raúl and Rubio Del Solar, Manuel (CETA-CIEMAT); Gonzalez Martin, Juan Manuel and Tcaci, Dorin (MAAT-G Knowledge)

Short overview: gLibrary/DRI (Digital Repositories Infrastructure) is a platform to host any kind of repository for digital content, providing a common infrastructure and a set of mechanisms (APIs and specifications) that repository providers use to define the data model, the access to content (by viewers, navigation trees and filters) and the storage model.The main goal of the platform is to reduce the cost in terms of time and effort that a repository provider spends in order to get its repository deployed

Analysis: A gLibrary/DRI repository is made of large digital content (as image files, video, etc) and metadata associated with it (annotations, descriptions, etc). In a typical scenario, new repository providers could use the built in mechanisms to store repository items (e.g. studies made of textual data and multiple medical images) in a combined Grid and federated RDBMS by simply describing the structure of their data in a set of XML files following the gLibrary/DRI specification. In a more elaborated scenario, repository providers can implement specific data management policies and use custom viewers for their specific data structures, still relying on the platform for navigation and management of their repository. As example, we present a repository based on mammograms, composed of both a repository and a viewer application, to manage patient's mammograms and diagnostics. This includes both the patient's data (stored as metadata) and the mammography digital content (large images stored in SE)

Impact: Repository providers describe the structure of the repository contents by following the DRI Data Model specification, indicating how the model is distributed into different relational entities (tables) and also marking what parts of it are to be stored in the federated database/metadata server and what parts are to be stored into Grid SEs. The Storage DRI API Specification provides method definitions for loading and persisting model nodes. Through this API we isolate data management from its storage technology. (However we provide an implementation of this API using Grid SRM SEs and AMGA technologies.) These methods are transparent to the node complexity and content, and also to the storage system chosen for storing the data. The GUI Navigation functions are used for providing to the user a quick and effective way of finding any node of the data model into the repository.The navigation system is based on categories trees and a set of filters that reduce the nodes search to the user.

Conclusions: We have developed a platform that reduces the cost for developing new digital repositories. It provides a set of API and specifications that decouples the repository developing from the underlying platform. Multiple repositories can be hosted, just by providing the UI and Storage modules. The architecture is totally Grid based (VOMS authentication/authorization, data federation and distribution, usage of the computing power in the future). A mammograms repository has been also developed.

Keywords: Digital Libraries, Metadata, Mammography, Medical Repositories, Data Management

52. A WS-DAIR compatible interface for gLite-AMGA

Authors: Javadzadeh Boloori, Ali (Royal Institute of Technology (KTH)); Koblitz, Birger (CERN)

Short overview:
AMGA is the gLite 3.1 Metadata catalogue and a widely used database access system by many groups and communities, ranging from High-Energy Physics to Biomedical and Earth Sciences. It recently started to offer the Web Service Data Access and Integration - The Relational realization (WS-DAIR) standard proposed by the Open Grid Forum. In our presentation we present the status of this work, which will greatly improve interoperability with other WS-DAI compliant components.

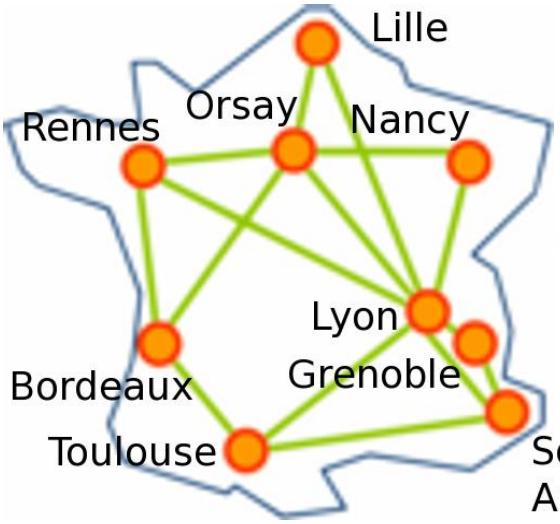
Analysis:
The addition of a WS-DAIR interface to the gLite AMGA metadata service will greatly improve the extensibility and interoperability with other Data access services based on the Open Grid Service Architecture. As the standard also defines the interaction of relational database services among each other, it will allow the integration of data access services of different types. We will present as an example the Avian Flue Drug Discovery application implemented by Academia Sinica Grid Computing (ASGC), which has been used as a test case for validation and evaluating the new interface, compared to the older TCP-Socket based of AMGA with respect to performance, scalability, fault tolerance, interoperability and ease of use for Grid applications. The result of the evaluation has also been presented at SC '07. As AMGA is in fact the first metadata service to adapt the WS-DAIR standard, we will present our findings on the usability of this standard as well as on its overall design.

Impact:
Adapting WS-DAIR in AMGA, which began as an exploratory project by the EGEE user community, and now is a part of glite 3.1 release, is another step towards interconnecting this data access system with other similar services. In other words, AMGA can communicate with other database access services on the Grid which has adapted to the WS-DAIR and vice versa, improving interoperability among database access services on the Grid by defining standard operations and encoding format of data, separating the functionality of the data access service from its operational representation, using service oriented architecture. On the other side, clients can use the service based on their own business logic. This will greatly improve the freedom of application writers to choose among suitable Grid services without the need to adapt the application. In addition, data source that are newly introduced to the Grid will be readily accessible with existing clients.

Conclusions:
We intend to further intensify the collaboration with the OGF in order to improve the WS-DAIR standard as it has already started, making AMGA fully compatible with the standard, such as supporting the Web Service Resource Framework. Interoperability test with other implementations of the WS-DAIR standard should be done in the future, which should further strengthen the growing community working on relational database access on the Grid.

Keywords: Relational database access, Standardization, metadata catalogue, Interoperability

Further information: http://cern.ch/



Grid'5000

From Research to Production Grids: Interaction with the Grid'5000 Initiative

From research to production Grids: interaction with the Grid'5000 initiative

Conveners: J.Montagnat (I3S Lab., CNRS), T.Glatard (CNRS)

Production Grid infrastructures are facing challenging problems related to the scalability of the system, security, heterogeneity, resources volatility, performance guarantees and fault tolerance in unprecedented large scale environments. Large scale applications developed for such environments similarly have to address Grid-specific problems related e.g. to deployment, distribution and performance in a highly competitive and distributed environment. The behavior of Grid systems, exploited under permanent and variable loads, is still little understood. Much research in this area is related to the modeling and the efficient exploitation of such infrastructures. They require an adapted testbed for model validation and large scale measurements in controlled experimental conditions.

Grid'5000 is a French research effort developing a large-scale, nation-wide infrastructure for Grid research. It aims at building a highly reconfigurable, controllable and monitorable experimental Grid platform gathering 9 sites geographically distributed in France. The current platform features 100 to a thousand PCs clusters, connected by the RENATER Education and Research Network through 1 Gb/s to 10Gb/s links. This infrastructure complements theoretical models, simulators and emulators, with a large scale testbed where real life experimental conditions hold.

The session aimed at fostering exchanges and collaboration between the EGEE production Grid experts and the research community. Talks described various aspects of the research made on Grid'5000 (including large scale application experiments, deployment and monitoring tools). Challenges identified by the EGEE experts in the area of middleware development, deployment and operations were proposed. The session ended with a round table discussion which outlined:

- The cost of migrating prototypes from research to production.
- The need to take into account the constraints of a production Grid in research (e.g. site security & networking policy restrictions, resources reservation is not possible).
- Bridging the gap from Grid'5000 to EGEE infrastructure can be tackled by:
    - Creating gLite images to deploy on Grid'5000
    - Creating a Grid'5000 VO, possibly on the pre-production service
    - An incremental approach is needed: work on a per service basis, impossible to re-deploy a complete middleware stack
- Scalability testing requires a large scale infrastructure. The BDII caused particular problems as the infrastructure was growing.
- Grid modeling is a point of junction between both communities: realistic workload patterns and system activity traces can be measured on production Grids (Grid observatory); models can be validated in controlled conditions on research Grids.

Overall it was agreed that the work on research and production Grids is complementary, and cooperation required ongoing discussions and planning involving both communities.

53. Modeling the EGEE latency to optimize job time-outs

Authors: Montagnat, Johan (CNRS); Lingrand, Diane (UNSA); Glatard, Tristan (CNRS)

Short overview:
Applications submitting a large number of jobs to the Grid infrastructure have to consider and recover from faulty jobs that are due to system failures or abnormally long job durations. A simple time-outing and resubmission strategy protects the application from very long durations in case outliers happen. However, determining the time-out value is not straight forward, especially for shorter jobs, as their execution time significantly depends on the Grid workload conditions.

Analysis:
Jobs submitted to a production Grid infrastructure are impacted by a variable delay resulting from the Grid submission cost (middleware overhead and queuing time). The actual execution time of a job will depend on the process execution time, which can be known through benchmarks, and the variable Grid latency duration, which is difficult to anticipate due to the complexity of the Grid infrastructure and the variable load patterns it is enduring. We aim at estimating the Grid latency through a probabilistic approach that is well adapted to complex system modeling. We derived a model of the expected execution time of a job function of the time-out value in a time-outing and resubmission setting. To follow on the variable load conditions, a monitoring service sends regular probe jobs to the infrastructure and measures their latency duration. This information is injected into the model and a numeric minimization provides the time-out value that minimizes the expected execution time.

Impact:
A study on the EGEE Grid workload pattern has shown that the latency endured by jobs follows heavy-tail distributions. Consequently, a non-negligible fraction of the jobs duration is likely to encounter very long latencies which are penalizing multi-job applications dramatically. Setting up the time-out strategies protects the application from these faults while introducing a very light overhead. The time-out estimation service is currently a prototype deployed on top of the EGEE middleware. The monitoring activity uses the workload management system to submit and monitor the jobs durations. The model computation is a lightweight numerical integration that can be integrated in any application. When their time-out expires, the application has to cancel and resubmit the faulty jobs to avoid abnormal computation times. An interesting perspective would be direct access to the RB logs to avoid applicationlevel probing of the infrastructure.

Conclusions:
The model was tested on the EGEE production infrastructure using thousands of probe jobs over hours of execution. A 2.5% faulty jobs ratio was measured. Recovering from these faults by time-outing protects the application from unbounded execution time. The model can be adapted to more or less reliable system by varying the outlier ratio. Simulation of a fault-less system (e.g. cluster) with similar load conditions than the Grid show that a minimum speed-up of 1.36 is achieved.

Keywords: Workload management, time-outing strategy

Further information: http://www.i3s.unice.fr/~glatard/publis/ccGrid07.pdf

54. Simple, fault tolerant, lightweight Grid computing approach for bag-of-tasks applications

Author: Georgiou, Yiannis (LIG Laboratory)
Co-authors: N.Capit and O.Richard (LIG Laboratory); B.Bzeznik (Projet CIMENT)

Short overview:
An alternative Grid computing approach for large scale computation is the exploitation of idle resources. We present a simple, scalable and fault tolerant Grid service of transparently harnessing idle cluster resources and idle diskless desktop workstations for executing large-scale scientific "bag-of-tasks" (BoT) applications.

Analysis:
Our approach consists by a (RMS) resource management system OAR, responsible for the efficient allocation of local cluster resources and a Grid lightweight service CIGRI that uses only the idle cluster resources by not interfering to the normal functionality of the interconnected clusters. The approach is based on the concept of "best effort" tasks, introduced by OAR. This type of jobs has the minimum execution priority and are submitted only if there is an idle resource. However, if during their execution the resource is requested by a local cluster user, the Grid "best-effort" job is killed by the local RMS. The CIGIR Grid fault-treatment mechanism can resubmit the killed jobs and thus guarantee a successful completion of the whole calculation. Features like web portal for Grid monitoring, checkpoint/restart, results collection, support of diskless PCs environment (ComputeMode) and application data transfer are implemented and provide ease of use and quality of service to the user.

Impact:
The mainstream Grid computing approach of Globus combines security, resource discovery and resource access in Grid environments. It provides standardized services o construct computational Grids. However, the installation, configuration and maintenance of this system, is a rather complicated task and requires a highly skilled support team, which not a lot laboratories are willing to afford. Lower-cost solutions were introduced by technologies like desktop Grid (Seti@home) which is based on the idea of harvesting the computing power (of individual desktop PCs) going idle on the Internet. In the case of multiple distinct administrative domains that want to share their resources, similar approaches are provided by OurGrid and Condor platforms. In a similar context our lightweight approach shares similarities with the above projects. As a matter of fact, the limited security measures and the support of simple BoT applications, makes CIGRI the lighter and simpler solution of both.

Conclusions:
CIGRI/OAR softwares have been active research projects since 2002. In one of the contexts where they are used (CIMENT), its users can benefit of the power of 6 different clusters with a total of more than 700 processors of heterogeneous machines, for execution of large-scale scientific applications. The experimental method used to study the CIGRI Grid service and evaluate the new functionalities is conducted upon Grid5000 experimental platform. OAR is the official RMS used on Grid5000 platform.

Keywords: alternative lightweight Grid, fault-tolerance, scheduling, BoT applications, besteffort tasks

Further information: oar.imag.fr/, cigri.imag.fr/, computemode.imag.fr/ , ciment.ujf-grenoble.fr/ , Grid5000.fr/

55. IV Grid plugtests: composing dedicated tools to run an application efficiently on Grid'5000

Authors: Besseron, Xavier (LIG - MOAIS project); Danjean, Vincent (LIG - MOAIS project); Gautier, Thierry (LIG - MOAIS project); Guelton, Serge (LIG – MOAIS project); Huard, Guillaume (LIG - MOAIS project); Wagner, Frédéric (LIG -MOAIS project)

Short overview:
This year, the IV Grid Plugtests took place in Beijing, China from October the 29th to November the 1st, 2007. Organized by ETSI and INRIA, it proposed a contest on the N-Queens problem in order to test Grid technologies.
We offer a feed-back about our experience of running efficiently our N-Queens application on a whole computing Grid like Grid'5000, composing tools from reservation and deployment to tasks scheduling.

Analysis:
Exploiting efficiently the resources of whole Grid'5000 with the same application requires solving several issues: 1) resources reservation; 2) applications' processes deployment; 3) applications' tasks scheduling. For the IV Grid Plugtests, we used a dedicated tool for each issue to solve. The N-Queens contest rules imposed ProActive for the resources reservations (issue 1). Issue 2 was solved using TakTuk which allows the deployment of a large set of remote nodes. Deployed nodes take part in the deployment using an adaptive algorithm that makes it very efficient. For the 3rd issue, we wrote our application with Athapascan API whose model is based on the concepts of tasks and shared data. The application is described as a data-flow graph using the Shared and Fork keywords. This high level abstraction of hardware gives us an efficient execution with the Kaapi runtime engine using a work-stealing scheduling algorithm to balance the workload between all the distributed processes. Impact : To run our N-Queens application on the Grid, we composed three tools : ProActive, TakTuk and Kaapi. The Grid's architecture was provided by Plugtests organizers through a deployment descriptor file which contains required information to reserve and contact nodes (gateways, resources managers). ProActive was in charge of reserving all the nodes and creating a tunnel to each cluster of the Grid. Then Taktuk just used these tunnels to connect all the nodes of all the clusters and started the Kaapi processes. Our N-Queens application ran successfully during this Plugtests. We deployed our Kaapi processes on 1364 nodes of Grid5000 (one process by node) in less than 3 minutes. The computation used 3654 cores (each Kaapi process creates one computation thread by core). Using this deployment during the one-hour slot, we computed all the solutions of one 23-Queens (35min 7s) and of six 22-Queens (about 2min 21s each). These results gave us the first place of the contest.

Conclusions:
We learnt two main lessons from these experiences: - Kaapi middleware allows us to scale up to thousands of heterogeneous cores while the efficiency is preserved. On going work is to increase the scalability on highly heterogeneous networks. - Fault tolerance is essential to run application at such a scale. Many times during the contest, our application crashed because some nodes in the Grid failed. Two fault tolerance protocols are currently in development for Kaapi.

Keywords: Grid, Deployment, Work-stealing scheduling, Tools for the Grids

Further information:
http://www-id.imag.fr/Laboratoire/Membres/Besseron_Xavier/IV_Grid_Plugtests/

56. DeployWare: a framework for automatic deployment of software systems on Grids

Author: Flissi, Areski (LIFL - UMR 8022 CNRS)
Co-author: Merle, Philippe (INRIA)

Short overview:
DeployWare is a framework allowing to automatically deploy and manage heterogeneous and distributed software systems, including middleware, application servers and applications, on large scale infrastructures such as Grids. It is independant of the paradigm/technology of the software that compose the system to deploy, automatically orchestrates the deployment process, dealing with software dependencies, and the heterogeneity of the targeted physical infrastructure (hardware, network, protocols).

Analysis:
Deployment, which can be defined as a set of tasks to orchestrate such as installation/uninstallation of software on remote nodes, configuration of nodes and software, starting/stopping of application servers or data collecting, is a nightmare for Grid Computing users. A first challenge is complexity of the orchestration of the several deployment tasks and software dependencies, and the administration of such large distributed software systems. A second challenge is heterogeneity of: - the software systems to deploy, which use different paradigms (parallel or objectoriented programming, component-based or services-oriented approaches) but also a plethora of runtime platforms/middleware (e.g. MPI, Globus, GridCCM, ProActive, SOAbased systems, etc.) - the targeted physical infrastructures in terms of hardware, operating systems, network, protocols. A third challenge is scalability: a typical scenario is to automatically perform the deployment of a software system on thousands of nodes.

Impact:
DeployWare addresses the complexity, heterogeneity and scalability challenges of deployment on Grids. The framework can be used by Grid Computing scientists coming from various disciplines (Physics, Earth Sciences, etc.), i.e. by non-computer science experts, to easily deploy and execute their applications on Grids. DeployWare provides a metamodel that captures abstract concepts of deployment, a concrete syntax to describe software system, a virtual machine (named FDF, Fractal Deployment Framework) that interprets this description and executes the deployment process, and a graphical console allowing to manage, at runtime, the deployed system. DeployWare, implemented using the component-based approach, can deploy itself in order to address very large scale deployment (thousands of nodes). Currently, DeployWare can deploy CORBA-based systems, SOA-based systems, JEE-based systems, Database systems, or Grid-based services such as the OAR tool used in the Grid'5000 platform to reserve nodes

Conclusions:
We have experimented DeployWare on Grid'5000, the French experimental Grid infrastructure with the automatic deployment of OpenCCM application servers on 1000 nodes of Grid'5000, on several clusters. Performance results have shown that, firstly, the execution time of the deployment process grows linearly with the number of nodes, secondly, the execution time decreases with the number of used DeployWare nodes. We plan to deploy more Grid-specific middleware such as GridCCM or the Globus Toolkit.

Keywords: Software Deployment, Middleware, Distributed Applications, Grid'5000

Further information: http://fdf.gforge.inria.fr/

57. Expo: an experiment framework for dedicated platforms

Authors: Videau, Brice (INRIA / LIG); Richard, Olivier (INRIA / LIG)

Short overview:
Expo is a framework to conduct and control experiments on platforms dedicated to experimentation like Grid'5000. Its primary goal is to help experimenter make reproducible experiments. Experiments are described through program written with a domain specific language (DSL). This language simplifies the development of complex experiments. This framework can be use on Grid'5000 platform, PlanetLab, DSLLab and will be extent to be used with Emulab and SensLab the future wireless sensor testbed.

Analysis:
Expo is used to analyze the performances of the file broadcasting tool Kastafior. Kastafior broadcasts a single file onto a given set of nodes. The aim of this experiment is to study Kastafior's performances across Grid'5000 when the file size and the number of nodes vary. The script used to conduct the experiment is only 15 lines long. Expo interprets this script and issues reservation commands. When the described resources are obtained they are checked to verify that they suit the experiment. Once used resources are determined, each measurement is launched by a command module. This module archives every outputs produced for future analysis. It also records the status of commands and thus monitors the proper unrolling of the experiment. When all measurements are done, resources are freed and a complete report on the experiment can be stored on disk. In the end the experimenter just has to analyze the results.

Impact:
Expo can be compared to other experiment framework like PluSH or ZENTURIO. There are many differences between Expo and those frameworks. For instance they are tied to a certain architecture. PluSH is tied to PlanetLab and ZENTURIO to Globus Grids, while Expo is not aimed at an architecture. Instead it uses a driver framework to manage resources. The type of experiments conducted on Grid'5000 is also not the same than those of PlanetLab and Globus Grids. PlanetLab experiments are network oriented, and thus PluSH design takes this into account. ZENTURIO aims at testing applications that are to be deployed on Globus Grids, while Grid'5000 experiments are more middleware oriented. And last but not least the languages used by those frameworks are rather complex, PluSH uses XML description while ZENTURIO is based on an imperative and very complete language. The domain specific language designed for Expo is derived from ruby and is very concise and powerful.

Conclusions:
The Expo framework enabled the design and the conduct of a complex experiment. Nonetheless the description of resources in a broad meaning is problematic. In order to manage transparently resources from Grid'5000 and PlanetLab the concept of resources has to be developed further. Resources have a number of properties like gateways, hardware configuration and software configuration that have to be accounted for when running an experiment.

Keywords: Workflows, Experiment Methodology

Further information: http://expo.imag.fr/



Grid Access

Grid Access

Conveners H.Kormayer (NEC Labs, Europe), E.Laure (CERN)

Grid infrastructures are now used routinely by many scientific communities, however, the inherent complexity of Grid technologies builds a serious threshold for new users to enter the Grid world and existing users to fully exploit its potential. The Grid promise of an easy and seamless access to heterogeneous resources can only be held if this threshold is lowered for non-Grid experts.

Different projects have developed tools to lower the threshold for Grid users. These tools include portals and command line tools for specific applications, generic tools to access a Grid infrastructure independent of the middleware as well as tools to manage security on distributed Grid sites. The integration of VO-based security concepts in the operating system is another promising approach. In addition, users often require support for interactive applications and the possibility to control scientific instruments remotely.

The "Grid access" session provided an overview of a variety of tools developed in different projects covering domain-specific tools as well as generic tools and infrastructures, which together provide important steps towards the vision of a seamless and easily accessible Grid infrastructure.

From the talks and discussions it was clear that:

- **For specific communities, tools exist for access to the infrastructure**
  - See talks on HEP (CRAB), Earth Sciences, RingGrid etc.
- **Communities often have specific requirements**
  - So we need customization according to needs
- **Generic CLI and Portals are missing!**
  - A portal is too cheap, so the wheel is often reinvented
  - The approach of g-Eclipse in using an existing reliable platform can be a blueprint for future developments.
  - It is worth to look at what happens beyond your community
  - Try to collaborate in tools
- **'Grid Access' should include Service Level Agreements documents and cost estimates**

58. XtreemOS: a Grid operating system providing native virtual organization support

Authors: Morin, Christine (INRIA); Jegou, Yvon (INRIA); Sanchez, Oscar David (INRIA)

Short overview:
XtreemOS is a Linux-based operating system that provides for the Grid what a traditional operating system offers for a single computer: abstraction from the hardware and secure resource sharing between different users. It thus considerably ease the work of users belonging to virtual organisations by giving them the illusion of using a traditional computer, and releasing them from dealing with the complex resource management issues of a typical Grid environment.

Analysis:
While much has been done to build Grid middleware on top of existing operating systems, little has been done to extend the underlying operating systems for enabling and facilitating Grid computing, for example by embedding important functionalities directly into the operating system. XtreemOS project aims at investigating and proposing new services that should be added to current operating systems to build a Grid infrastructure in a simple way. This approach can be seen to have some advantages over conventional Grid middleware toolkits, which may have different programming interfaces and lack of a unifying model. A common interface can be provided to simplify the task of the application developer on the Grid by making the Grid support native to the operating system, and also by removing layers of abstraction, leading to higher dependability of services.

Impact:
XtreemOS provides native support for the management of VOs in a secure and scalable way, without compromising on flexibility and performance. VO Management (VOM) covers all the infrastructural services that are needed to manage the entities involved in a VO and ensure a consistent and coherent exploitation of the resources, capabilities, and information inside the VO under the governance of the VO policies. VOM is implemented as an operating system service that can be integrated directly with existing authentication infrastructure. This approach reduces the management and performance overheads introduced by the layers of controls. Local user accounts in XtreemOS are allocated dynamically on each resource to match the actual global users exploiting that resource. The dynamic allocation of user accounts ensures XtreemOS scalability and reduces the complexity of VO management: no need to configure resources when users are added or removed from VOs.

Conclusions:
Users, developers and system administrators of Grid applications and services benefit from XtreemOS in terms of ease of management, scalability and dynamicity. Applications can run in the context of a VO even if they are not VO-aware, and take advantage of a secure environment that provides logging, auditing and accounting. XtreemOS is currently under implementation and the first public release will be available in June 2008. XtreemOS is 4-year project funded by the European Commission.

Keywords: Grid Operating System, Virtual Organization

Further information: http://www.xtreemos.eu

59. Exploitation path of interactive European Grid on user communities

Authors: Campos Plasencia, Isabel (Instituto de Fisica de Cantabria CSIC); Marco de Lucas, Jesus (Instituto de Fisica de Cantabria CSIC)

Short overview:
We will summarize the main achievements of the project Interactive European Grid from the point of view of middleware oriented to advanced application support. We will also address the exploitation path of the project in what concerns support to user communities and middleware repositories perspective in the context of RESPECT. We will discuss several models of Service Level Agreements (SLAs) oriented to serve research centers and SMEs interested in using Grid infrastructures

Analysis:
The Interactive European Grid project (int.eu.Grid) aims to deploy and operate a production quality Grid infrastructure oriented to service research communities with specific needs regarding parallel MPI support and interactive access to Grid resources. Over the past user forums (Geneva 2006, Manchester 2007) it has been observed that there is a clear need and interest in the scientific community for the services being developed by int.eu.Grid on top of gLite as well as for an infrastructure that deploys these services for the user communities.

Impact:
The sustainability of Grid infrastructures beyond the project lifetime relies on the capacity to provide a service with quality standards. In this context it is important to understand what the possibilities are for the Service Level Agreement for users and resources to cluster in a usable Grid infrastructure.

Conclusions:
The development of a Grid infrastructure targeting advanced services such as parallelism and interactivity has proved to be attractive for user communities. The experience gathered by the inteuGrid consortium needs now to be consolidated in a well defined exploitation path.

Keywords: Exploitation of Grid Infrastructures, Service Level Agreements

60. CRAB, the CMS tool to allow data analysis in a distributed environment

Authors: Fanzago, Federica (CERN-CNAF); Cinquilli, mattia (INFN-Perugia); Codispoti, giuseppe (university bologna); Corvo, marco (CERN-CNAF); Fanfani, alessandra (university bologna); Farina, fabio (Univesity Milano Bicocca); Kavka, carlos (INFN-TS); Lacaprara, stefano (INFN-LNL); Spiga, daniele (INFN-PG); Vaandering, Eric (FNAL)

Short overview:
The CMS collaboration is developing a tool to allow physicists to access and analyze data stored in geographically distributed sites, simplifying the data discovery and hiding details related analysis job creation, execution and monitoring in the Grid environment. With this presentation we would like to show the progress of our work and some statistics about its usage.

Analysis:
The CMS experiment will produce few PBytes of data each year to distribute and store in many computing centres spread in the countries participating to the CMS collaboration and made available for analysis to world-wide distributed physicists.CMS will use a distributed architecture based on Grid infrastructure to analyze data stored at remote sites, to assure data access only to authorized users and to ensure remote resources availability.Data analysis in a distributed environment is a task that assume to know which data are available, where data are stored and how to access them.To simplify analysis job creation and management the CMS collaboration is developing CRAB (CMS Remote Analysis Builder) a tool to allow users with no specific Grid knowledge to be able to run analysis in the distributed environment as data were in their local farm. CRAB is developed as tool standalone and client-server to improve the throughput, the scalability and to automatize most of CRAB functionalities.

Impact:
Users have to provide CRAB with the name of the dataset to analyze and the total number of events, their analysis configuration file and libraries.They must belong to the CMS Virtual Organization and have a valid Grid certificate.CRAB creates a wrapper of the analysis executable including CMS environment setup and output management.CRAB finds data location querying specific CMS catalog and splits the number of events in jobs according with data block distribution.CRAB packs the user code and send it to remote resources together with the wrapper.The job submission is done using Grid workload management commands.The resources availability, status monitoring and output retrieval of submitted jobs are fully handled by CRAB.For job submission CRAB is interfaced with gLite WMS and with OSG, based on Condor-G. CRAB uses the voms-proxy server to create the user proxy certificate and its delegation.CRAB uses the LB Api to check the status of jobs and the UI command to manage jobs.

Conclusions:
During the last year the number of users and jobs submitted via CRAB increased.This result shows that CRAB is useful to run analysis in Grid environment and the development of server-client architecture is needed to guarantee scalability.Our experience using CRAB shows some weakness of some Grid services as WMS constrains, problem with sandboxes dimension, problem with the protocol for copy the produced output to remote mass storage.Remote sites need continuous checks to guarantee availability.

Keywords: CMS distributed data analysis, workload management, high energy physics, Grid

61. Deploying e-infrastructures for new user communities in DORII project

Author: Norbert, Meyer (PSNC)

Short overview:
We will summarize the main goals of the project Deployment of Remote Instrumentation Infrastructure from the point of view of application support. We will show challenges and present expected results. We will present our relation with EGEE project and gLite middleware.

Analysis:
The DORII project aims to deploy e-Infrastructure for new scientific communities, where the ICT technology is still not present at the appropriate level. The DORII is focusing on the following selected scientific areas: earthquake community, with various sensor networks, environmental science community, experimental science community, with synchrotron and free electron lasers. Working closely with end-users, DORII will build solution upon the success of past and ongoing projects in such areas as remote instrumentation (GRIDCC, RINGrid), interactivity (int.eu.Grid), software frameworks for application developers (g-Eclipse) and advanced networking technologies (GN2) with EGEE based middleware.

Impact:
By offering support to three mentioned different communities, DORII will contribute to the consolidation and expansion of eInfrastructures addressing the specific needs of these communities, in particular the challenge of integration of their experimental equipment. The deployment of the specific services will allow the exploitation of the relevant layers of eInfrastructures, from networking to Grids and middleware.

Conclusions:
DORII is oriented to support researchers with experimental equipment and instrumentation, which are not integrated or integrated only partially with the European infrastructure. DORII capitalises the previous projects achievements and is going to use according to the demands and requirements of the scientific communities. The scientific groups are intended to empower their daily work with the functionality available in modern eInfrastructure, with certain enhancements delivered by DORII.

Keywords: Grid project, e-Infrastructures, remote-instrumentation, interactivity

Further information: http://www.dorii.eu/

62. g-Eclipse - easy access to Grid infrastructures

Author: Kornmayer, Harald (NEC Laboratories Europe)
Co-author: Stuempert, Mathias (FORSCHUNGSZENTRUM KARLSRUHE (FZK))

Short overview:
Grid infrastructures, build over the last years, offer basic service (i.e. computing, storage) as well as high level services to make the underlying infrastructure transparent (i.e. RLS, RB). Many different application domains started to use Grid infrastructures for their research, but at the same time facing the common problems due to the inherit complexity of Grid infrastructures. The g-Eclipse framework will help the developers from different domains to port their applications to the Grid.

Analysis:
The usage of a common and reliable tool eco system will help the developers from different domains to port their legacy applications to Grids. But not only developers will benefit from a general tool Eco System, but also Grid users and Grid resource operators can integrate their use cases in such a general Grid Tool Eco System. The g-Eclipse project built such an general, middleware independent tooling framework for Grid infrastructures on top of the well known Eclipse Eco System. The first release of the framework is available and exemplary support for the gLite middleware is available. The GRIA middleware support is currently be implemented. The g-Eclipse framework requires stable and reliable basic Grid services like information systems, data replication systems and resource brokers. g-Eclipse is a JAVA application and requires either JAVA APIs or well defined WS descriptions for the basic Grid services, which are independent of the Grid operation system.

Impact:
The g-Eclipse framework provides an extensible architecture based on the Eclipse mechanisms of extension points, plugins and bundles. By defining the extension points the g-Eclipse framework gets middleware independence and can connect to every middleware service available. The framework is flexible enough to develop plugins to new and emerging Grid services. g-Eclipse provides already plugins and bundles to interact with existing Grid resources running gLite (i.e. EGEE, D-Grid). These implementation use existing API, WS interfaces or - where needed - own implementations to access the gLite services. g-Eclipse extends the eco system of the Eclipse framework by using its components and by providing extension points for Grid functionality. i.e. g-Eclipse provides a new Grid Project View analogue to the Java Project View of Eclipse. The development of Grid applications is not limited to JAVA only, but to other programming languages too, as g-Eclipse is using results from other projects.

Conclusions:
With the help of the g-Eclipse framework, the Chinese wall between local and Grid resources will be broken and the Grid user can access Grid resources seamlessly by managing data, defining and submitting jobs, visualize data, etc. Furthermore the time-to-application will be shortened with the help of Grid development and Grid deployment tools. Last but not least, the Grid resources provider will be able to reduce the time-to-service of their offered resources and services.

Keywords: Tooling, Eclipse, middleware independent, Generic applications, Visualisation, Development, deploy.

Further information: www.geclipse.org www.eclipse.org/geclipse

63. Grid website vulnerabilities and the Gridsite security framework

Author: Mcnab, Andrew (University of Manchester)

Short overview:
This talk describes Cross Site Request Forgery (CSRF) and Cross Site Scripting (XSS) attacks which can be attempted against administrative websites and portals used in Grid projects. It explains how the X.509 certificates used in Grid projects actually make these attacks easier, and then describes a solution implemented by the GridSite project.

Analysis:
CSRF and XSS attacks have been used against major public websites, such as Google's GMail, for several years, and generally involve "confused deputy" scenarios in which an authenticated user's web browser is deceived into carrying out an action desire by the attacker. Due to the support for Javascript functions such as XMLHttpRequest in browsers, it can be possible for an attacker's script to communicate with a website using the user's credentials without their knowledge. The credentials involved have typically been HTTP cookies issued by websites to legitimate users, and the attacks have relied on users being logged-in at the time of the attack. However, in Grid environments many websites authenticate users with their X.509 user certificates, and so users are always logged-in from the point of view of an attacker's script.

Impact:
This class of vulnerabilities has the potential to allow some severe escalation attacks against web-based management components of Grids, as the sessions of users with lower credentials are used to inject attacker's scripts into wikis, bug tracker sites, monitoring messages etc. When users with higher administrative privileges view pages containing these scripts, their credentials could then be used to modify access policies, group memberships, site configurations etc. This talk explains how the GridSite Security Framework prevents these attack modes using a combination of X.509 user certificates, the established double-submit cookie method and cross-domain limitations on cookie sharing and creating XMLHttpRequest connections. This method involves inserting an additional login page step, which also allows the integration of non-X.509 authentication systems such as Kerberos and Shibboleth on an equal footing with X.509.

Conclusions:
Support for this system is included in the mod_Gridsite extension to Apache, and can be used as the basis of third-party portals, management sites etc in any language supported by the Apache HTTP server. Furthermore, this mechanism for limiting CSRF/XSS attacks can also be implemented by other web application hosting environments, or by applications themselves.

Keywords: Gridsite security x.509 csrf xss websites portals

Further information: http://www.Gridsite.org/

64. Portals for earth science

Author: Linford, Julian (ESA)
Co-authors: Plevier, Camiel (DutchSpace); Lecca, Giuditta (CRS4); Poliakov, Andrey (GCRAS); Simo, Branislav (UISAV); Gotab, Benoit (IPGP)

Short overview:
Earth Science (ES) is an all-embracing term for sciences related to planet Earth, covering a large and diverse user community. Since several years the ES applications show an increasing need for access to intensive computing facilities and to large and heterogeneous sets of data, in general via web portals. DEGREE is a consortium of ES partners aiming at promoting the uptake of Grid technology in ES and defining the requirements of ES applications on Grid technologies, including portals.

Analysis:
Large sets of ES data are available and distributed all over the world. The data come from satellites, ground-based network and sensors aboard balloons, aircrafts, and/or sounding rockets. A critical requirement is the organisation of the data, their accessibility and in some cases tools to define the workflow of the application. From a very large number of existing ES portals, a survey was done to focus on, analyze and document those of particular interest and relevance. The focus is on ES portals which are employing, to a greater or lesser extent, some combination of the following relevant technologies and methodologies, Grid, e-collaboration, Service oriented architecture, semantic web and Ontology. This survey provides a clear picture of wide range of emerging technologies in ES portals. The high-level of web-based portal services, provided to end-users, permits to define requirements for implementation on gLite and for development of new services.

Impact:
Some ES portals have appeared with different tools for discovery, download, and local computation. Grid infrastructure offers the capability to explore those large sets of data that could not be analysed before due to computing power limitations and the inability to deploy complex calculations based on a combination of various large sets of data. Portals enormously increase the number of Grid potential users because they mirror most established usage patterns without requiring any specific expertise of the technological background to be understood.

Conclusions:
By full exploration of the data, the combination of data web services and Grid via a portal will open new fields and discovery, not limited to Earth science alone.

Keywords: Earth Science, portal, Data management, Grid

Further information: http://www.eu-degree.eu

65. RINGrid: conceptual design of the remote instrumentation systems

Authors: Lawenda, Marcin (Poznan Supercomputing and Networking Center)
Co-authors: N.Meyer (Poznan Supercomputing and Networking Center); C.Kotsokalis (GRNET); F.Davoli (Italian National Consortium for Telecommunications); T.Prokosch (GUP); Y.Kalvachev (CLMC)

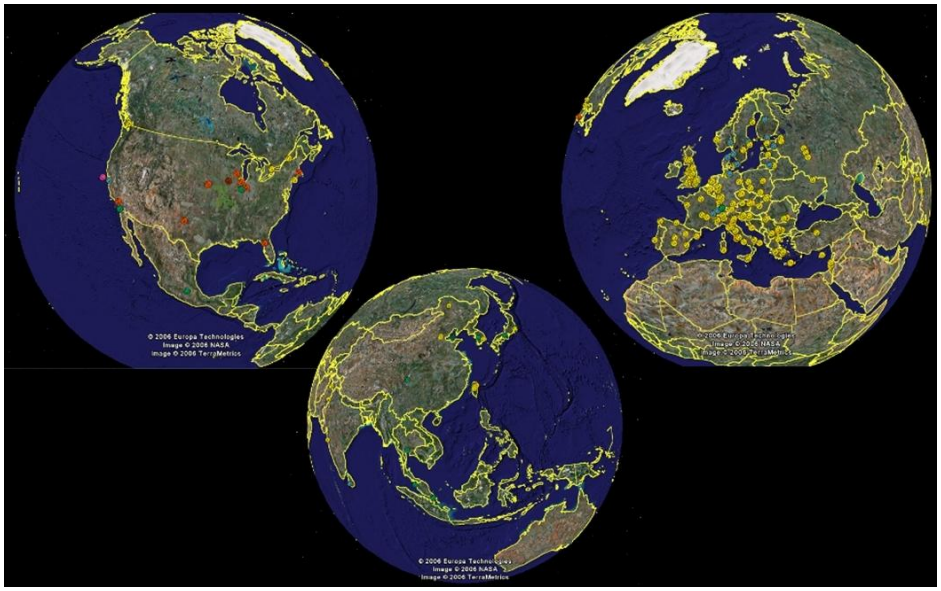
Short overview:
A number of problems in science, industry and commerce may be addressed by using sophisticated equipment and top-level expertise, which is often locally unavailable. The answer for some of these problems is conception of Remote Instrumentation Services (RIS). RIS supports activities related with using rare equipment remotely e.g. workflows, post-processing, visualization, data management. This idea is especially attractive for: radio astronomy, chemistry, physics and medicine.

Analysis:
The analysis of the wide implied RIS aspects are under of interest of the RINGrid (Remote Instrumentation in Next-generation Grids) project. This activity is part of 6th European Framework Programme and has been launched in October 2006. Briefly, the RINGrid project will provide systematically identification of instruments and corresponding user communities, the definition of their requirements as well as careful analysis of the remote instrumentation synergy with next-generation highspeed communications networks and Grid infrastructure. These results will be the basis for the definition of recommendations for designing next-generation RIS. RINGrid associates partners coming from Europe and Latin America from 10 institutions. On the one hand it allows to achieve required level of generality and on the other hand gives desired impact by gathering scientists from different research domains. User communities are related with unique laboratory devices e.g. NMR spectrometers.

Impact:
All RINGrid effects will be practically verified in the last stage of the project. Prototype installations will be set up, by taking into consideration user communities and instruments as well as used software. One of the systems which will be used in validation process is PSNC Virtual Laboratory (VLab). VLab (vlab.psnc.pl) project is developed by Poznań Supercomputing and Networking Center in collaboration with the Institute of Bioorganic Chemistry since 2002. The main research goal of the VLab is definition of a framework for building many different types of laboratory. It will facilitate and automate building new laboratories using existing modules with their functionality. The PSNC Virtual Laboratory system should not be comprehended solely as a set of mechanisms to submit, monitor and execute jobs. It is also a possibility to give access to the resources of the digital library, communication, and e-Learning systems.

Conclusions:
Basing on the demands and requirements and taking into account the state of the art, future needs and trends will be analyzed in respect of RIS. Guidelines concerning the design, development and use of next-generation RIS will be provided. Special attention will be paid to present and on-going research activities (e.g. EGEE, gLite), enabling a cooperative and integrated use of Grid technologies and selforganizing, self-configuring, self-optimizing, self-healing networks with QoS support.

Keywords: remote instrumentation, virtual laboratories, expensive instruments, instrument virtualization.
Further information: http://www.rinGrid.eu



Interoperability and Resource Utilization

Interoperability and Resource Utilization

Conveners: C. Germain-Renaud (LRI/AL, Paris), C. Grandi (CERN/INFN)

With the deployment of production Grids, defining roadmaps towards the future e-infrastructures becomes a practical issue. While resource integration on the European scale is required in order to sustain the needs of e-science, a fully integrated ("monolithic") Grid is not a realistic perspective, nor is it desirable: various independent actors already have integrated hardware, software and immaterial resources, into community, local, or regional Grids. Interoperability is now a central objective, with the ultimate goal of building an ecosystem of resources. While Service Oriented Architectures provide a technological framework, interoperability requires standards, to define the infrastructure and the services themselves.

On the other hand, the chasm between the standardization processes and even the skilled professionals remains very large. The session Interoperability and Resource Utilization offered some insights on the subject through case studies, which are also a needed component of the standardization process.

The complete e-infrastructure ecosystems encompass volunteer computing, ultra-high performance resources, and EGEE as the paradigm for institutional Grids. Given the heterogeneity of applications and middleware, the goals of interoperability were revisited. The session also reported on lessons learned from implementing compliance of gLite-based utility components in various areas, including information systems and resource discovery, to OGF specifications. The rationale for a large part of the current stack of standards is to shield the end-user from infrastructures; however, factoring the applications logics across e-science applications requiring collaborative, on-demand, and intensive information processing, are of equal importance, and were exemplified. Finally, meta issues, such as the critical question of reliable and automated evaluation of interoperability and compliance to standards, as well as the access to platforms not directly supported by the middleware stack were presented.

EGEE strategy towards interoperability:

- The best solution is to have *common interfaces* through the development and adoption of *standards*.
- The gLite reference forum for standardization activities is the Open Grid Forum
    - Many contributions (e.g. OGSA-AUTH, BES, JSDL, new GLUE-WG, UR, RUS, SAGA, INFOD, NM, etc.)

Problems with this strategy:

- Infrastructures are already in production
- Standards are still in evolution and often underspecified
- OGF-GIN follows a pragmatic approach

How to achieve interoperability now while standards are developing:

- Parallel Infrastructures
    - User driven: the user joins different Grids (uses different tools)
    - Site driven: the site offers different access methods to resources
- Gateways
    - Bridges between infrastructures
- Adaptors and translators
    - Single API for users. Plug-ins provide translation

66. Partnership for advanced computing in Europe (PRACE)

Authors: Vartto, Saara (CSC - Finnish IT center for science); Koski, Kimmo (CSC -Finnish IT center for science)

Short overview:
The Partnership for Advanced Computing in Europe (PRACE) prepares the creation of a persistent pan-European HPC service, consisting of several tier-0 centres providing European researchers with access to capability computers and forming the top level of the European HPC ecosystem. PRACE will start on 1st January 2008 and is funded by the EC's 7th Framework Program.

Analysis:
The objectives of PRACE are to:
• Create and implement by 2009/2010, a persistent, sustainable pan-European HPC service with several HPC leadership systems of petaflop/s performance.
• Define and establish a legal and organizational structure involving HPC centers, national funding agencies, and scientific user communities.
• Prepare for the deployment of petaflop/s systems in 2009/2010 under the responsibility of European supercomputing centers having the expertise, competency, and required infrastructure to provide a comprehensive service to industry and academia user groups.
• Collect requirements and demands from the user community about future challenging applications.
The infrastructure will be complemented with network and Grid access, and the services required to enable applications. These include development of parallel application software expertise, packages, and data handling. It will use concepts and services from EC-funded projects, such as EGEE, GÉANT2 and DEISA.

Impact:
Utilizing high-end computing centers necessitates the development of the whole European HPC ecosystem. Close collaboration with other European flagship e-Infrastructure projects, such as EGEE and DEISA, IT industry and potential users in order to deploy technical and user-level interoperability within all levels of the performance pyramid. Technical interoperability (middleware work together, etc.) depends on user needs and obviously the same middleware may not be suitable for all types of usage. However, technical interoperability will be taken into account and maximized during the implementation phase. User-level interoperability (the same user groups can use different resources depending on their needs) between research infrastructures will benefit the whole ecosystem.

Conclusions:
The PRACE project starts in January 2008 and continues until the end of 2009. The first petaflops center should be in production in 2009/10. In addition, aims at defining and setting up a legal and organisational structure involving HPC centres, national funding agencies, and scientific user communities to ensure: adequate funding for the continued operation and periodic renewal of leadership systems.

Keywords: Supercomputing, HPC ecosystem, petascale, interoperability, European competitiveness

Further information: http://www.prace-project.eu

67. WLCG-RUS: an extensible solution to resource usage service

Author: Chen, Xiaoyu (Brunel University)
Co-author: Akram, Khan (Brunel University)

Short overview:
The main goal of WLCG-RUS project is to provide a development framework facilitating implementations of OGF Resouce Usage Service. The WLCG-RUS is designed to be extensible and allows usage records to be persistent in various storages, either XML or Relational database. With a set of abstract components implementations can provide custom solutions in accordance to deployment requirements. In addition to RUS core features, the WLCG-RUS allows advanced operations on summary usage records.

Analysis:
The project originated from providing a RUS compliant solution for WLCG accounting, which requires collection of usage data from three operational Grids, the Open Science Grid (OSG), EGEE and NorduGrid. The collection of usage data are to be stored centrally and summarized for usage reporting on per site, per VO, per month basis. These collected usage data are persistent in relational database based on WLCG accounting schema. At present, usage providers from each operational Grid simply email SQL statements for insertion of summary usage records to project manager who runs a simple script to populate usage data into storage. The WLCG-RUS project is therefore proposed to automate and standardize usage data sharing and reporting processes with interoperability to RUS implementations available or being developed in operational Grid projects.

Impact:
The WLCG-RUS design is based on the proposed framework of “Review of Grid Accoutning and Usage Monitoring”, a three-month review project funded by JISC in UK. The WLCG-RUS framework is composed of a set of abstract components that enable implementation of standard RUS core operations while allowing customization on usage data persistence in various storage format (either XML and relational database). A component known as XML-Object Mapping (XOM) is used to convert custom usage representation to standard OGF URF format, or vise versa during the execution of RUS data operations. WLCG-RUS also allows implementations to provide custom functionalities on authorization, usage filtering, operational logics, data access pattern, and summarization. Therefore the WLCG-RUS provides a flexible and extensible development framework for RUS implementations.

Conclusions:
In summary, the WLCG-RUS project provides an extensible framework for RUS implementations that bridges the gap between relational usage representation and OGF URF standard. The WLCG-RUS is going to be deployed at Rutherford Tier 1 sites and London Tier 2 sites for performance and interoperability test.

Keywords: Usage Record Format, Resource Usage Service, XML-Object Mapping, WLCG

68. gCube Grid services

Authors: Andrade, Pedro (CERN); Pagano, Pasquale (CNR-ISTI)

Short overview:
gCube is a service-based framework for eScience applications requiring collaboratory, on-demand, and intensive information processing. It provides to these communities Virtual Research Environments (VREs) to support their activities. gCube is build on top of standard technologies for computational Grids, namely the gLite middleware. The software was produced by the DILIGENT project and will continue to be supported and further developed by the D4Science project.

Analysis:
gCube reflects within its name a three-sided interpretation of the Grid vision of resource sharing: sharing of computational resources, sharing of structured data, and sharing of application services. As such, gCube embodies the defining characteristics of computational Grids, data Grids, and virtual data Grids. Precisely, it builds on gLite middleware for managing distributed computations and unstructured data, includes dedicated services for managing data and metadata, provides services for distributed information retrieval, allows the orchestration of workflows, and offers a novel approach for managing these services. Rather than interfacing the infrastructure, the gCube services are transparently deployed across its constituent nodes. This is genuinely ambitious and entirely novel: like computational resources and data before, application logic in gCube becomes a pervasive commodity within an infrastructure which abstracts over its physical location at any point in time.

Impact:
The dynamic deployment mechanisms of the gCube services allow the creation and management of VREs, i.e. aggregations of users, computational, data, and service resources which characterize the activities of distributed research collaborations. Users interface VREs in order to select resources, define the policies which control their sharing, and to interactively orchestrate services into executable workflows to satisfy their domain specific needs. Through the D4Science project, gCube will offers VREs to users from two distinct eScience areas: Environmental Monitoring and Fishery resources Management. By supporting these communities, gCube will provide them a powerful, innovative, reliable and easy-to-use infrastructure allowing the shared access to data, services and applications that will dramatically reduce the time needed to perform their scientific activities.

Conclusions:
The gCube system, as developed by the DILIGENT project, already offers a basic framework to support scientific collaboration as it provides mechanisms to create VREs that support on-demand sharing of resources and application services. However, in order to fully address the requirements of the two D4Science communities, the gCube application framework will be appropriately consolidated and expanded in particular with respect to service performance, dependability, and resilience.

Keywords: Virtual Research Environments, Collaboratories, Grid Computing

Further information: www.gcube-system.org

69. Towards a WBEM-based implementation of the OGF GLUE information model

Authors: Andreozzi, Sergio (INFN-CNAF); CANAPARO, Marco (INFN-CNAF); Carpene, Michele (INFN-CNAF)

Short overview:
In the context of the Open Grid Forum, the GLUE Working Group is defining the next generation information model for the description of Grid resources targeted at enabling resource awareness, discoverability and selection. The OMII-Europe project is engaged in this activity and is developing a modular framework for managing the information providers based on WBEM (Web-Based Enterprise Management). In this presentation, we will describe the details and the advantages of this approach.

Analysis:
The current gLite middleware relies on the GLUE 1.3 information model and its implementation in LDAP in order to advertise the available resources and their characteristics in the EGEE infrastructure. In the context of the Open Grid Forum, the GLUE Working Group is defining the evolution of this information model to improve the current design and to unify a number of existing approaches in a community standard. The OMII-Europe project is engaged in this activity and is developing a modular framework for managing the information providers based on WBEM (Web-Based Enterprise Management) technologies. A client supporting multiple renderings is being developed in order to be useful for different consumers (e.g. LDAP for BDII, XML for Web Services, SQL for R-GMA). Impact : WBEM technologies are a suite of standards for the management of resources wellestablished in the enterprise area and with mature implementations both as commercial and open source products. These technologies well suite the need for handling information providers and for exposing them via a standard management interface. When adopted in the proper way, they can simplify the addition of information providers from various developers responsible for the software component to be advertised. Moreover, it can reduce the amount of bad data via a stronger control at the metering side.

Conclusions:
A WBEM-based framework for managing information providers of Grid resources is an important test for improving the quality of the produced data and for symplifing the development and deployment of the providers. The support for multiple renderings eases the exposure of such information via different types of services using different concrete data models.

Keywords: information modeling, information discoveryinformation modeling, information discovery

70. SAGA API for gLite service discovery

Authors: FISHER, Steve (RAL); Paventhan, A (RAL)

Short overview:
The Simple API for Grid Applications (SAGA) from the Open Grid Forum (OGF) defines standard APIs to allow Grid applications to be middleware independent. We have contributed a Service Discovery specification to SAGA and an implementation as a generalisation of the existing gLite component. The purpose of service discovery is to locate services based on various characteristics. The API supports a very general selection mechanism and is built on the GLUE notion of a service.

Analysis:
The API returns a list of service descriptors matching search criteria. A random choice can then be made from the URLs returned. Information about the individual services can be obtained from the descriptors if it is desired to rank the services returned or produce a web page of some subset of services. The search criteria are specified by means of three filters – service, VO and data. The service filter selects on the basis of some GLUE attributes such as the "type" of service. The VO filter allows the user to select from those services he is allowed to use and the data filter makes use of a GLUE feature of key/value pairs associated with each service. SAGA components have a "plugin" architecture. In the case of Service Discovery, a plugin is required for each underlying information system; so far we have R-GMA and BDII support in C++.

Impact:
The existing gLite Service Discovery API is being used by components of the Workload Management System (WMS) and Data Management Systems. The Logging and Bookkeeping service developers have expressed an interest in using the new SAGA API because of the extra functionality it offers. The SAGA approach is useful from a user perspective because it frees end users from dependency upon specific Grid middleware. We expect that the use of SAGA will grow making the interface increasingly valuable. The SAGA Service Discovery API has been designed to be very easy to use with SQL style filter expressions. It also means that services that use other services require less error-prone configuration as they can find the actual services when they need them. This in turn leads to increased reliability.

Conclusions:
The SAGA based Service Discovery C++ API supporting SQL style filters has been implemented within gLite. We provide a C wrapper that is compatible with the old gLite API however this is mainly useful for testing to check that the returned set of services is the same. In future we will provide Python and C wrappers and a Java implementation. The wrappers avoid the need for rewriting the plugins. JNI will be considered for a Java wrapper as a short term solution.

Keywords: Grid, API, SAGA, OGF

Further information: http://forge.ogf.org/sf/go/doc14875?nav=1 http://hepunx.rl.ac.uk/egee/jra1-uk/index.html

71. A simple SPAGO implementation enabling the connection of heterogeneous computational resources to a gLite based Grid

Authors: Bracco, Giovanni (ENEA FIM, 00044 Frascati, Roma, Italy); Santoro, Andrea (ENEA FIM, 00044 Frascati, Roma, Italy); Migliori, Silvio (ENEA FIM, 00044 Frascati, Roma, Italy); Scio', Carlo (ENEA FIM, 00044 Frascati, Roma, Italy); Quintiliani, Andrea (ENEA FIM, 00044 Frascati, Roma, Italy); Rocchi, Alessio (ENEA FIM, 00044 Frascati, Roma, Italy)

Short overview:
SPAGO (Shared Proxy Approach for Grid Objects) is a methodology which relies on standardized tools for file-sharing and remote process execution to build a proxy system providing a simple solution to connect to the EGEE Grid a local computational resource without strong requirements on the architecture or operating system compatibility with the gLite middle-ware. SPAGO has been developed in the context of the interoperability solution between EGEE and ENEA-GRID.

Analysis:
The success of the Grid depends also on its flexibility in accommodating the computational resources available over the network. A big effort is underway to develop accepted Grid standards but in the meanwhile solutions have to be found to include into EGEE infrastructure resources based on platforms or operating systems which are not currently supported by gLite middle-ware. SPAGO concept has been developed in the implementation of the ENEA Gateway which now provides access from EGEE to the ENEA AIX SP systems. Although the ENEA Gateway implementation requires a solution for the interoperability between ENEA-GRID and EGEE (due to the different authentication mechanisms, AFS and Kerberos 5 vs. X509), a much simpler solution has been found for standard UNIX/Posix systems where NFS and ssh can be adopted as the base for the proxy implementation. This simplified solution is the object of this presentation.

Impact:
The SPAGO architecture allows the EGEE user to submit jobs that are not necessarily based on the x86 or x86_64 Linux architecture, thus allowing a wider array of scientific software to be run on the EGEE Grid and a wider segment of the research community to participate in the project. On the other way round, the SPAGO approach provides a simple way for local resource managers to join the EGEE infrastructure without strong requirements on architecture/ platform/ operating system distribution and with advantages also concerning the firewall configuration requirements. This fact can widen significantly the penetration of gLite middle-ware outside its traditional domain of the distributed and capacity focused computation. For example the world of the High Performance Computing, which often requires dedicated system software, can find in SPAGO the easy way to join the large EGEE community.

Conclusions:
This paper presents a new simplified implementation of the SPAGO architecture, describing the guidelines that allow any Grid manager to integrate into EGEE his own non-standard machines. The result relies on the experience of the ENEA EGEE site, where AIX resources are seamlessly integrated into the EGEE production Grid (successful tests also conducted for IRIX and MacOSX). The SPAGO approach will be also used for the new ENEA HPC system (CRESCO, ~2500 cores, initial operation early 2008).

Keywords: Interoperability, heterogeneous platforms, computing element

Further information: http://www.afs.enea.it/project/eneaegee/

72. An application of ETICS co-scheduling mechanism to interoperability and compliance validation of Grid services

Authors: Ronchieri, Elisabetta (INFN CNAF); Aguado Sanchez, Carlos (CERN); Diez-andino Sancho, Guillermo (CERN); DI Meglio, Alberto (CERN); Marzolla, Moreno (INFN)

Short overview:
Grid software projects require infrastructures in order to evaluate interoperability with other projects and compliance with predefined standards. Interoperability and compliance are quality attributes that are expected from all distributed projects. ETICS is designed to automate the investigation of this kind of problems. It integrates well-established procedures, tools and resources in a coherent framework and adaptes them to the special needs of these projects.

Analysis:
Interoperability and compliance to standards are important quality attributes of software developed for Grid environments where many different parts of an interconnected system have to interact. Compliance to standard is one of the major factors in making sure that interoperating parts of a distributed system can actually interconnect and exchange information. Taking the case of the Grid environment (Foster and Kesselman, 2003), most of the projects that are developing software have not reached the maturity level of other communities yet and have difficulty to identify and adopt standards. Validating the compliance with standards often requires the design of custom test suites and a constant attention to any proposed change. Interoperability amongst middleware and application software developed in order to be used on Grid and other distributed environments is usually a very complex issue.

Impact:
ETICS provides a single reference for software configuration information, which separate projects can use to validate basic interoperability assumption when developing the code. The co-scheduling mechanism has been developed in ETICS in order to automatically deploy and run distributed tests in different platforms. By coscheduling it is understood the automation of the deployment of the different services and clients, the execution of the tests and the gathering of information such as test results, metrics, and logs. A typical scenario to be faced by the coscheduling is composed of several services that interoperate among them, clients that contact the various services and tests that require servers and clients to be in place. This functionality has been applied for testing the interoperability between job submission engines (like CREAM) by using their conformance to the OGSA-BES recommendation. ETICS has therefore been adopted to perform this test automatically.

Conclusions:
We presented the co-scheduling mechanism used to execute complex distributed tests requiring the deployment of many interacting services on different physical nodes. A practical application to the interoperability testing of the CREAM-BES service has been presented. Additional work on this technology is being performed to expand its use to other types of tests, middleware, services and applications.

Keywords: Interoperability, Co-scheduling mechanism, Automatic Test

73. Interconnecting Grid, desktop Grid and network

Author: Georgakopoulos, Kostas (University of Macedonia)
Co-authors: Stefanidis, Vassilis (University Of Macedonia); Margaritis, Kostas (University Of Macedonia)

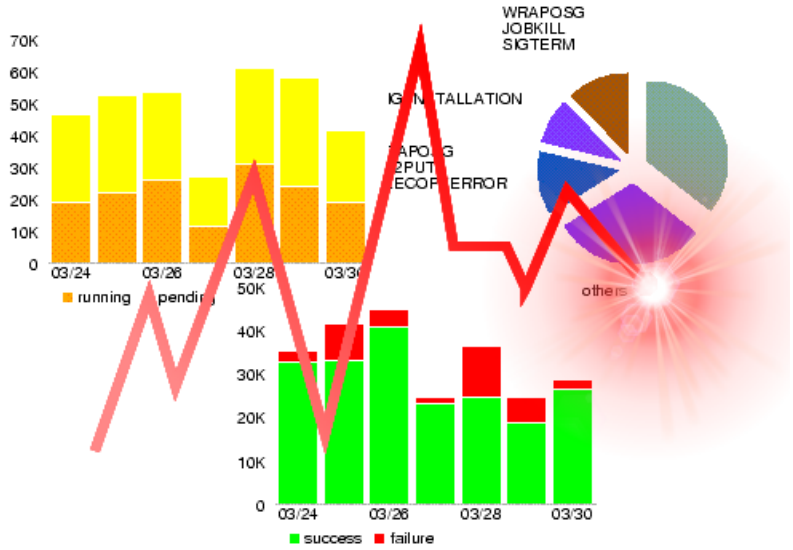
Short overview:
Grid infrastructures today are expanding slowly because adding computing resources is sometimes a difficult, costly and bureaucratic procedure. Some high standards must be met so that a new cluster or high performance system can be added to the Grid. We are investigating the interconnection of the main Grid infrastructure to other Gridlike systems (like Condor) or network computing systems (like B.O.I.N.C.) that provide inexpensive computing power by exploiting idle computing resources.

Analysis:
We are researching and evaluating systems that can provide a bridge to non-dedicated resources for the Grid. We focused on the Condor system because it is a technology that has been around for many years. Furthermore, computing elements (CE) that use the LCG or gLite middleware can be configured to interact with Condor pools and forward jobs to be executed. Our aim was to test the functionality of this bridge and also to research issues like security, reliability and network functionality. Our testbed for this research was a Condor pool we set up and the gLite Pre-Production site we administer as part of the EGEE project. Additionally we researched,to some extent, other systems that provide a non-dedicated resources computing model like B.O.I.N.C and the LiveWN project. Our end goal is to provide some case studies that document the possible solutions for expanding the Grid with non-dedicated resources and also to investigate the restrictions and boundaries imposed by these solutions.

Impact:
Computing power that can be collected from idle computing resources can be a great benefit for the Grid. It will provide an inexpensive way of expanding the present infrastructure and also gives countries a way to exploit their current computing resources that are located in places such as university or school labs and remain idle for the most part of the day. This can affect other areas as well: by increasing the computing power of an institution (e.g a university) one can provide the means to advance scientific research and knowledge. Furthermore, by using public computing resources, Grid technologies are brought closer to the public and also to the scientific community. Finally, there can be a significant reduction to public expenditure, since it will be possible to have better utilisation of the large numbers of workstations being purchased every year in large public organisations, such as universities, research institutes, schools etc.

Conclusions:
The results so far are promising: the Condor system interacts well with our Grid site and Condor's features of checkpointing and rescheduling in case of systems failing for some reason provide a very flexible and reliable service. Condor also provides many reliable security features. Future plans include extended scalability and reliability tests and also development of methods and tools that will ease the deployment of such an infrastructure.

Keywords: Grid, Middleware, Bridge, Idle Resources, Condor, B.O.I.N.C, Network Computing, LiveWN, Case Study



Monitoring, Accounting & Support

Monitoring, Accounting & Support

Conveners: F.Schaer (CEA, Paris), G.Sipos (MTA SZTAKI, Budapest)

With 250 partner sites in 50 countries, providing more than 64000 CPUs and 20 petabyes of active storage, the EGEE infrastructure is now the major worldwide production Grid infrastructure. Thus, EGEE needs to maintain a high quality of service, including tools with excellent functionality and performance.

Among these are monitoring tools: regardless of the quality of the middleware, a service can break because of hardware, software or human failure. And while the service is degraded, it is the monitoring applications that allow rapid detection and reaction. For managing the infrastructure, the question of managing resource allocation is another key to success: without such management, users cannot be given their fair share of resources, and without this capability, users are reluctant to invest resources in the Grid. The last, but not least, requirement that was addressed in this session was support. Considering that neither software nor infrastructure can be perfect, users need to be guided when services fail. Not only do users need support, but the infrastructure itself needs a communication channel with its users.

The session allowed attendees to have an overview of the forthcoming enhanced Grid services, and of what these have to offer. A major part of the session was user oriented, through user support, user side monitoring and user communication presentations, as it is the users' experience that measures the success of an infrastructure.

Some key concepts emerged from the talks and discussions:

- **User friendliness**
    - The use of GUI/Portal tools with simple building block structures is important
- **Scalability and reliability**
    - Use solid tools such as Oracle/APEX are used , and intensive tests are conducted
- **Provide active services**
    - Authentication servers can query accounting servers and lock users
    - Job or Service monitoring trigger notifications
    - Service monitoring must be able to exclude failing nodes/clusters
    - LHCb uses SAM to check AND install software
- **Provide different level user views**
    - Basic view
    - Advanced user view
    - Programmer view
    - Administrative view

- **Advanced features**
    - SAM framework allows user defined tests
    - Dashboard shows logs for advanced users
    - Monitoring results can be shared with applications
    - Reporting tools and graphs are necessary
- **Feedback, communication, improvement**
    - There are monthly GGUS releases
    - Monitoring tools developers become users to better comprehend the monitoring needs

74. gUSE: Grid User Support Environment

Authors: Lovas, Robert (MTA SZTAKI); Kacsuk, Peter (MTA SZTAKI); KaroczkaiI, Krisztian (MTA SZTAKI)
Co-authors: Schnautigel, Andras (MTA SZTAKI); Marton, Istvan (MTA SZTAKI); Sipos, Gergely (MTA SZTAKI); Hermann, Gabor (MTA SZTAKI)

Short overview:
gUSE provides a high-level Grid service layer in order to support Grid application development. gUSE is based on the lessons we learned from the P-GRADE portal and significantly extends its objectives. The main goal of gUSE is to provide a set of high-level Grid services by which interoperation between Grids and user communities could be achieved. Workflow interoperability and user collaboration is supported by application repository. gUSE as a collection of web services is highly scalable.

Analysis:
Users of gUSE can be either Grid application developers or end-users. Application developers can develop sophisticated workflow applications where workflows can be embeded into each other at any depth. Even recursive workflows allowed. gUSE enables to embed workflows derived from other workflow systems (e.g. Taverna, Triana, Kepler, etc.). gUSE supports the concept of workflow templates, abstract workflows, concrete workflows and workflow instances. All of them can be published in a workflow repository. Members of a developer community can import workflows from the repository and can continue the work on them. End-users can import completed workflow applications from the repository and can execute them based on a simple user interface that hides Grid details from them. Grid is exposed only for the application developers. Parametric sweep nodes and normal nodes can be used in a mixed way in the workflows enabling very complex applications to develop in gUSE.

Impact:
gUSE is based on the lessons we learnt from the P-GRADE portal and significantly extends its objectives and features. The workflow concept of gUSE is much more flexible than other workflow systems. Its DAG topology is extended with
- embeded WFs and even recursive embeded WFs
- parameter sweep nodes
- conditional control mechanism
- special workflow starting control mechanisms based on external events or periodic timing.

It supports not only Grid interoperation but also workflow interoperation. It can be easily connected to any known Grid middleware. It is already connected to GT2, GT4, LCG-2, gLite and WS based Grid systems but it can also be connected to local systems like clusters or supercomputers. It contains a built-in Grid broker that can automatically distribute the jobs of a workflow into any of the connected Grids. Of course, it can use other Grid brokers like the gLite broker or GridWay.

Conclusions:
Its implementation is highly scalable, can be distributed on a cluster or even on different Grid sites. Stress tests show that it can simultaneously serve several thousand users. gUSE can be installed with or without a portal interface. The portal interface developed for gUSE is called WS-PGRADE. Its user interface provides a graphical workflow editor that is much faster than the one in P-GRADE portal. WSPGRADE also supports a workflow repository and its use by end-users and appl. developers.

Keywords: Workflows, Repositories, Brokers, Grid interoperation, Workflow interoperation

Further information: http://www.lpds.sztaki.hu/gUSE/

75. Strategies for experiment-specific monitoring in the Grid

Authors: Mendez Lorenzo, Patricia (CERN IT); Sciaba, Andrea (CERN IT) ; Campana, Simone (CERN IT); Santinelli, Roberto (CERN IT); Lanciotti, Elisa (CERN IT); Miccio, Enzo (CERN IT); Magini, Nicolo (CERN IT); Di Girolamo, Alessandro (CERN IT).

Short overview:
This contribution describes how the LHC experiments implement their own Grid resource monitoring, either by internally developed tools, or by reusing tools used for Grid operations, like the Service Availability Monitor (SAM) used for the EGEE operations.

Analysis:
The LHC experiments perform most, if not all, of their computing activities on Grid resources. This requires an accurate and updated picture of the status of the Grid services used by them, and of the services which are specific to the experiment. To achieve this, a common method is to periodically execute tests on the services, where the functionalities tested may be different from a VO to another. The SAM framework, developed for the EGEE operations, can be easily used to run and publish the results of arbitrary tests, from basic functionality tests, to high-level operations from real production activities. This contribution describes in detail how the monitoring system of each LHC experiment has taken advantage of SAM.

Impact:
The work covered by this contribution has largely improved the usage efficiency of Grid resources by the LHC experiments. A more accurate and prompt discovery of problems allows to fix them as soon as they appear, thus increasing the overall reliability of the Grid resources from the experiment point of view. This information also allows the experiment applications to make better decisions whenever they are given a choice of the resources to use, avoiding for example to send jobs to problematic or overloaded computing resources.

Conclusions:
The necessity to commission the computing resources available to the experiments before the start of the LHC data taking in 2008 requires a constant effort to improve the quality of the monitoring information. This is why the work described here is still ongoing and we foresee an increasing usage of the SAM framework by the experiments, both by expanding the current tests, and by adding new tests for services that are not yet tested with this methodology.

Keywords: LHC, Monitoring, SAM, High Energy Physics

Further information: https://lcg-sam.cern.ch:8443/sam/sam.py

76. Increased productivity for emerging Grid applications: the application support system

Authors: Maier, Andrew (CERN IT); Lee, Hurng-Chun (CERN IT); Mendez Lorenzo, Patricia (CERN IT/GD); Moscicki, Jakub (CERN IT); Lamanna, Massimo (CERN IT); Muraru, Adrian (CERN IT)

Short overview:
Recently a growing number of various applications have been quickly and successfully enabled on the Grid by the CERN Grid application support team. This allowed the applications to achieve and publish large-scale results in a short time which otherwise would not be possible. We present the general infrastructure, support procedures and tools that have been developed. We discuss the general patterns observed in supporting new applications and porting them to the EGEE environment.

Analysis:
The CERN Grid application support team has been working with the following real-life applications: medical and particle physics simulation (Geant4, Garfield), satellite imaging and geographic information for humanitarian relief operations (UNOSAT), telecommunications (ITU), theoretical physics (Lattice QCD, Feynman-loop evaluation), Bio-informatics (Avian Flu Data Challenge), commercial imaging processing and classification (Imense Ltd.) and physics experiments (ATLAS, LHCb, HARP). Using the EGEE Grid we created a standard infrastructure - set of services and tools - customized for the emerging applications. This includes creation of a generic Virtual Organization easily accessible by small communities and adding resources and services to it. We provide the consultancy service to help the porting of the applications to the Grid using the Ganga and DIANE tools. The system may be operated with only small maintenance and support overhead and is easily accessible by new applications.

Impact:
The various parts of the application support system developed by the CERN Grid application team were used by more than 1000 individual users in the year 2007. More than 10 new applications have been successfully enabled and produced large scale results. We consider that the efficient application support is the key point for further development of the Grid as it allows to continuously attract new application communities, strengthen the Grid infrastructure and enhance the productivity of the users.

Conclusions:
We plan to further consolidate the application support system in order to minimize the maintenance overhead and further increase the autonomy of the application communities in the efficient Grid usage.

Keywords: Grid applications, users, interoperability

Further information: www.cern.ch/arda

77. New monitoring applications in the experiment dashboard

Authors: Andreeva, Julia (CERN); Gaidioz, Benjamin (CERN); Maier, Gerhild (CERN); Ricardo, Rocha (CERN); Saiz, Pablo (CERN; Catalin, Cirstoui (CERN); Sidorova, Irina (CERN/JINR); Wakefield, Stuart (IC); Herrala, Juha (CERN)

Short overview:
The Experiment Dashboard is a monitoring system initially developed for the LHC experiments in order to provide the view of the Grid infrastructure from the perspective of the virtual organization. The presentation will focus on the recently developed applications, in particular monitoring systems for the Monte Carlo production for ATLAS and CMS experiments.

Analysis:
The LHC experiments ALICE, ATLAS, CMS and LHCb are preparing for data acquisition planned to start in 2008. The LHC experiments are relying on several Grid infrastructures (LCG/EGEE, OSG, NDGF). Providing the reliable monitoring system which enables the transparent view of the experiment activities across different middleware platforms and combines the Grid monitoring data with information which is specific for the experiment/activity/application is a vital and challenging task. The Experiment Dashboard is used by all four LHC experiments to follow their activities on the Grid. There are multiple monitoring applications of the Experiment Dashboard which are in production and are widley used by the LHC VOs. At the same time the project is in active development phase. Existing applications are evolving and new applications are developed following the suggestions of the user community.

Impact:
The focus of the presentation is monitoring for the Monte Carlo production of the ATLAS and CMS experiments. Monte Carlo production is a very important activity of the LHC VOs which is fully relying on the distributed infrastructure. The main users of the system are production managers and operators and the monitoring system should allow them to follow the production progress and detect problems in a straight forward way. Due to the close collaboration with the user community and the resulting feedback it was possible to make major improvements in the functionality compared to previous production monitoring system.

Conclusions:
The Experiment Dashboard is an evolving system which is covering more and more areas of the experiment activities on the Grid. The main goals of the future development are to improve the reliability, the completeness of the provided monitoring data and to satisfy better the exact needs of the user community.

Keywords: Monitoring, LHC Experiments, dashboard, Monte Carlo production monitoring Monito

Further information:

http://dashb-atlas-prodsys-test.cern.ch/dashboard/request.py/overview-taskjobs

78. The national Grid service user accounting system

Author: Weeks, Katie (STFC)
Co-authors: Haines, Kevin (STFC); Richards, Andrew (STFC)

Short overview:
The UK's Grid, the National Grid Service (NGS), has developed and implemented a User Accounting System to automate the processes of user registration and account approval as well as provide automatic policing of accounts that go over quota. The User Accounting System queries the Resource Usage Service to obtain usage details for each individual user, inputting the data into an Oracle database which performs automatic policing. Oracle Application Express is used as the web interface to the system

Analysis:
The User Accounting system has simplified administration of users on the NGS. Users who go over their allocated CPU hours find themselves warned when they reach 90% of their allocation, and automatically locked out when they reach 100%. They can apply for further resources using the online form. Since the system entered production in October 2006, it has locked 74 users out, of which 80% successfully reapplied for more time. 183 new users have applied using the system, enabling the NGS to collect more valuable information on users than before. This automatic collection of data and the use of the Oracle Apex system mean statistics can be produced daily. Figures on how much CPU time is allocated and used, where our users are located, how they found out about the NGS and who funded them are available. The users themselves have benefited from the Accounting System, using the online interface to update their contact data, see their allocations or apply for more resources.

Impact:
Early 2006, the NGS had the tools to monitor account usage by way of the Open Grid Forum standards Resource Usage Service (RUS) and the policing policies for account usage, but not the tools to enforce those policies. The User Accounting System was developed by the NGS to address this problem. User account details are kept on an Oracle database. Oracle Application Express (Apex) was used to develop various interfaces to this data for NGS staff, reviewers and users. When the Accounting System was developed, no other monitoring or accounting system satisfied the needs of the NGS. The NGS User Accounting System does this and more. As well as CPU accounting, the system performs automatic policing (locking users out when they exceed their limit), statistical analysis, SRB account creation upon account approval and provides a web interface for users to access their own data.

Conclusions:
The introduction of the User Accounting System has satisfied the NGS accounting needs and will continue to expand to do so. Administration of individual accounts is possible using the Oracle Apex interface. Users now have the important ability to manage their own accounts through the web. Future plans for the system are many and include incorporating Storage use into the automatic policing and the support for Virtual Organisations and their accounting needs.

Keywords: National Grid Service, Accounting, Policing, Oracle, user account

Further information: www.ngs.ac.uk

79. R-GMA: now with added authorization

Authors: Wilson, Antony (RAL); Fisher, Steve (RAL)
Co-authors: Chidambaram, Arun (RAL); Duncan, Alastair (RAL); Jiang, Ming (RAL); Kuseju, Adebiyi (RAL); Bhatti, Parminder (RAL)

Short overview:
R-GMA permits users to define their own data structures along with the fine grained authorization rules specifying who can write and read the data. They can then publish data via a producer API without knowledge of potential consumers. A consumer API is used to retrieve the permitted view of information published by the producers. Previous releases of the server have been patches to the original prototype. The new code has been re–engineered for robustness and scalability.

Analysis:
R-GMA is currently being used by APEL, the ARDA Dashboard and Service Discovery on the LCG Grid and by Grid Ireland. APEL uses a producer at each site to publish accounting data. A consumer is used to accumulate all of the data in a central location where it is migrated off line for later analysis. The ARDA dashboard has a consumer that pulls in monitoring data about the status of Grid jobs as published by resource brokers. This enables real time monitoring of the progress of jobs on the Grid. The Service Discovery API has an R-GMA plugin. A producer at each site publishes information about available services and their current status. This enables other middleware components to select required services. Grid Ireland are using R-GMA to monitor TCP logs. With the increased robustness of the code and the fine grained authorization we expect that users will find new applications for R-GMA.

Impact:
The latest version of the R-GMA server improves on the current implementation. It is based around a new design that was derived from our experiences from the initial prototype and subsequent patches to it. Robustness and scalability are at the centreof the new design. Single points of failure have been removed and the servers have been made as autonomous as possible. Reliance on the delivery of individual control messages has also been removed. From a user's perspective, the improvements in functionality are the introduction of fine grained authorization and virtual databases (VDB). The authorization is done using SQL views of tables constructed dynamically from user defined rules and VOMS attributes. VDBs allow for the partitioning of data. We envisage that each VO would have one or more VDBs.

Conclusions:
From the existing deployment we learned not to rely upon any single message being transmitted successfully. For the new deployment there will no longer be a central registry and schema service. Instead there will be several registry replicas per VDB. For the schema there will be a replica for each VDB at each site supporting that VDB with one defined as the master schema. The design permits alternative databases to be used. Currently we only support MySQL but Oracle will be added in the future.

Keywords: monitoring, information, message, relational

Further information: http://hepunx.rl.ac.uk/egee/jra1-uk/index.html

80. New developments on the LHCb bookkeeping

Authors: Lanciotti, Elisa (CERN IT); Maier, Andrew (CERN IT); Santinelli, Roberto (CERN IT); Koblitz, Birger (CERN IT)

Short overview:
The LHCb Bookkeeping is the service which aims to keep the data of the LHCb experiment coherently organised. It provides information on the provenance of data and all kinds of metadata to allow for the characterisation of the data. This service is undergoing a restructuring and reorganization to optimise its functionality and to make it suitable for handling the forthcoming data taking. In particular, the functionality which allows users to search for datasets has been replaced with a new client

Analysis:
The Bookkeeping (Bkk) is a crucial component in the LHCb software infrastructure, both for the production, as it registers and uploads to the database all newly produced files, as well as for the data analysis, since it is the tool which allows physicists to retrieve datasets and their metadata. The motivation for this activity on the Bkk arises from requirements of the physicists, who outlined a lack of efficiency of the service. Issues raised include the current user interface, implemented as a web page, is not flexible enough and has broken functionality. Furthermore, the service does not provide exhaustive information on the metadata and returns the output to the user in a rather cumbersome way. The objective now is to provide a new client to allow physicists to search for data and relative metadata in the most flexible and efficient way possible. The new client is implemented in Python, for consistency with the rest of the LHCb software infrastructure

Impact:
The impact of a restructuring of the Bkk is immediate for the physics community of the LHCb experiment since physicists are direct users of this service. The new client of the Bkk will be also implemented in the Ganga framework, easing the way LHCb physicists can construct their analysis jobs and improving the functionality to search for replicated data at different sites

Conclusions:
A new client for the BKK is being developed. The client is implemented as a python module, and includes all the functionality required by the LHCb physicists. The implementation of the module inside Ganga is still ongoing

Keywords: Bookkeeping, LHCb, Metadata Catalog, Data Management, Ganga

81. Communication tools between Grid virtual organisations, middleware deployers and sites

Author: Dimou, Maria (CERN)

Short overview:
Grid Deployment suffers today from the difficulty to reach users and site administrators when a package or a configuration parameter changes. Release notes, twiki pages and news' broadcasts are not efficient enough. The interest of using GGUS as an efficient and effective intra-project communication tool is the message to the user community presented here. The purpose of GGUS is to bring together End Users and Supporters in the Regions where the Grid is deployed and in operation.

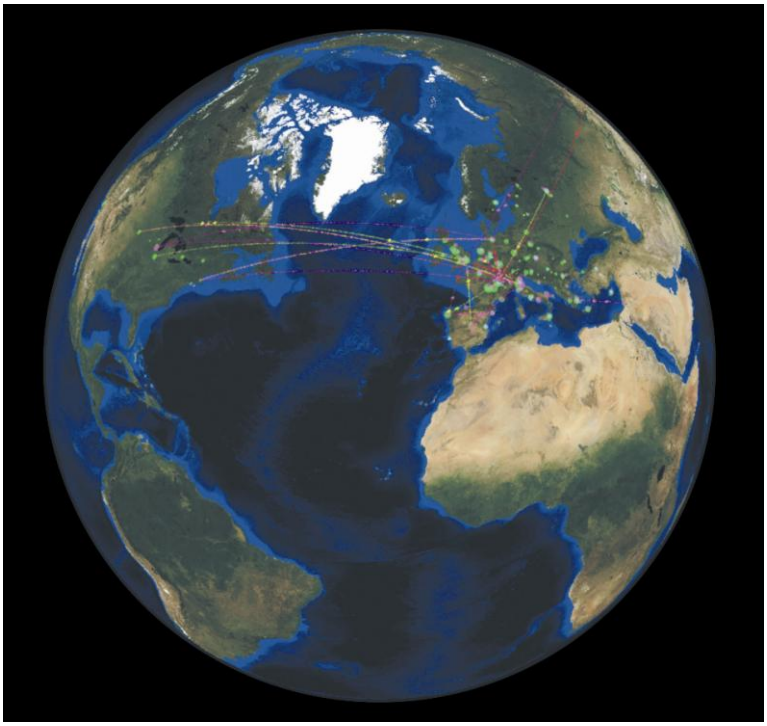
Analysis:
Today's Grid usage is still very far from the simplicity and functionality of the web. While pressing for middleware usability, we try to turn the Global Grid User Support (GGUS) into the central tool for identifying areas in the support environment that need attention. To do this, we exploit GGUS' capacity to expand, by including new Support Units that follow the project's operational structure. Using tailored GGUS database searches we obtain concrete results that prove where we need to improve procedures, Service Level Agreements and deployment methods. These are reliable indicators of the health status of all Grid services. They are also useful to anticipate and plan changes of direction in the required strategy and procedures. It is via regular reporting to the ROCs and the users within the VOs that we show the value of using GGUS. It is also by using user input for GGUS improvement that we try to make this a truly useful tool.

Impact:
The expansion of VOs, sites, users and applications is unavoidable as well as the passage to new middleware releases. This rapidly changing environment leaves holes in the way it tries to pave. Ensuring the necesssary centralised (or coordinated) effort for supporting these candidate areas efficiently, will increase the popularity of the Grid. GGUS contributes in this effort by: offering the users a uniform and simple way to submit problems, using supporters from the Regions on shift as Ticket Process Managers (TPMs) to dispatch problems to the appropriate supporters, addressing all Grid services when a problem is in their area of expertise and responsibility, cross-referencing other web-based tools for monitoring Grid deployment progress, e.g. the savannah trackets for registering bugs and patches, offering documentation links, including FAQs to save supporters' time in reoccurring problems . Publishing escallation reports for the ROCs, TPMs and experts.

Conclusions:
From Grid users to application developers, a whole chain of people who need information and help is often left frustrated. Solid middleware is, of course, the indispensable basis of any successful operation. Nevertheless, the use of GGUS is in the users' interest because, it is the central point of recording 'evidence', so it helps spotting areas for improvement in the products and the processes. This approach proved useful for VOs and should expand further in usage and functionality.

Keywords: Sites, Procedures, Release, Monitoring, GGUS, Global Grid User Support, VO, Virtual Organisation

Further information: http://ggus.org



Workflow and Parallelism

Workflow and Parallelism

Conveners C.Loomis (LAL, Orsay), V.Floros (GRNET, Athens)

Complete scientific analyses are complex, often involving multiple stages and multiple applications. As Grid technology and infrastructure have matured, users find that more and more of the applications making up a full analysis can be run on the Grid. As a consequence, the full analysis workflow becomes a tangible object on the Grid and a prime target for high-level Grid services.

One goal of this session was to provide an overview of job and workflow management tools that can accommodate the scientific analysis workflows. These tools can, for example, manage dependencies between different applications, provide data-driven workflows, and call application- level services "outside" of the Grid infrastructure. Additionally, individual stages of the workflow (or individual jobs) require higher quality-of-service guarantees: for example, low-latency scheduling for pseudo-interactive jobs or multiple CPU reservations for parallel applications.

This session also explored some of these high-level capabilities of the infrastructure and their expected evolution. In summary, the session covered job management capabilities provided by the middleware, the spectrum of quality-of-service guarantees provided by the infrastructure, and concrete example applications to highlight real-world requirement and to focus discussion.

The main outcomes of this session were:

- **Real scientific analyses are typically complex**
  - Multiple codes with data or execution dependencies
  - Large numbers of jobs
  - Branch points within analysis

- **Scientists want their results with short turnarounds**
  - Reduce latencies via optimization, workflow, parallelism
  - Need improved middleware functionality, capturing common patterns
  - Need better understanding of Grid and its use in order to model application on Grid
  - What is the best model for Grid optimization may not easily match the application model

- **Grid technology is maturing**
  - Scientists asking for complete analysis to run on the Grid
  - Asking for differing qualities of service

- Must develop MPI service, including multi-site capabilities
- Follow the use of interactive modeling of workflow as in int.eu.Grid, mixing MPI, agent scheduling
- Want interoperability with different languages, engines
- Variety of workflow engines exist or are in development. Range of complexity. Go for the most simple, and those with proven track record

82. MPI support on the Grid

Author: Dichev, Kiril (High Performance Computing Center Stuttgart)
Co-author: Keller, Rainer (High Performance Computing Center Stuttgart)

Short overview:
MPI-Start is a layer of scripts to support the workload management system in running MPI applications on different clusters with different configurations. Open MPI is an open-source implementation of the MPI 2 standard. PACX-MPI is a library for support of inter-cluster MPI applications. Marmot is a correctness checker for MPI applications.

Analysis:
MPI-Start was developed for the Interactive European Grid project in order to improve MPI support for its infrastructure. MPI-Start supports different MPI implementations (currently Open MPI, MPICH, MPICH2, LAM-MPI). Also, it offers support to different batch systems (currently PBS, SGE, LSF). In addition, support for MPI tools like Marmot is already integrated into MPI-Start. PACX-MPI supports any implementation of the MPI 1.2 standard and delivers the support for seamlessly running one large MPI application on heterogeneous clusters or supercomputers. Marmot can be useful for different MPI correctness checks at runtime like using correct data types, deadlocks etc.

Impact:
MPI-Start greatly improves the MPI support on the Grid. Previous solutions for MPI support required the workload management system to use a hard-coded approach. This approach was not flexible and it also required a complete test and validation of the middleware for configuration changes of MPI/scheduler of a site. Currently, MPI-Start is successfully integrated into the EGEE middleware. Regarding the use of different MPI tools, support for such tools could be integrated into MPI-Start as well, which spares the user from sending additional instructions along with every job. Open MPI is a modern MPI 2 implementation with a component-based design and many features. PACX-MPI can optimally be used when running large-scale MPI applications which do not fit a single cluster.

Conclusions:
MPI-Start will be further used to integrate other MPI oriented tools into the Grid like some tools for performance measurement or debugging. Open MPI is being actively developed. Marmot is currently implementing better support for graphical viewers and fixing bugs.

Keywords: MPI, inter-cluster, scheduler, workload management system, runtime checks

Further information: http://www.open-mpi.org/ http://www.hlrs.de/organization/amt/projects/

83. Towards a statistical model of EGEE load

Authors: Germain-Renaud, Cecile (LRI & LAL/IN2P3, France); Vazquez AZQUEZ, Emmanuel (Supelec); Colling, David (Imperial College London)

Short overview:
The comprehensive monitoring data provided by EGEE makes it possible to analyze from a statistical point of view two characteristics of the activity on the Grid, namely the frequency of the arrivals of the jobs on resources and the load on the computer elements. The results of this analysis are relevant in various areas, such as resource dimensioning, providing differentiated Quality of Service (QoS), middlewarelevel and user-level scheduling.

Analysis:
Preliminary results indicate that EGEE job traffic shares some properties with the Internet traffic: the distributions of the inter-arrival times seem to be heavytailed and the time series of the loads indicate long-range power-law correlations. Precise characterizations are currently investigated on two aspects. a) Marginal distributions. Modeling the distributions at different spatial and temporal scales will provide an insight into the way the flow of jobs is actually dispatched on the resources. Relevant statistical approaches are parametric modeling of the nominal behavior as well as the tail behavior of the distributions, and specifically, extreme value theory. b) Time-dependent structures in the time series. We explore two kinds of well-known stochastic models: Poisson processes, with a possibly non homogeneous or stochastic intensity; and self-similar stochastic models such as fractional Gaussian noises (FGN) and fractional ARIMA processes (ARFIMA).

Impact:
All of the attempts to provide a differentiated QoS to the EGEE user community share two common problems: 1) accurate, complete publishing of the state of the Grid resources and 2) propagation of the scheduling policies implemented on the constituent CEs. Both the state and policy are required by the various scheduling systems at work on the EGEE infrastructure to determine the optimal resource for a particular task. This work addresses the first of these issues. The WMS, and workflow enactors or overlay systems as well, may exploit our results in order to get a more accurate estimation of the expected waiting time at a CE. On the other hand, confirming our initial observations about heavy-tailed distributions and long-range power-law correlations should impact Quality Insurance and Control by proposing concise and meaningful indicators that capture the dynamics of both the collective behavior of users (input flow), and the reaction of the middleware services to these requests.

Conclusions:
The data have been gathered by the GridPP Real Time Monitor. The MATLAB analysis tools will be released through the future Grid Observatory activity, together with updated data from the same source. The statistical characteristics of usage and load will likely undergo significant changes in the near future (LHC activity, communities joining or expanding). The public availability of data and tools will help tracking these evolutions.

Keywords: Job management, Grid Observatory, Statistical Models

84. Grid-aware Optimal data Warehouse design (GROW)

Author: Jakimovski, Boro (University of Sts. Cyril and Methodius)
Co-authors: Velinov, Goran (University of Sts. Cyril and Methodius); Cerepnalkoski, Darko (University of Sts. Cyril and Methodius)

Short overview:
Grid-aware Optimal data Warehouse design uses Gridified genetic algorithm to solve the problem of optimal data warehouse design. The main problem is to select the optimal set of physical objects (Views and Indexes) materialization (VIS) of a data warehouse for a specified database design, considering specified queries and additional parameters. This can significantly increase the performance of any large database. The Grid is used for parallelization of genetic algorithm optimizations.

Analysis:
The application is implemented as a Java framework for executing genetic algorithms in a distributed fashion using a Grid. The framework consists of two parts: genetic algorithm framework and Grid tools. The first part enables researchers to easily implement new optimization problems by simply extending several classes. The second part enables researchers to make their application Grid-aware. In other words it enables easy Grid job submission, job status and output retrieval. The GROW application is a VIS optimization. The chromosomes are bit sequences, each bit representing weather particular view or index is materialized in the database. The chromosomes are evaluated on a set of database queries, where for each query we estimate the time and memory usage for its execution. The parameters for the GA optimization influence both per population GA execution and Grid execution workflow. Some parameters are: mutation and crossover probability, islands, epochs, seasons, migration width.

Impact:
The framework uses the following Java Grid features: WMProxy job submission, VOMS proxy init, DAG (Workflow) execution and LBProxy. Because the framework is implemented in Java, it makes the applications implemented in it portable on all operating systems supporting java 1.5. Also by using Java implementation of the Grid job management functions, the developed applications does not need an installed UI machine. For the Java Grid tools to work the application user needs to have: his certificate in p12 format, CA certificates, VOMS certificates and specification. For the implemented GROW application, the user needs to put the formerly mentioned files in different folders and specify their location in the application properties file. When the application loads, and the user wants to submit a job, he first must generate a VOMS proxy. For this he provides a password for the p12 file, VOMS name and FQAN. After this the other functionalities for the Grid tools are available.

Conclusions:
The porting process was in two phases. The first phase was the implementation of the Genetic algorithm framework. This was mainly to enable researchers reuse the already implemented GA structures. The second phase consisted of implementation of tools for automatic generation of JDL workflows, job submission, job status reporting and job output retrieval. Further development should enable automatic retrieval of CA certificates, VOMS configuration and infrastructure information (BDII).

Keywords: Workflow, Java WMProxy, Java LBProxy, Genetic Algorithms

85. Optimizing a Grid workflow for the EGEE infrastructure: the case of Wien2k

Author: Berger, Maximilian (University of Innsbruck)
Co-author: Fahringer, Thomas (University of Innsbruck)

Short overview:
Wien2K is a package for electronic structure calculation of crystals. After porting Wien2K to the gLite environment we discoverered a severe performance drawback: Scheduling in the real life EGEE infrastructure provides proved to take too long to manage a small workflows efficiently. We have already presented some optimization work through aggregation and will now present other optimization techniques.

Analysis:
In real production Grids the time between submitting a Grid activity and its execution ranges from 10 to 60 minutes. When porting a complex workflow to the Grid, such as Wien2K, this overhead does not only appear once, but repeatedly, and increases the execution time of workflows largely. In our previous presentation we showed aggregation of Grid activities. Since then we have also experimented with other means of reducing overhead through scheduling: Worker nodes may be scheduled without an active task, which they request through a pull model from a coordinator. These workers would be submitted once, and thus the overhead of scheduling them would only appear once. However, this mechanism is unfair towards other users, as it occupies resources for a longer period than one task. We will show results of our experiments, and classify them according to speed and fairness.

Impact:
While similar research has been done for simple parameter studies, complex workflows have not yet been studied at this level of detail. Although the optimization techniques shown here are applied to the Wien2K workflow in particular, they are generic enough to be applied to other complex Grid workflows. The lessons learned from porting the Wien2k application can provide guidance for other future work: Porting other applications should become much easier, as the same patterns can be applied to other work. The Wien2K application is currently used by thousands of scientists: Optimizing the Wien2K worfklow for the Grid would enable these scientists to use the Grid for their calculations, resulting in significantly lower simulation time.

Conclusions:
We plan to continue to optimize and improve our Grid version of Wien2K. During the EGEE III project we plan to work towards the user: Providing a user-friendly interface through the use of a web portal, and providing an "easy" downloadable package, without violating the original Wien2k license. We are also continuesly working on new ideas of workflow improvement.

Keywords: Workflows, Computational Chemistry, Wien2K, Application Porting

Further information: http://www.dps.uibk.ac.at

86. Extension of DIRAC to enable distributed computing using windows resources

Authors: Tsaregorodtsev, Andrei (Centre de Physique des Particules de Marseille); Coles, Jeremy (University of Cambridge); Harrison, Karl (University of Cambridge); Li, Ying Ying (University of Cambridge); Lyutsarev, Vassily (Microsoft Research); Parker, Andy (University of Cambridge)

Short overview:
We give details of the implementation, deployment and testing of a distributed computing system that provides transparent access to both Linux and Windows resources. The system presented is an extension of the DIRAC Workload and Data Management System, developed in the context of the LHCb experiment, and used successfully with Linux machines for several years. We have added the possibility to also use Windows resources, significantly increasing the experiment's dataprocessing capabilities.

Analysis:
The LHCb experiment, designed for high-precision studies of matter-antimatter asymmetries in the decays of b-hadrons, is one of the four main experiments at the CERN Large Hardon Collider (LHC). DIRAC has been developed to meet the experiment's need for processing petabytes of data per year, using globally distributed resources. It can be used either as a standalone Grid implementation, or as an optimisation layer on top of another system, such as the EGEE Grid, and has performed impressively in data challenges held since 2002. Although mostly written in Python, which is largely platform-independent, various features of the implementation have previously limited use of DIRAC to Linux machines. We have extended DIRAC to allow its use also on Windows platforms, making the core code more generic in a number of places, integrating Windows-specific solutions for certificate-based authentication and secure file transfers, and enabling interaction with Microsoft Windows Compute Clusters.

Impact:
An initial, small-scale deployment of the new system allows jobs submitted through DIRAC to be run on 100+ Windows CPUs, distributed between the Universities of Bristol, Cambridge and Oxford, and allows jobs to be submitted from Windows machines to run at the 120+ sites with Linux nodes made available through DIRAC. We have tested the different submission paths, and have successfully used the distributed Windows resources to optimise selection criteria for one of the b-hadron decay channels of interest in LHCb. Some sites are able to offer dedicated Windows clusters, not previously accessible through Grid systems, and others have large numbers of Windows machines that may be idle at certain periods, for example in teaching laboratories. The Windows-enabled version of DIRAC allows these resources to be added to existing Grid-based Linux resources, under a single workload management system, increasing data-processing capabilities by a significant factor.

Conclusions:
The DIRAC system continues to evolve, and we are helping ensure that newer releases are portable across platforms. We plan to deploy DIRAC at more sites with Windows machines available, and in particular aim to demonstrate the gains that are possible by using non-dedicated resources. Tests so far under Windows have involved running only a single application per job, and as a next step we will be running chained applications, covering simulation, digitisation and reconstruction.

Keywords: Workload and Data Management, Distributed Windows Resources, Cross-platform Job Submission

87. Interactive workflow management in int.eu.Grid

Authors: Simo, Branislav (Institute of Informatics, Slovak Acedmy of Sciences); Mr. Habala, Ondrej (Institute of Informatics, Slovak Acedmy of Sciences); Hluchy, Ladislav (Institute of Informatics, Slovak Acedmy of Sciences)

Short overview:
The Grid service in development allows users to manage interactively and comfortably complex jobs composed of multiple program executions. It is a modification of a system developed previously in the project K-Wf Grid as a management tool for application composed of web and Grid services. The system uses the interactive channel of the Int.eu.Grid project architecture to forward commands from a GUI to the on-site workflow manager to control the job during execution.

Analysis:
Grid computing is a useful tool for complex scientific applications, enabling their execution over a large pool of resources. Many of the deployed applications are a complex workflow composed of many smaller parts. However, most of these applications appear to their users as a monolithic black box, usually driven by a complicated and finely tuned shell script. Once the job starts executing, the user has no finer control over it than being able to abort it or to wait until it finishes. The described tool is able to visualize the inner workflow of the application. The user can completely control the job during execution, can see partial results, and can even alter it while it is still running. This allows not only to associate the produced data to the job workflow, to extend it, or to shorten it, but also to interactively debug and tune the job—something that would otherwise be possible only for a domain expert, and would be more time-consuming.

Impact:
The tool is suitable for applications for which the user may want to adapt their execution during runtime using to partial results. Instead of repeatedly trying to run, tune, debug, and change a master script of the application, the user can modify the application workflow at runtime. If the need arises, another analysis to process any interesting partial results that were computed may be added. Or, if a simulation provides uninteresting data, the rest of the workflow subtree may be cancelled, and resources shifted to other parts of the job. Any application that currently uses a shell script calling several components (binary modules or other scripts) can be easily converted to a visually controlled workflow. The workflow can then be saved, exported to an XML file, and later reused. Such reuse is very simple even for nonexperts.

Conclusions:
This tool for interactive workflow management of complex jobs is under development within the Int.eu.Grid project. It is able to visualize a workflow of application components, to change the workflow during its execution, to display partial data results, and to store and later reuse any workflow, at any stage of execution. In the future, it will be extended with additional capabilities—containers for workflow steps—that will enable closer integration with other Grid tools.

Keywords: workflow management, semantic annotation, GUI, interactivity

Further information: http://www.interactive-Grid.eu/

88. The gLite workload management system

Author: Giacomini, Francesco (INFN)
Co-authors: Cecchi, Marco (INFN) ; Ghiselli, Antonia (INFN); Gianelle, Alessio (INFN); Guarise, Andrea (INFN); Maraschini, Alessandro (Elsag Datamat); Monforte, Salvatore (INFN); Perini, Laura (INFN); Sgaravatto, Massimo (INFN)

Short overview:
The gLite Workload Management System has been designed and developed with the ambition to represent the main access point to the computing resources made available on a Grid. The goal is to provide a reliable, effective and efficient service responsible for the distribution and management of computational jobs, hiding the intrinsic complexity of the infrastructure to its users. The abstraction provided by the WMS is generic enough to support applications coming from largely different domains.

Analysis:
The WMS accepts requests concerning the execution of a computation, whose description is expressed in a flexible language, based on Condor ClassAds, as a set of key - value pairs. The WMS is then responsible to translate the logical description to concrete operations, in order to bring the execution of a job to a successful end. Several types of jobs are supported: simple, intra-cluster MPI, interactive, collections, parametrics, simple workflows in the form of DAGs, with on-going development of a generic workflow engine. Additional benefits concern sandbox management, with support for multiple transfer protocols, data-driven match-making, the availability of multiple mechanisms of error prevention and management, isolation from the heterogeneity of the infrastructure, the capability to implement optimizations based on non-local information, such as bulk submission and matchmaking. The progress of the job is safely recorded into the complementary Logging and Bookkeeping Service.
Impact:
Managing a job, from submission to completion, usually involves the interaction with several other services: computing elements, storage elements, information systems, data catalogs, authorization, policy and accounting frameworks, credential renewal. Unfortunately their convergence towards standard solutions has not shown fast progress in the past, with the consequence that multiple implementations with different interfaces are available on the same infrastructure. The complexity that stems from this situation is also a major cause of errors. An important goal of the WMS is then to hide as much as possible to end users both the heterogeneity of infrastructure components and the occurence of non-fatal errors, without sacrificing generality and performance during request processing. In order to ease the integration with higher-level middleware and application frameworks, the WMS itself exposes a Web Service interface compliant with the WS-I specification.

Conclusions:
The WMS has been deployed in a number of different multi-user and multi-VO scenarios, thanks to the neutrality of its design. The recent introduction of features like the bulk match-making has shown that it can cope with sustained high loads. When used in demanding production environments it has nevertheless shown some limits in terms of stability and usability. With the experience gained in the past years, parts of the WMS are now being revised in order to fully comply with the expectations.

Keywords: Workload Management, interoperability, integration, abstraction, error management

Further information: http://egee-jra1-wm.mi.infn.it/egee-jra1-wm/

89. Execution time prediction of imperative paradigm tasks for Grid scheduling optimization

Authors: Lim, Mei Kuan (Mimos Berhad); Yap, Yee Jiun (Mimos Berhad)
Co-authors: Kiran, Maleeha (Mimos Berhad); Lai, Weng Kin (Mimos Berhad)

Short overview:
An efficient functioning of a complicated Grid environment requires a resource manager to monitor the idling resources and to schedule users' submitted jobs accordingly. However, at present, the execution time prediction depends mostly on pure guesswork. The inaccuracy of guesswork leads to inefficient resource usage, incurring extra operation costs. Thus, we propose a job execution time prediction module that estimates the execution time of jobs to optimize the scheduling system in the Grid.

Analysis:
The proposed system is intended to be implemented in the KnowledgeGrid Malaysia to improve the efficiency of the scheduling system. The work is focused on imperative paradigm tasks since they are commonly used in the aforementioned Grid. Imperative paradigm refers to a sequence of commands for the computer to perform and the normally used imperative paradigm programming languages are R!, Fortran and C. In the current phase, all testing and evaluation is done via a web-based wrapper which is developed specially for this purpose. The testing and evaluation involves test cases ampled from jobs submitted to the aforesaid Grid.

Impact:
We proposed a novel methodology and architecture to predict the execution time of jobs. In this phase, the proposed prediction module works as a standalone system which would estimates the execution time of jobs to assist scheduling in existing middleware used in the Grid. A mathematical model and benchmarked data are used to forecast the time required to execute jobs. An incoming job is categorized according to its application, and is then parsed and broken down into smaller units known as tokens. The complexity and relationship amongst these tokens are then analyzed. The execution times for the tokens are then combined to give an estimate of the execution time of the entire job. An accurate estimation of jobs' execution time in advance allows allocation of resources into appropriate queues, which eventually leads to effective scheduling. Also, a mathematical model has been developed for the purpose of comparing the theoretical optimized scheduling system with that of the actual Grid.

Conclusions:
The experimental results from the sampled test cases and developed prototype show that the technique is successful in achieving an accuracy of greater than 80%. As this work focuses on imperative paradigm programming, perhaps future work may suitably involve other paradigms such as object-oriented and data-intensive programming. Also, further research may look into integrating the prediction module into the real Grid environment instead of a standalone, web-based system.

Keywords: Prediction module, Grid scheduling, Job execution time, Grid queue length distribution

90. Parallel execution of chemical software on EGEE Grid

Author: Sterzel, Mariusz (CERN)

Short overview:
Constant interest among chemical community to study larger and larger molecules forces the parallelization of existing computational methods in chemistry and development of new ones. These are main reasons of frequent port updates and requests from the community for the Grid ports of new packages to satisfy their computational demands. Unfortunately some parallelization schemes used by chemical packages cannot be directly used in Grid environment. Here we present a solution for Gaussian package.

Analysis:
The current state of development of Grid middleware allows easy parallel execution in case of software using any of MPI flavour. Unfortunately many chemical packages do not use MPI for parallelization therefore special treatment is needed. Gaussian can be executed in parallel on SMP architecture or via Linda. These require reservation of certain number of processors/cores on a given WN and the equal number of processors/cores on each WN, respectively. The current implementation of EGEE middleware does not offer such functionality therefore the only solution is to enforce required configuration via Maui scheduler. The solution we present does not require Linda for parallel execution. It allows utilization of maximum number processors/cores on a given WN. Taking in to consideration the WNs supporting Gaussian VO parallel execution on maximum 8 processors/cores is possible. The main disadvantage of our solution is necessity of local Maui configuration on each site by an administrator.

Impact:
The port of parallel version of Gaussian packages on the Grid has been shown as a next step towards better Grid utilization and better community satisfaction. As the simplicity of the usage of the parallel version of the software on EGEE Grid remains unchanged we expect a quick switch to the usage of the parallel version of the software not only in case of Gaussian but also for other packages like NAMD, GAMESS or Turbomole for which parallel versions have been ported to the Grid recently. It is also important to note that our solution may serve as a prototype for other difficult cases where there is no direct support for specific parallel execution model by the middleware.

Conclusions:
The Grid port of the parallel version of Gaussian package has been developed to fulfil community needs especially for large molecular system studies as easy for use as the serial version was in the past. At the same time we have demonstrated the possibility of execution of parallel versions of chemical software on the Grid even if the middleware does not support the parallelization model directly. Our future work will focus on other parallel versions of packages as required by the community.

Keywords: parallel execution, commercial software, license issues

Further information: http://egee.Grid.cyfronet.pl/gaussian

91. Non-parametric parallel Grid Harris-affine detector

Author: Bellavia, Fabio (Univ. Palermo)
Co-authors: Valenti, cesare (Univ. Palermo); TEGOLO, domenico (Univ. Palermo)

Short overview:
A new nonparametric Harris-affine detector is introduced here. This is an image processing algorithm for extracting a particular kind of image features. The new proposed implementation automatically tries to select best features with respect to local-to-global image properties in a scale-space domain. An unusual parallel Grid implementation has been developed to avoid unbalanced computational workload distribution among different processors.

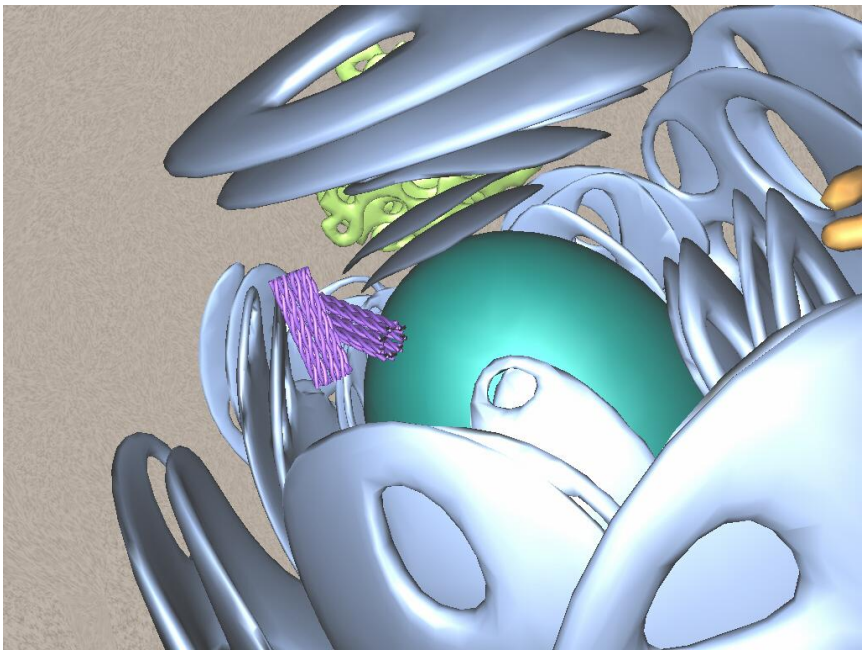
Analysis:
Because most-wanted of image analysis applications as three-dimensional reconstruction, mosaicing, object recognition and classification can rely on feature detection methodology as a primary stage, it can be used to satisfy many requests of these items and more in general in the field of computer vision. Feature descriptors can be applied to identify similar regions on different images; it is clear that some characteristics have to be owned of good descriptors. One of the most appropriate questions in match methodology regards which detector has to be used to characterize the region of interest. They can be classified as global or local, some of them are characterized by global information and other is modeled on local values. In this contribution, based on local information, a detector will be used. It rejects the same model of the parametric Harris Affine detector with the peculiarity to have no parameters and to be focussed on the each sections of the image.

Impact:
The proposed algorithm consists of the following steps: image enhancement and feature mask computation by using z-scored local windows, simple Harris-corner extraction and selection, and refinement of the final result by an iterative procedure computed on every feature without computational approximation. The algorithm uses statistical filters with a variety of kernel, which cause a bottleneck on a serial implementation. Right now, our application has been developed under MPI paradigm and a corresponding porting for PI2S2-Grid is under construction and we foresee that the final Grid version will be tested by a couple of weeks. The system will use the support of Genius for dissemination on a naïve scientific community and also to display the results of large data. Given the latency of standard network we assume a improving of the performance with the use of Infiniband network. The efficiency of our MPI methodology has been test on a set of images and it has been evaluated about 80%.

Conclusions:
Good results have been obtained considering that for some sections the parallelism degree is bounded by the numbers of used scales and also the bottleneck of very heterogeneous data. From a technical point of view, our application needs an useful installation of FFT library; such installation has been inquired to the PI2S2- Grid technical team, and it will be running by the next few days. We will discuss the resource required for it, the performance and its scalability on Grid paradigm.

Keywords: parallel image analysis, MPI feature detector, scale-space theory, no-parameters algorithms, Genius

DEMONSTRATIONS



Demonstrations

The 19 practical demonstrations were a highlight of the event. The demo session provided the ideal place for live performances showcasing mature scientific work and Grid tools. It gave a great opportunity for scientific teams to present their results and interactively discuss the finer details and potentially build bridges for collaboration and further interaction with the participants. The work presented spanned all scientific disciplines and appropriately complement the relevant oral sessions.

There was a very high quality of demonstrations, which were all evaluated by the EGEE EAC (External Advisory Committee). There was thus a very lively competition for the 'best demo prize', resulting in 5 runners-up awards in addition to the overall winner. The awards were as follows:

Best Demo

'The Health-e-Child (HeC) Gateway and Case Reasoner, a Concrete Implementation and Use-Case of a gLite-based HealthGrid for European Paediatrics'

Manset, David (MAAT GKnowledge) Huber, Martin (SIEMENS AG)

- Genuine Grid project
- Perfect example of cooperative/collaborative application
- Data distribution by nature
- Validation of gLite middleware in a production environment
- Follows the Service Oriented Architecture paradigm
- Successfully deals with all non-functional requirements: security, performance, fault tolerance
- High social impact
- Keeping close touch with the industry

Runners Up

'WISDOM'

Salzemann, Jean (IN2P3/CNRS), Bloch, Vincent (IN2P3/CNRS), Kasam, Vinod (SCAI Fraunhofer)

'A Telemedicine platform for information and image management on the Grid'

Diarena, Matteo (CNRS IN2P3 LPC Clermont-Ferrand), Nowak, Simon (CNRS IN2P3 LPC Clermont-Ferrand)

'GRelC DAIS: Towards Data Access and P2P Data Integration in gLite based Production Grid

Fiore, Sandro (SPACI Consortium & University of Salento), Aloisio, Giovanni (SPACI Consortium & University of Salento), Barbera, Roberto (INFN Catania)

'fMRI analysis on EGEE with the VBrowser and MOTEUR'

De Boer, Piter (Institute of Informatics, University of Amsterdam,) Olabarriaga, Silvia (Institute of Informatics / Academic Medical Center, UvA), Glatard, Tristan (Institute of Informatics / Academic Medical Center, UvA), Boulebiar, Kamel (Institute of Informatics / Academic Medical Center, UvA)

‘**Design, implement and deploy Grid oriented applications in a cooperative way: a biomedical use case’**

Porro, Ivan (University of Genoa), Scifo, Salvatore (COMETA Consortium)

92. WISDOM

Author: Salzemann, Jean (IN2P3/CNRS)
Co-authors: Bloch, Vincent (IN2P3/CNRS); Kasam, Vinod (SCAI Fraunhofer)

Short overview:
During 2005, 2006 and 2007 four biomedical data challenges were run on the EGEE Grid: two on malaria and two on avian flu. These deployments, based on relevant biological needs, were successfully achieved using most of the available resources on the Biomed virtual organisation. As a total, almost 700 years of computations were achieved during these 4 deployments using the WISDOM production environment and some in vitro tests have been already started with really interesting results.

Analysis:
The environment evolved throughout the development: It was first made of a set of scripts that generate the jobs, submit the files and check regularly their status while they are on the Grid. Through this abstract we want to present the new environment that is based on the AMGA metadata catalog for more flexibility and on a Java environment that can be used through web services. The environment is very flexible and can be used for any type of bioinformatics application. In this new environment we control the job distribution, maintaing the choice of directly submitting the executable (push mode) or implementing a two-way submission where the system submits generic wrapper jobs which request their paylod (the executable and the input data) only when they start to be executed (pull mode).

Impact:
With WISDOM we wanted to create a robust framework to allow biologists to integrate their software with and run it on EGEE. The system was designed to deploy high throughput experiments on the Grid, and is being reengineered to offer a fully interoperable web services interface, with connections to databases to store and query, in quasi-real-time, the statistics and results. One of the major added values of this new architecture is that the whole system can be easily integrated in workflow engines that just call the ad-hoc operations. The developments were focused on fault-tolerance, flexibility and scalability but several issues arose during the experiments. The relatively slow information system refresh rate can also cause outdated ranking when the job submission rates are high, this is the reason why we decided to introduce an internal rank system to address these information system issues.

Conclusions:
As a matter of fact, the environment has proved many times that it is adapted to run hi-throughput docking experiments on the Grid. During the last deployment we successfully managed up to 70000 jobs producing almost 2TB during 10 weeks corresponding to more than 400 cpu years on a single computer. The next challenge will be to integrate WISDOM in whole workflows to apply to other bioinformatics activities.

Keywords: Drug-Discovery, Large scale deployment, Bioinformatics

93. Interactive European Grid: advanced applications support demo

Authors: Campos Plasencia, Isabel (Instituto de Fisica de Cantabria CSIC); Hardt, Marcus (Forschungszentrum Karlsruhe); Plociennik, Marcin (Poznan Supercomputing and Networking Center); Garcia, Lino (CESGA)

Short overview:
The purpose of the demonstration is to show the capabilities of the int.eu.Grid middleware and services deployed on top of glite. We have prepared an I2G on-line Demo Package, consisting of a set of applications targeting different research areas: Physics, Environment and Medical Science.

Analysis:
The package includes an enhanced version of fusion application that won the last User Forum Best Demo award in Manchester. In environmental sciences we will show the integration of an open source Geographical Information Systems on the Grid, GRASS, which is used for environmental analysis of water in reservoirs. Also in the environment sector we will show the application to analyze the evolution of pollution clouds. In medical science we will show how to optimize radiotherapy plans by computing the amount of radiation absorbed by the human body organs in cancer treatments. The total computing time goes down from a few days to few minutes when MPI job submission to several sites is used. In particular we will show the submission of MPI jobs distributed between different clusters using PACX-MPI. A second application of the field of medical science will be shown. It presents a prototype of running Matlab Applications for Ultrasound Computer Tomography (USCT) on interactive Grids.

Impact:
The purpose of the demonstration is to show to the researchers that the Grid can be used as an everyday working tool also for advanced applications, meaning MPI parallel applications or those requiring from graphical or interactive capabilities, and in general, going beyond the serial batch job submission supported already by glite middleware.

Conclusions:
This demonstration and the oral presentation we have submitted will help us to stablish a discussion framework with the users present in the meeting. The idea is to have a well defined document for what are the requirements for Quality of Service from the user point of view. We will translate the results of our discussions into the exploitation path of the project.

Keywords: Generic applications; visualization on the Grid; MPI applications

94. The Health-e-Child (HeC) gateway and case reasoner, a concrete implementation and use-case of a gLite-based healthGrid for European paediatrics

Authors: Manset, David (MAAT GKnowledge); Huber, Martin (SIEMENS AG)

Short overview:
HeC aims to integrate and exploit heterogeneous biomedical information for improved clinical practice, medical research and personalized healthcare. It brings together 3 major paediatric medical centres with several European institutions specialized in Grid biomedical technologies. Aiming at turning the healthGrid vision into reality, it is developing a platform that can federate distributed data sources over the Grid, where the Grid also serves as a technological glue and collaboration facilitat

Analysis:
The HeC prototype is the result of 2 years of active R'nD, which has matured inside a private Grid infrastructure. Amongst the 1st contributions, a security prototype was delivered as well as innovative domain specific client applications. Through a userfriendly singe sign-on, clinicians access resources independently of their geographical location and connectivity.It allows them to enter, from within their hospital, the large Grid spread over Europe to store anonymously patient records and further manipulate these. Medical images are processed, stored in the Grid and referenced within the integrated case database. The system enables clinicians to look for similar patients and further process corresponding images, e.g. to extract 3D and 4D models of the heart, useful for better making decisions over particular cases. In cardiology, a 4D-mesh representing the right ventricle is computed and stored in the Grid, from which various clinically relevant parameters can be further derived.

Impact:
The HeC project uses the gLite Grid middleware. As it is used and functionallyaugmented through the Gateway, it can be compared to a distributed Picture Archiving and Communication System (PACS), with additional capabilities such as medical image processing, patient similarity search as well as a distributed database management system for structuring and federating multi-centre data. The Grid technology makes use of the shared medical centres' computing resources to solve clinicians' requests and is made available through the so-called Gateway installed at each institution. HeC therefore makes use of most of the gLite Grid middleware services since it runs its own private Grid infrastructure. The middleware core services such as tBDii, LFC, VOMS, WMSLB have been deployed and a proper VO created. Every site is featured with a common set of gLite site services ranging from CE, to SE, to WN. The Gateway materialises under the form of a SOA.

Conclusions:
From intensive prototyping efforts, HeC has started materializing in several concrete outcomes. It has demonstrated at the hospital Necker in Paris, its first prototype of the Gateway and gLite-based Grid infrastructure. The proposed demo illustrates the successful port of similarity search and Grid-based feature extraction over different data sources ranging from clinical records to medical images. It also introduces a framework for simplifying Gridification of complex applications.

Keywords: HealthGrid, Gridification, distributed data, security, privacy, image processing, data mining

Further information: www.health-e-child.org

95. The EGEE user support infrastructure

Author: Antoni, Torsten (GGUS, Institut für WissenschaftlichesI Rechnen, Forschngszentrum Karlsruhe)
Co-authors: Mills, Alistair (CERN)

Short overview:
Grid user support is a challenging task due to the distributed nature of the Grid. The variety of users and Virtual Organisations adds further to the challenge. Support requests come from Grid beginners, from users with specific applications, from site administrators, or from Grid monitoring operators. With the GGUS infrastructure, EGEE provides a portal where users can find support in their daily use of the Grid. The current use of the system shows that the goal has been achieved with success.

Analysis:
The Grid user support model in EGEE can be captioned "regional support with central coordination". This model is realised through a support process which is clearly defined and involves all the parties that are needed to run a project-wide support service. This process is sustained by a help desk system which consists of a central platform integrated with several satellite systems belonging to the Regional Operations Centres (ROCs) and the Virtual Organisations (VOs). The central system (Global Grid User Support, GGUS) interconnects the ROCs and VOs and the other project wide groups like middleware, network, and service groups. Additionally the central system acts as a portal for users, offering the possibility to document problems and requests in the form of trouble tickets. Since all trouble tickets pass through the GGUS system it is the perfect place to store information on problems and of course also their solution in a knowledge base, available to users and support staff.

Impact:
A well established and functional user support service permeates the whole EGEE project and it is one of the core non-middleware services and as such one of the key success factors in running a production quality infrastructure. Over the course of the series of EGEE projects the GGUS system and the management of the support process has been professionalised by applying proper change and process management strategies. The GGUS system is being improved through a series of regular new releases, which are well planned and documented including release notes. A coordinating body involving all relevant parties meets regularly to plan the future strategy. Applying these processes, the GGUS system has been constantly improved and its acceptance throughout the project has constantly increased. With this presentation of the GGUS system at the User Forum, we aim at a better understanding of the importance of a proper support infrastructure and show the major achievements of EGEE in this area.

Conclusions:
At the end of 2007 a major release of the GGUS portal took place. Included in this release were several new features whose implementation included modifications of the interfaces of the regional help desks. A new search engine which performs semantic searches of the ticket data base and several other data sources will improve the search results will be available by the time of the User Forum. We want to present to the audience the new as well as the established features.

Keywords: User support, operations support, help desk

Further information: www.ggus.org

96. Fusion demonstration: ion kinetic transport and stellarator optimization

Authors: Castejon, Francisco (CIEMAT); Voznesenskyi, Vladimir (Inst. of Information Systems, RRC "Kurchatov Inst.")

Short overview:
Grid computing has demonstrated to be very useful for a kind of special application that is customary within the fusion community. A stellarator optimisation application has demonstrated the efficiency and the ability of the EGEE Grid to meet the demands of such computations. The Ion Kinetic Transport application has opened new lines of research and has shown the limitations of some customary approximations that have been developed in Fusion research.

Analysis:
Two representative fusion applications have been chosen to show the power of Grid computing for this community. The first is the Grid-based stellarator optimization, run in the RDIG VO; the second is Ion Kinetic Transport, which is running in the fusion VO.
Both applications have been successfully ported from a supercomputer to the EGEE infrastructure. The porting of the first implied the use of mathematical methods that allow asynchronous completion of parallel jobs without loss of efficiency, implying a shift from iterative (gradient-based) methods to results-based, spool-driven (genetic, stochastic interpolation) ones, together with tools for applicationspecific job and data management. The second application was tailored to run in this kind of architecture. In its first version, all the jobs are serial and the huge amount of information needed for every job is sent to the catalogue. In its second phase, an iterative method is developed.

Impact:
A Grid portal prototype, Grid InterFace (GIF), is presented, which is designed to be a complete solution for the Stellarator optimisation application. A Python script that generates several calculations of the target function was created. Another script is spawned after every job completion. It adds the calculated function value and gives the current best genome to the user, selects the parents from the pool to breed and generates a new job to spawn. The Ion Kinetic Transport application is based on a script that launches the number of needed jobs, composed of the calculation of 1000 trajectories in the plasma. Then the trajectories are analysed and used to update the plasma background. A new set of jobs is launched by the script according to this background and so on, until the calculation converges (about 30 iterations are needed). Finally the transport properties of the device are obtained without any approximation.

Conclusions:
Stellarator optimization applications in fusion science need a special applicationdriven, non-predictable workflow manager not fullfilled by existing middleware. The authors present a prototype that serves as an interface and a driver environment for such application. Ion Kinetic Transport application, suited to run in the Grid infrastructure, produces novel scientific results and avoids the customary approximations that are used to solve the 5D kinetic fusion equation.

Keywords: Fusion, Non-predictable workflow, Grid portal, optimisation, workflow, stellarator, Kinetic Theory

Further information:
http://vo.nfi.kiae.ru/pmwiki/pmwiki.php?n=Main.StellaratorOptimization
http://www-fusion.ciemat.es

97. Utilization of EGEE Grid as a computational platform for chemistry

Author: Sterzerl (ACC CYFRONET AGH)
Co-authors: A.Lagana and O.Gervasi (University of Perugia); J.Kmunicek (CESNET); M.Berger (University of Innsbruck)

Short overview:
The current focus of computational chemistry far exceeds the traditional interest of studying properties of small molecules. Fast development of new materials like polymers or drugs not only requires numerous applications of computational chemistry methods to study their properties but also helps to design new materials with desired properties. Such simulations demand however, huge computational resources. Thus a Grid platform can be seen as one of the answers to these demands.

Analysis:
A huge amount of work has been devoted to satisfy chemical community requirements on the Grid. The activity of CompChem, Gaussian and VOCE VOs has been mainly focussed on the Grid ports of chemical software packages and on the development of Grid tools that simplify job manipulation and workflows, automating complex data management tasks. The ports targeted commercial software packages like Gaussian, Turbomole or Wien2k, in particular as the community is highly accustomed them. The main difficulty concerned licenses for which Grid solutions had to be developed. In parallel, Grid ports of other packages for ab initio, molecular dynamics and quantum dynamics (including time) has been developed mainly for the GEMS project. The development in job management resulted in the Charon Extension Layer, the latest version of which allows easy job manipulation via a web browser. Workflows are mainly available to the Wien2k and GEMS communities to solve their complex data submission issues.

Impact:
The availability of variety of above mentioned software packages on the Grid resulted in their application to many areas of computational chemistry including chemical reactions studies like N+N_2 or Cl+CH_4 with help of very accurate ab initio and quantum dynamics methods, modelling of catalytic centres and possible reaction paths to understand the way active centre interacts with substrates and products, analysis of ions flowing through a carbon nanotube to later apply similar models for ions transfer through molecular membranes or attempts of charge transfer modelling between carotenoids and chlorophyll during photosynthesis process. The EGEE Grid utilization by these applications places computational chemistry in third position just after HEP and life sciences. Also, it is worth noting that other communities like solid state physics, pharmacy or climate are interested in usage of chemical packages.

Conclusions:
The chemical software ports, easy job handling systems and use of workflows to manage complex data resulted in numerous applications ported to the Grid infrastructure. We have also enabled chemical software for other communities and we are working now to make software ported by these communities available for chemists. Our future work will include further development of Grid license models and web portal with software plug-ins to enable the Grid platform for non-expert users.

Keywords: computational chemistry, license issues, commercial software, software porting

Further information: http://compchem.unipg.it;
http://egee.cesnet.cz/en/voce; http://egee.Grid.cyfronet.pl/gaussian.

98. GANGA - powerful job submission and management tool

Authors: Maier, Andrew (CERN IT); Lee, Hurng-Chun (CERN IT); Mendez Lorenzo, Patricia (CERN IT); Moscicki, Jakub (CERN IT); Lamanna, Massimo (CERN IT); Muraru, Adrian (CERN IT)

Short overview:
The computational and storage capability of the Grid are attracting several research communities, also beyond HEP. Ganga is a lightweight Grid job management tool developed at CERN. It is a key component in the distributed Data Analysis for ATLAS and LHCb. Ganga`s open and general framework allows to plug-in applications, which has attracted users from other domains outside HEP. In addition, Ganga interfaces to a variety of Grid and non-Grid backends using the same, simple end-user interface

Analysis:
Ganga has already gained widespread use, the incomplete list of applications using Ganga include: Imaging processing and classification (developed by Cambridge Ontology Ltd.), Theoretical physics (Lattice QCD, Feynman-loop evaluation), Bio-informatics (Avian Flu Data Challenge), Geant4 (Monte Carlo package), HEP data analysis (ATLAS, LHCb). All these communities have different goals and requirements and the main challenge is the creation of a standard and general software infrastructure for the immersion of these communities onto the Grid. This general infrastructure is effectively "shielding" the applications from the details of the Grid. Finally, it is flexible and general enough to match the requirements of the different productions without including mayor changes in the design of the tool. Ganga supports a large number of backends without the underlying knowledge of each one: EGEE gLite and NorduGrid ARC middlewares, Condor and Cronus (Condor/G), various batch systems, etc

Impact:
From January to end of 2007 Ganga has been used by around 1000 users and has been installed locally in more than 50 sites around the world. Recently also the educative aspect of Ganga has been recognized and Ganga has become a part of the official EGEE tutorials. Contrary to other portals or tools, Ganga is not limited to specific VOs or infrastructures allowing new users to quickly exploit the EGEE infrastructure. It also allows for the interoperability of various Grid backends.

Conclusions:
Ganga has demonstrated to be a powerful job submission tool able to allow a fast merge of any new community onto the Grid. Its value has been demonstrated also by HEP communities that have adopted Ganga as the submission tool for their productions. In the new phase of the EGEE project the fast immersion of new communities will continue being a central goal and we will continue working for the confirmation of Ganga as the Gridification tool for new communities.

Keywords: job submission, job management, user interface, interoperability, applications

99. GRelC DAIS: towards data access and P2P data integration in gLite based production Grids

Authors: S.Fiore, G. Aloisio (SPACI Consortium & University of Salento); R.Barbera (INFN Catania)
Co-authors: S.Vadacca (CMCC); A.Negro (ISUFI Settore Nanoscienze e Grid Computing); M.Cafaro (SPACI Consortium & Univ. of Salento); E.Giorgio, (INFN Catania)

Short overview:
The GRelC Data Access and Integration Service (GRelC DAIS) aims at transparently and securely integrating heterogeneous, distributed and geographically spread Grid data sources (through P2P connected GRelC DAIS nodes) decoupling routing aspects from data access and so defining a very general and robust Grid data integration architecture. It is WS-I based, GSI and VOMS enabled, compatible with Globus and gLite Grid middleware/environments, and it represents the evolution of the GRelC DAS.

Analysis:
Decoupling routing aspects from data access, the GRelC DAIS can be used in several data integration scenarios. Some examples are: integration of information stored within several distributed metadata DBs for Earth Science to perform queries across distributed collections described by a common metadata model; distributed queries on accounting services deployed at several sites (e.g. APEL or DGAS within EGEE) to infer “global reports” on the Grid infrastructure usage (ordered list - per job, cputime, etc. - of VOs/GridUsers which are mostly using the Grid). The architecture is very modular, query language independent and easily extensible, so the integration can be related to a set of XML DBs (using XPath), distributed Relational DBs (using SQL), distributed BDII (using LDAP), distributed flat files (using GFAL libraries), distributed Monitoring of the GRelC DAIS P2P Network (retrieving a KML files for client-side Google-Earth based visualization), etc.

Impact:
The GRelC DAIS service is the extended and improved evolution of the GRelC DAS, it allows managing Grid databases (relational, XML, flat-files) containing data/metadata carrying out data access and integration activities. gLite does not provide services so widely addressing these issues even though accounting, monitoring, database access and integration is really important for end-users/VO (astrophysics, bioinformatics, ES community, etc.). Supporting GSI/VOMS security model for authentication and authorization, this service can be naturally integrated within the gLite farm model together with CE and SE. Moreover, the GRelC DAIS provides Glue Schema extensions for the BDII to ease database discovery and publishing. Client side can be part of the UI (i.e. GILDA UI). For end-users the GRelC DAIS Portal allows managing and querying via web distributed data sources (very easy and attractive for end users). Submission through broker is also supported and SLC3 & SLC4 releases are available.

Conclusions:
The GRelC DAIS is very versatile so it can be used both at VO and site level. It can/was used in both ways depending on VO/user/database constraints and requirements. There is no single point of failure and no centralized management for this service due to the scalable P2P architecture. This service is currently successfully deployed and positively evaluated by end-users and sysadmins on the GILDA t-Infrastructure. It is part of the GILDA release and will be included within the INFNGRID release.
Keywords: Grid Data Management service, Data Access and Integration Service, P2P Architecture, GRelC Portal

Further information: www.grelc.unile.it https://Grid.ct.infn.it/twiki/bin/view/GILDA/GRelCPortal

100. fMRI analysis on EGEE with the VBrowser and MOTEUR

Authors: De Boer, Piter; Olabarriaga, Silvia; Glatard, Trista; Boulebiar, Kamel (Institute of Informatics/ Academic Medical Center, University of Amsterdam)

Short overview:
The application aims at analyzing fMRI data to compute brain activation maps. Such an analysis is well-known for healthy subjects but performing it on pathological brains (e.g for neurosurgery planning) is challenging because the optimal software parameters are still unknown. The Grid has already been used to address this parameter search problem (1). Yet, it is still hardly possible for end-users to be autonomous with it. We demonstrate here our current solutions to enhance usability.

Analysis:
Data management requirements The data has to be handled directly by end-users. It is thus mandatory to set up a high-level data management tool providing a uniform view of distributed storage. A user-level file access control is also required to prevent users from ruining someone else's experiment because of wrong data manipulations. Although the Logical File Catalog provides a uniform view of the SEs, a layer is missing to make them usable by end-users. In an experiment, several file transfers need to be performed between local and Grid storage, which must be hidden. Moreover, file access control is based on the VO membership and not sufficiently fine-grained. The needs of the application in this area are:
- Intuitive parameter sweep specification
- Intermediate status check-pointing
- Fault tolerance mechanisms

The first point is addressed by a dedicated GUI. The two last points are expected to benefit from the use of a workflow management system.

Impact:
Our deployment is based on the VBrowser for data management and on MOTEUR for workflow management. The VBrowser (2) is an interactive tool that enables browsing local and remote resources from a single application. User-level file access control is yielded by the use of the Storage Resource Broker (3) through the VBrowser. A plug-in allows to easily manage parameter sweep experiments for fMRI data. The workflow description relies on the Scufl language used in Taverna (4). The interface between Taverna and EGEE is done using the MOTEUR engine (5). In addition to a command-line wrapper that handles basic application-level errors, it allows to exploit service parallelism, which is particularly important on variable platforms such as EGEE. An interface between MOTEUR and the VBrowser has been implemented to enable:
- Executing workflows processing files managed by the VBrowser
- Easily accessing results through the VBrowser

Conclusions:
This software architecture is a step towards an autonomous usage of the EGEE infrastructure by medical image analysts. In our future work, we plan to study the integration of solutions such as the Medical Data Manager or the Globus MEDICUS in this architecture to enable the use of EGEE Storage Elements in a secure way.

Keywords: Medical image analysis, data management, parameter sweep, workflow.

Further information: http://www.vl-e.nl

101. The G-DSE (Grid-Data Source Engine)

Author: Vuerli, Claudio (INAF-OA Trieste)
Co-authors: Taffoni, Giuliano (INAF-OA Trieste); Barisani, Andrea (INAF-OA Trieste); Pasian, Fabio (INAF-OA Trieste)

Short overview:
Astronomical Database resources are of crucial importance for astronomical community and their applications; almost all of them need to access a database to get input data and/or to store final results. Therefore Grid infrastructures that don't offer this capability are not particularly useful for astronomers. The G-DSE extends the Grid middleware so that databases become a new embedded resource in Grid. Any scientific community can benefit of the G-DSE to access database resources via Grid.

Analysis:
The I/O of Astronomical Applications almost always involves one or more databases. Grids unable to directly access databases force users to access databases off-line and transfer data of interest in classical SEs before the execution of the applications. Similarly, output will be stored in classical SEs and transferred to a database off-line after the termination of the application. This way of working is extremely uncomfortable and discourages users to choose the Grid as a collaborative tool. The G-DSE is one of the proposed solutions; with G-DSE a database becomes an embedded resource of the Grid. Grids extended through the G-DSE allow users to submit special jobs containing instructions to get data from databases, process them and store the processing results in one or more databases. In this way users can intermix database-related and processing related directives in their jobs. A database in fact is one of the shared resources in Grid as a CPU, a disk space storage and so on.

Impact:
The G-DSE is an extension of the Grid middleware. Unlike other proposed solutions to access databases via Grid, G-DSE is entirely based on the Grid technology. Its implementation was achieved by modifying some components of the middleware. The GRAM component was extended by introducing the new "Query Manager" besides the original "Job Manager"; this new manager takes in charge all jobs that require to access databases. The MDS Grid service, in particular its Glue Schema, is also extended; a new set of metadata characterizing and describing the new database resource is introduced so that users can take advantage of the Grid discovery capabilities to find and locate these new resources in Grid. The authentication and authorization mechanism of the Grid, instead, was left unchanged. In Grids extended with the G-DSE, users continue to authenticate as usual and user's rights defined in VOMS are mapped at DBMS level. The most recent releases of the G-DSE are both GTk and gLite compatible.

Conclusions:
The main target for the deployment of the G-DSE is the EGEE Grid infrastructure. The final goal is to make possible the exploitation of the G-DSE by all EGEE users and this requires that all Grid sites of all EGEE VOs install the G-DSE. Intermediate scenarios are also possible where only some of the EGEE VOs provide the G-DSE support (the VOs of those communities for which the interoperability between the Grid and databases are relevant like the astro VO).

Keywords: Database, Interoperability, Query Manager, Metadata, Glue Schema, Authentication, Authorization.

Further information: http://wwwas.oats.inaf.it/Grid/G-DSE

102. All-in-one graphical tool for Grid middleware management

Author: Caron, Eddy (ENS-Lyon / INRIA / CNRS / UCBL)
Co-authors: Amar, Abdelkader (ENS-Lyon / INRIA / CNRS / UCBL); Loureiro, David (ENS-Lyon / INRIA / CNRS / UCBL)

Short overview:
The DIET project is focused on the development of scalable middleware with initial efforts dedicated to the distribution of the scheduling problem across multiple agents. DIET consists of a set of elements that can be used together to build applications using the GridRPC paradigm, standard from the OGF. To evaluate the performances of DIET on the french Grid Grid'5000 and present its functionnalities in a demo, the DIET DashBoard and its fork GRUDU are very useful.

Analysis:
When dealing with Grid environments, Grid middelware are powerful tools for the development of computational servers able to exploit the available resources. But managing a Grid middleware, and a fortiori the Grid environment itself can be a hard task when no dedicated tools exist. Some are usable through nice graphical interfaces, but they are all dedicated to one or some limited tasks and do not fulfilled all the needs of a Grid end-user wanting to deploy Grid applications easily and fastly. The aim of this paper is to present all-in-one software, designed for the management of Grid middleware gathering user-friendly graphical interfaces answering to the various needs of a end-user. The software moreover eases the use of the Grid by avoiding the scripting layer under a nice GUI enabling the user a faster and more efficient use of the Grid environment. By this way they demonstrate how the DIET Dashboard fulfilled all the needs of a unified tool for the Grid management.

Impact:
From the knowledge of DIET Dashboard we have provided a tool, called GRUDU, to ensure deployment and reservation on the french Grid Grid'5000. For the EGEE community and the Grid'5000 community it could be intersting to share around how to use a Grid.

Conclusions:
The DIET Dashboard is designed to be a complete, modular, portable and powerful set of tools dedicated to a Grid context. With this tool user can manage Grid resources, monitor the Grid itself and manage the Grid middleware by designing your Grid applications or using workflows and then deploying these Grid applications on the Grid environment. The DIET Dashboard offers a large number of modules, created to answer the different needs of tools appearing in a Grid context.

Keywords: Vizualisation, Deployment, Resource reservation, Workflow

Further information: http://graal.ens-lyon.fr/DIET

103. g-Eclipse - Grid in five minutes

Author: Kornmayer, Harald (NEC Laboratories Europe)
Co-author: Stuempert, Mathias (Forschungszentrum Karlsruhe (FZK))

Short overview:
The threshold for new Grid users to access existing Grid infrastructure is still to high due to the complexity of the whole system including different protocols, cryptic commands with many options, distributed resources in different administrative domains, etc. Grid users needs new and innovative tools to access existing Grid infrastructures in just five minutes. The g-Eclipse framework provides an eco system to seamlessly access Grid resources built on top of Eclipse (www.eclipse.org).

Analysis:
The g-Eclipse framework requires stable and reliable basic Grid services like information systems, data replication systems and resource brokers. g-Eclipse is a JAVA application and requires either JAVA APIs or well defined WS descriptions for the basic Grid services, which are independent of the Grid operation system. For the demo, only a computer with JAVA and an arbitrary OS (Windows, Linux, MacOS) is needed.

Impact:
The demo will prove hat the g-Eclipse framework remove the Chinese wall between local and Grid resources. Grid user can access Grid resources seamlessly by managing data, defining and submitting jobs, visualize data, etc. The demo will show that the submission of a simple job to the Grid is now possible within a few minutes with only a small knowledge about Grids. Furthermore the shortening of the time-to-application will be demonstrated by Grid development and Grid deployment tools. A new application will be developed loacally and compiled and debugged remotely as transparent as the developer would use his local machine. Last but not least, the benefit of the g-Eclipse framework for Grid resources provider will be demonstrated by managing remote queuing system from a graphical managing system. Such wizards will help the resource providers to reduce the time-toservice of their offered resources and services.

Conclusions:
The g-Eclipse framework offers a middleware independent Grid access tool for existing Grid infrastructure. The current state of the framework will be presented by its developers including the exemplary support for gLite. The g-Eclipse framework benefits from the solid and reliable Eclipse eco system. In the future the g-Eclipse team expects more middleware supporting plugins and will therefore be able to access any existing Grid infrastructure. This will be proven with the GRIA middleware.

Keywords: Tooling, Eclipse, middleware independent, Generic applications, Visualisation, Development, deploy.

Further information: www.geclipse.eu www.eclipse.org

104. Solving data transfer level Grid interoperability among SRM, SRB and OGSA-DAI data resources

Authors: Lovas, Robert (MTA SZTAKI); Sipos, Gergely (MTA SZTAKI); Kiss, Tamas (University of Westminster)
Co-authors: Cevat, Sener (Middle East Technical University)

Short overview:
The GIN VO of OGF defined 4 levels of solving interoperation among different Grids. It was demonstrated several times how P-GRADE portal can support job submission level interoperation. In the current demonstration we show how P-GRADE portal was extended with SRM, SRB and OGSA-DAI portlet support in order to solve the interoperation problem at the data movement level. Moreover, interoperation of SRM, SRB and OGSA-DAI data resources are supported among nodes of a workflow.

Analysis:
The input files of a node (job or service call) of a P-GRADE workflow can come from file systems, like SRM or SRB, or from database management systems via OGSA-DAI and the results can also be fed into any of these solutions. Both the file systems and the databases can be located in different production Grids, and the jobs of the workflow can also be mapped to different Grids. These Grids can be based on different Grid middleware and may require different user certificates for authentication. The workflow level data resource integration allows the seamless interoperation of SRB catalogues, GridFTP file systems and EGEE storage elements (based on SRM) at the level of P-GRADE workflows. We will demonstrate that jobs of an urban traffic simulation workflow are running in different Grids (US OSG, UK NGS, EGEE) and utilize data resources based on different technologies (SRB, SRM, GridFTP, local) from these different Grids.

Impact:
Grid portals typically do not provide SRM, SRB and OGSA-DAI portlets or they provide only one of them in a limited form. We have developed intelligent versions of these portlets and showed how to integrate them into a single portal (P-GRADE). As a result users of P-GRADE portal can easily access all the major Grid-related file and database systems without learning the different command line interfaces. Moreover, Grid workflow systems are typically tailored to one particular Grid concerning both job submission and data file access mechanisms. P-GRADE portal is the first multi-Grid portal where not only the job submission is supported among different Grids but also the data resource access mechanisms of different Grids can become interoperable at workflow level. Intra-workflow interoperation of Grid data resources allows data to be input from or output to different file storage systems or database solutions, located in several different Grids.

Conclusions:
There are several variants of P-GRADE portal deployed for different user communities. For SEE-GRID and EGEE VOs P-GRADE portal is deployed with GridFTP file systems and EGEE storage elements (based on SRM). For the UK NGS P-GRADE portal is deployed with full access to GridFTP, SRB and SRM file systems. Another experimental version of the portal contains additionally the OGSA-DAI portlet. A new version of the portal that integrates all these features is planed for the first half of 2008.

Keywords: Grid workflow, interoperation, Grid data resources, SRB, OGSA-DAI

105. Mathcell.Ru: integrated mathematical model of living cell in Grid infrastructure

Author: Ustinin, Mikhail (IMPB RAS); Lakhno, Victor (IMPB RAS)
Co-authors: Nazipova, Nafisa (IMPB RAS ; Filippov, Sergey (IMPB RAS); Zaitsev, Aleksandr (IMPB RAS); Fialko, Nadezhda (IMPB RAS); Tyulbasheva, Gayane (IMPB RAS); Teplukhin, Alexander (IMPB RAS); Ustinin, Dmitriy (IMPB RAS) Session

Short overview:
The purpose of the Mathematical Cell Project (http://www.mathcell.ru) is to create the integrated mathematical model of eukaryotic cell based on Grid and distributed bioinformatics' resources. This model will help to solve some scientific and practical problems, such as novel drug design (prediction of their direct and mediated influence on cell), or the development of nanostructures and nanomaterials.

Analysis:
The MathCell Project includes 3D interactive living cell model, encyclopedia on mathematical modeling of cell and software for modeling of basic processes in living cell. Within the limits of the Project the interactive environment was developed, which allows to perform calculations of mathematical models using Grid infrastructure. The special Job Maintenance System was developed which automatically allows User Logging & Accounting, Job Submission, Job Status Monitoring, Job Queuing, Results Obtaining. At the present three models are deployed in Grid infrastructure:
- software for mathematical modeling of electron transfer in DNA molecule;
- simulation model of electron transfer on inner photosynthetic membrane in chloroplasts;
- software for calculation of dissolution energy of biomolecules in water by Monte Carlo method.

Impact:
The Mathcell Project was developed to provide biologists with powerful resources for calculation of extremely complicated models. It gives a novel functionality to different Grid services, creating a specific interface for users from computational biology.

Conclusions:
Further development of the MathCell Project is closely associated with advance of Grid infrastructure, and implies integration of individual components of the model into a program system which would simulate cell processes at different levels – from microscopic to macroscopic scales and from picoseconds to the cell lifetimes.

Keywords: Computational Biology, Mathematical Modeling, Bioinformatics

Further information: http://www.mathcell.ru

106. A telemedicine platform for information and image management on the Grid

Authors: Diarena, Matteo (CNRS IN2P3 LPC Clermont-Ferrand); Nowak, Simon (CNRS IN2P3 LPC Clermont-Ferrand)
Co-authors: Breton, Vincent (CNRS IN2P3 LPC Clermont-Ferrand); Legre, Yannick (CNRS IN2P3 LPC Clermont-Ferrand); Maigne, Lydia (CNRS IN2P3 LPC Clermont-Ferrand); Dao, Van Tuyet (Ho Chi Minh City Institute of Information Technology); Boire, Jean-Yves (ERIM INSERM ERI 14); Bilbao, José Roman (University of Almeria)

Short overview:
Constant growth of Grid technology opened the way for new opportunities in terms of information and data exchange in a secure and collaborative context. These new opportunities can be exploited to offer physicians new telemedicine services in order to improve their collaboration capabilities. Our platform gives physicians an easyto- use telemedicine environment to manage and share patient information between remote locations.

Analysis:
The medical field offers a wide and challenging scenario in which new Grid applications can be developed to improve collaborative work between scientists. The development of Grid-based medical applications needs to take into account some key factors such as the need to conform to strict legal constraints in terms of data privacy and security. Moreover physicians are quite reluctant to use new applications that change their way of working, for this reason applications developed on this context need to be as intuitive and user friendly as possible.

Impact:
To allow physicians to manage and exchange medical data and images, the platform uses web services technology and Grid services provided by gLite middleware. Physicians access the platform using a web portal developed with the GridSphere portlet container that presents to them a user-friendly interface to access several distributed medical services that manage images and medical information. Medical information is stored locally in the user's hospital using the AMGA metadata catalogue and information between services deployed in different location is exchanged using the SOAP messaging protocol. Medical images are stored anonymized and encrypted on the Grid while their corresponding metadata are stored in the local AMGA server. The proposed medical platform allows submitting, monitoring, and managing medically-related jobs such as dosimetric simulations. These jobs are CPU-intensive simulations using a physician’s medical images to predict the result of a cancer dosimetric treatment.

Conclusions:
Our platform is mainly based on data management services provided by gLite middleware with particular regard to AMGA for medical information management and GFAL APIs for image storage and management on the Grid. Our experience with these services is overall positive but the increase in Grid reliability, stability and performance opens the way for new features and improvements in order to offer physicians more reliable medical services.

Keywords: Medical Data Management, Data Management, Medical Imaging, Web Services, GridSphere

Further information: http://clrwww.in2p3.fr/PCSV/

107. What can the CIC portal do for end users?

Authors: Cordier, Helene (CNRS/IN2P3); Aidel, Osman (CNRS/IN2P3); Mathieu, Gilles (CNRS/IN2P3) ; L'Orphelin, Cyril (CNRS/IN2P3)

Short overview:
The CIC Portal, or Operations Portal, is meant to be useful to any user of the Grid, namely to VOs. Information about existing VOs, including requirements, resources and services is made available. Also, Grid wide communication tools are there to ease up operations and broadcasting important information in a transversal way to the different communities involved in EGEE operations. The demo will show how to access and use all this, will address questions and record feedback from the attendance.

Analysis:
The CIC portal added value to the Grid infrastructure is for all the EGEE actors, whether scientist, VO or site manager, or Grid operator. Every type of group has its own entry point to the portal. The information on the operational state of the Grid is filtered and presented according to the usefulness for a particular group. The tools presented to a given group are those which could be useful for it, like VO ID card updates for VO managers, EGEE broadcasts for various communities, dashboards for Grid operators and so on. For instance, any new VO can immediately, directly and simply benefit from the portal: a given VO manager defines indeed its "VO ID card" in the portal, which is the starting point for any site administrator to configure and allow VOs' access to his sites' resources.

Impact:
Key services essential to operations in EGEE are numerous and the CIC portal is an integration platform for them. Indeed, it interfaces with operational tools like GGUS, GOCDB, gstat, the Grid's information system, FCR, and SAM. Consequently, the CIC portal is in itself a key service for various Grid activities. Indeed, the range of tools and information proposed by the CIC portal over the last 3 years has allowed major improvements in daily work and procedures for various actors. The best example of this is the work of "Grid Operators on Duty" (COD) who use the CIC portal as their central operational tool. Tools and procedures established to support their work have proven to be stable and scalable, as the number of sites they have been taking care of has been multiplied by 5 in less than 3 years. Moreover, in order to ensure the High-Availability of their service, COD teams have set-up internal working groups to elaborate, namely, failover processes of the operational tools.

Conclusions:
We intend to advertise the latest functionalities of the CIC portal available to the user community e.g downtimes announcements via subscription released late October 2007 and to collect feedback from end-users as well as VO managers. This approach will enable us to enhance the usefulness and the efficiency of the CIC portal in easing up more and more EGEE operations at a global level and thus making the production Grid infrastructure more and more reliable.

Keywords: EGEE operations, sites monitoring dashboards, VO configuration at sites, VO resources assessment.

Further information: http://cic.Gridops.org/

108. Enginframe genius Grid portal and VOMS proxy creation

Authors: Venuti, Nicola (NICE srl); Falzone, Alberto (NICE srl); Ardizzone, Valeria (INFN Catania)
Co-authors: Roberto, Barbera (INFN Catania AND University of Catania); Scardaci, Diego (INFN Catania)

Short overview:
Grid and their associated tools must be presented to novice users in terms of applications, without needing to know the underlying details of Grid middlewares. Genius and EnginFrame Grid portal are an increasingly popular mechanism for creating customizable, Web-based interfaces to Grid services and resources. This work describes the new portal's capabilities and a new service for VOMS Proxy creation through the portal.

Analysis:
With Enginframe user can interact with files on the UI, can submit and monitor jobs to Grid and manage data and job output inside the VO belongs to. The Web portal eliminates any problems and needs about particular Operating System running on the client, the user can interact with the Grid from everywhere and with everything: a Java compliant web browser is only required. The purpose of VOMS ProxyInit service is to create the user's Grid proxy file, with or without VOMS Extensions, using its personal certificate and private key from his usb pen drive attached to the local workstation, and finally, by means of an encrypted and mutually authenticated connection, transfer just the created proxy file to the server where is installed Enginframe with GENIUS on top. Globus Security Infrastructure provides communication integrity between elements of a computational Grid and support for single sign-on for users and it was implemented in the VOMS ProxyInit service to client-server communication

Impact:
With the new VOMS ProxyInit service, given a user already belongs to VO, is now possible to create its proxy file using its personal certificate and private key directly form its “local computer”, then by means the Global Security model implementation, it is transferred to the server installed on GENIUS. In this way, the user’s private key is kept completely secure and not required to be copied on remote UI machine. The command line complexity is hidden to users that are able to create a valid Grid proxy with few clicks from the GENIUS portal. Furthermore, VOMS service accepts both P12 and PEM formats so any certificate’s conversion and management is needed from user now. The proxy obtained is fully compatible with the standard Globus proxy format and can contain additional VO-related attributes using from Grid services to perform decision based on their values about the user’s request and its authorization.

Conclusions:
Given the modularity and flexibility of EnginFrame Framework, which acts as a general-purpose framework underneath GENIUS, the portal can be easily customized and adapted to interact with other Grid middlewares, even non-Glite based, new Virtual Organization, Scheduler at the same time. Acting as a simple and intuitive "gate" to access the Grid, the portal brings with itself a huge dissemination power, in fact, it is the official portal of GILDA VO.

Keywords: Grid portal, voms, proxy, authentication, genius, enginframe, virtual organization, gilda,

Further information: https://genius.ct.infn.it/ https://gilda.ct.infn.it/ http://www.nice-italy.com/

109. Bioinformatics portal on Grid: the GPSA - Grid Protein Sequence Analaysis - case

Author: Blanchet, Christophe (CNRS IBCP)
Co-authors: Michon, Alexis (CNRS IBCP); Eloto, Christelle (CNRS IBCP); Combet, Christophe (CNRS IBCP)

Short overview:
Although Grid computing offers great potential for executing large-scale bioinformatics applications, practical utilization is constrained by the middleware's ease-of-use. Biologists are generally unwilling to use command-line interfaces or complex toolkits consisting of numerous components, such as most current Grid middlewares. Integrating the required applications in a Web portal is then an efficient way to bring these scientists to the Grid.

Analysis:
Bioinformatics analysis of data produced by high-throughput biology, for instance genome projects, is one of the major challenges for the coming years. Two of the requirements for this analysis are access to up-to-date databanks (of sequences, patterns, 3D structures, etc.) and access to relevant algorithms (for sequence similarity, multiple alignment, pattern scanning, etc.). Since 1998, we have been developing the Web server NPS@ (Network Protein Sequence Analysis), that provides the biologist with many of the most common resources for protein sequence analysis, integrated into a common workflow. We have adapted this portal to the EGEE Grid. The bioinformatics Grid portal GPS@ ("Grid Protein Sequence Analysis") simplifies and automates the EGEE Grid job submission and data management mechanisms using XML descriptions of available bioinformatics resources: algorithms and databanks.

Impact:
One major problem with a Grid-computing infrastructure is the distribution of files and binaries, as for the BLAST or ClustalW algorithms, through the job submission process. Sending a binary of the algorithm to a node on the Grid is quite simple because of its size (few kilobytes) and can be done at each execution. Putting on the Grid a databank, ranging from tens of megabytes (as Swiss-Prot) to gigabytes (as EMBL), consumes a large part of network bandwidth, and greatly increases the execution time if done inappropriately. The GPSA interface hides the mechanisms involved for the execution of bioinformatics analyses on the Grid infrastructure. The bioinformatics algorithms and databanks have been distributed and registered on the EGEE Grid and GPS@ runs its own EGEE interface to the Grid. In this way, the GPS@ portal simplifies the bioinformatic Grid submission, and provides biologists with the benefits of the EGEE Grid infrastructure to analyze large biological datasets.

Conclusions:
The GPS@ Grid Web portal (Grid Protein Sequence Analysis) is a bioinformatic integrated portal that provides a biologist with a user-friendly interface to the Grid resources (computing and storage) made available by the EU-EGEE project. The GPS@ portal will be used as case study in the context of the EGEE PORTAL group to implement the recommendations raised by this group.

Keywords: Bioinformatics, Portal.

Further information: http://gpsa-pbil.ibcp.fr

110. Design, implement and deploy Grid oriented applications in a cooperative way: a biomedical use case

Authors: I.Porro (University of Genoa); S.Scifo (COMETA Consortium)
Co-authors: L.Torterolo, L.Corradi, M.Fato (University of Genoa); R.Barbera (University of Catania and INFN); S.Parisi (IR & T engineering s.r.l.); N.Venuti (NICE s.r.l.); D.Scardaci, A.Calanducci (INFN Catania); G.Scuderi (Unico Informatica s.r.l); S.Gatti (Aitek S.p.A.)

Short overview:
The BMPortal is a flexible Grid application container designed and developed at BIOLAB, DIST, and University of Genoa. The project was born in early 2007 as a container for Bioinformatics application and then evolved in a more general biomedical portal. Furthermore, it is currently used to re-engineer previously developed biomedical applications. The Grid is presented here not only as the underlying technical infrastructure but also as a new paradigm shift in software development.

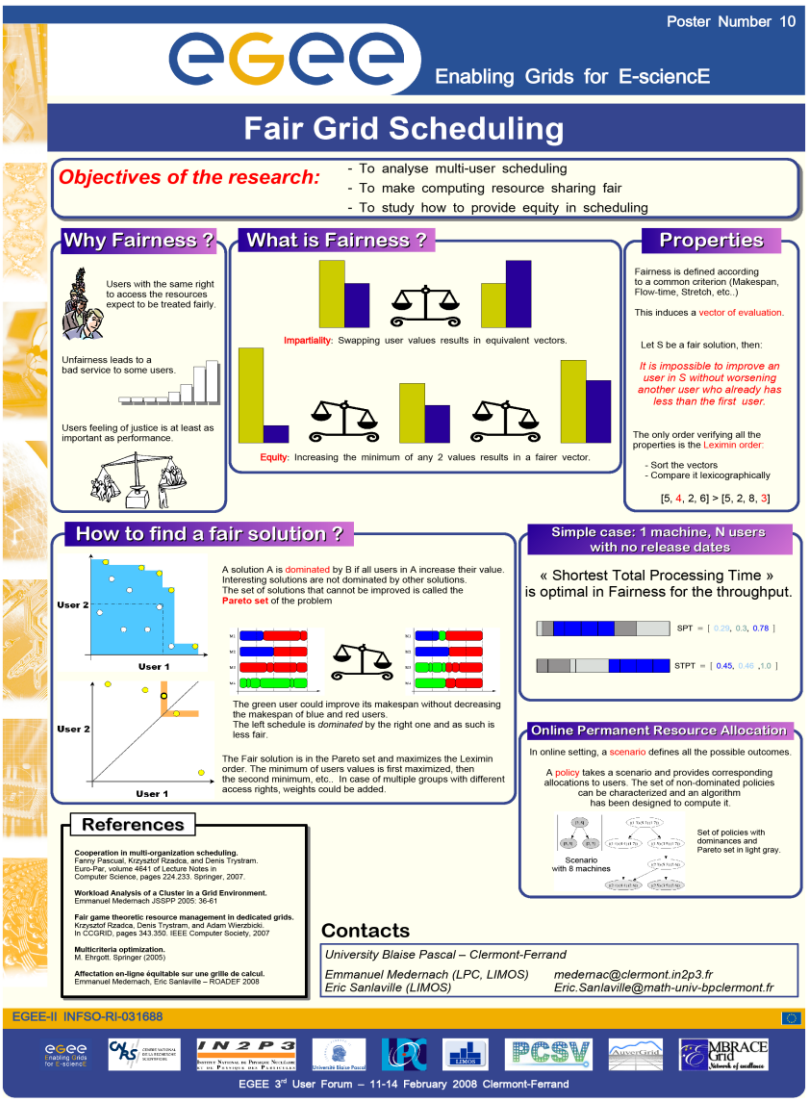
Analysis:
Nowadays, many biomedicine studies are dealing with large, distributed, and heterogeneous repositories as well as with computationally demanding analyses. Complex integration techniques are more often required to handle this complexity, even if for small sized applications, when they are intrinsically distributed: this particular scenario is frequently found in medical informatics applications, where the health care provider is not a single institution but a collection of actors that play different roles in the territory. The BMPortal is a platform thought to promote collaboration and cooperation among scientists and healthcare research groups, enabling the remote use of resources integrated in complex software platform services forming a virtual laboratory. It is designed to host several medical use cases and it is able to deploy several analysis that can be combined in large applications using a workflow strategy: here, the engineering of BIOLAB SPM Alzheimer application is presented

Impact:
The work is undertaken at BIOLAB with the cooperation of some Italian SMEs (AITEK, NICE, IR, UNICO) and the INFN (Department of Catania) as well as the Official Training and Support Team of EGEE. A set of independent applications could be published on the portal sharing a common data and metadata infrastructre based on gLite. Data Management capabilities are made up by the adoption of the GSAF software layer developed and the Data Violation is avoided thanks to the interoperation with the Secure Storage Service. Security, data and metadata management components are developed by researchers and SMEs in Catania while the overall platform, interfaces and application deployment is performed in Genoa (researchers and SMEs too). Researchers and SMEs work at the development deploying services in their laboratories and contributing to a distributed build of the project in a really collaborative and secure way, sharing the gLite security context.

Conclusions:
The BMPortal provides tools for accessing distributed data in a secure way without moving files on the net, for managing related metadata, for building and maintaining catalogues, for submitting jobs to the Grid and to local computing cluster, for organizing services into workflows. The scope of this work is both to present a Grid application with its own medical use case and empathize the benefit that a new design paradigm based on Grid could provide to distant research groups.

Keywords: Data and metadata Management, Workflows, Portal, cooperative development

Further information: http://Grid.bio.dist.unige.it


Poster Number 10
Enabling Grids for E-sciencE
Fair Grid Scheduling
Objectives of the research:
- To analyse multi-user scheduling
- To make computing resource sharing fair
- To study how to provide equity in scheduling
Why Fairness ?
Users with the same right to access the resources expect to be treated fairly.
Unfairness leads to a bad service to some users.
Users feeling of justice is at least as important as performance.
What is Fairness ?
Impartiality: Swapping user values results in equivalent vectors.
Equity: Increasing the minimum of any 2 values results in a fairer vector.
Properties
Fairness is defined according to a common criterion (Makespan, Flow-time, Stretch, etc..)
This induces a vector of evaluation.
Let S be a fair solution, then:
It is impossible to improve an user in S without worsening another user who already has less than the first user.
The only order verifying all the properties is the Leximin order:
- Sort the vectors
- Compare it lexicographically
[5, 4, 2, 6] > [5, 2, 8, 3]
How to find a fair solution ?
User 2
User 1
A solution A is dominated by B if all users in A increase their value. Interesting solutions are not dominated by other solutions. The set of solutions that cannot be improved is called the Pareto set of the problem
The green user could improve its makespan without decreasing the makespan of blue and red users. The left schedule is dominated by the right one and as such is less fair.
The Fair solution is in the Pareto set and maximizes the Leximin order. The minimum of users values is first maximized, then the second minimum, etc.. In case of multiple groups with different access rights, weights could be added.
Simple case: 1 machine, N users with no release dates
« Shortest Total Processing Time » is optimal in Fairness for the throughput.
SPT = [0.29, 0.3, 0.78]
STPT = [0.45, 0.46 ,1.0]
Online Permanent Resource Allocation
In online setting, a scenario defines all the possible outcomes.
A policy takes a scenario and provides corresponding allocations to users. The set of non-dominated policies can be characterized and an algorithm has been designed to compute it.
Scenario with 8 machines
Set of policies with dominances and Pareto set in light gray.
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Contacts
University Blaise Pascal – Clermont-Ferrand
Emmanuel Medernach (LPC, LIMOS) medernac@clermont.in2p3.fr
Eric Sanlaville (LIMOS) Eric.Sanlaville@math-univ-bpclermont.fr
EGEE-II INFSO-RI-031688
EGEE 3rd User Forum – 11-14 February 2008 Clermont-Ferrand

POSTERS

Posters

Convener: Vangelis Floros (GRNET, Athens)

The poster session was integral part of the Forum providing the opportunity for face to face discussions and lively presentation of ongoing research, early project results and other activities of the Grid computing community. The 36 posters were available for viewing throughout the User Forum.

The voting for the 'best poster' was performed by all the User Forum participants. Again the competition was tight, but the prize was awarded to a contributor who managed to illustrate a solution to a key Grid issue in a poster with good, clear graphics and simple messages.

'Fair Grid Scheduling' Medernach, Emmanuel (LPC - Clermont, France)

111. Problem solving environment for stereological modeling of muscle cells

Authors: Ciglan, Marek (Institute of Informatics, Slovakia); Parulek, Julius (Institute of Molecular Physiology and Genetics, Slovak Academy of Sciences)
Co-authors: Simo, Branislav (Institute of Informatics, Slovak Academy of Sciences); Sramek, Milos (Austrian Academy of Sciences, Austria); Hluchy, Ladislav (Institute of Informatics, Slovak Academy of Sciences); Zahradnik, Ivan (Institute of Molecular Physiology and Genetics, Slovak Academy of Sciences)

Short overview:
The presented work is aimed at creation, verification and visualization of muscle cell models. Generated cell models should meet the requirements established by stereological measurements of real cell images. These requirements necessitate evaluation of volume and surface densities, which is a rather time consuming process, requiring Grid computational power. In addition, visual inspection of the model is necessary to reveal possible morphological and structural inconsistencies.

Analysis:
From the viewpoint of Grid computing, SM-PSE requires: Computing Intensive Parametric Studies: The created cell tools enable users to repetitively create hundreds of huge models, which, consecutively, will be stereologically verified. The computation of volume and surface densities of a single model can take up to hours; i. e., computation of all the models would last for days. Heterogeneous Computing Platform Support: Visualization rendering platform is limited to Windows OS. Therefore, combining model solving with model visualization on Windows platform has to be provided. Moreover, rendering requirements are not the only ones that define the platform demands. Several existing tools, capable of working with stereological data that are considered to extend our PSE are available also solely on the Windows platform.

Impact:
EGEE infrastructure utilizing the gLite middleware and MEDIGRID middleware were identified as the ideal solutions for computationally intensive model verification tasks and for multi-platform infrastructure support (visualization on Windows platform), respectively. Each of those middlewares provides different tools and different APIs. This might be quite confusing for the user and impedes construction and execution of the Grid activity workflow, spanning both middlewares. Interoperability of the two middlewares is required at the level of job submission and data exchange. We address interoperability by providing specialized MEDIGRID job service (gL-service) that can submit jobs to gLite powered infrastructure and transforms the job state of a gLite job to MEDIGRID job state while the computation is running. The user can thus use MEDIGRID toolkits and APIs to manage the jobs in MEDIGRID based infrastructure as well as in gLite based infrastructure.

Conclusions:
Presented effort is still work-in-progress. Compute intensive tasks in the development version were tested in Gilda testbed. Before moving to the production environment, specialized, application specific portlets have to be developed to facilitate the utilization for end users, and thorough evaluation of middlewares interoperability modules has to be conducted. We plan to move to the production environment in the first quarter of 2008; the application will be used in VOCE VO.

Keywords: Biomedicine, Molecular Physiology, Implicit surfaces, middleware interoperability

Further information: http://www.sccg.sk/~parulek/cell/

112. Enabling distributed access and parallel processing of bioinformatics data in Grid environment: the EKTORAS platform

Author: Maglogiannis, Ilias (University of Aegean)

Short overview:
In this work we present a Web based platform called EKTORAS (http://www.icsd.aegean.gr/ektoras), which enables distributed access and parallel processing of biological data in Grid environments. The deployed software aims at creation of tools for processing data from microarray experiments over the Hellenic Grid infrastructure. This work serves as a starting point for building a more complete and integrated Grid enabled microarray experimentation environment.

Analysis:
Users, accessing the platform's Web interface through the implemented portal, are given the ability to submit their experiments, retrieve their results and also compare them with formerly submitted experiments. Access to services is enabled by parsing input files and accordingly activating the 'Gridified' algorithms for processing the microarray experiments. Both data parsing operations and launching of experiments are specified as Grid jobs, using the Job Description Language (JDL). The provided microarray input files, which are usually structured according to formats that are standard for the microarray bioinformatics community, are pre-processed so as so to be usable by the range of algorithms available. The results of this preprocessing step are directed to the Grid's storage elements (SE). Then the data are being processed by parallel applications distributing the parallel chunks & jobs to various nodes-processors of the Grid.

Impact:
The described EKTORAS platform for microarray data analysis helps scientists and research groups with limited or no experience in microarray analysis to significantly reduce the processing time of large experiments. In the meantime the EKTORAS platform aims to bridge and integrate distributed databases storing multi-faceted biological and medical information (gene sequences, homology across species, proteins encoded and relevant biochemical pathways) about gene function and structure, enabling ubiquitous access to bioinformatics data. The original architectural design will be constantly updated, based on the early feedback from experiments on the prototype infrastructure. However the already implemented modules have clearly proven the
feasibility of the envisaged system.

Conclusions:
This work serves as a starting point for building a more complete and integrated Grid enabled microarray experimentation environment. In this context the EKTORAS access portal will be enhanced to allow end-users to retrieve experiment files from public biological databases such as the EBI microarray library (http://www.ebi.ac.uk). To this end the portal will provide an adapter to the EBI database system, allowing to view, browse and select EBI files and then process them in the Grid.

Keywords: cDNA microarray experiments, Bioinformatics, Data Management, MPI (Message Passing Interface)

Further information: http://www.icsd.aegean.gr/ektoras, http://hellasGrid.gr/

113. Batch service management tool within g-eclipse

Author: Gjermundrod, Harald (University of Cyprus)
Co-authors: Dikaiakos, Marios (University of Cyprus)

Short overview:
Eclipse provides a powerful platform for tool building and the g-Eclipse project uses this platform to create a middleware-independent Grid framework for users, developers, and operators. For the operator perspective of this framework a tool to monitor and manage batch services of Grid sites has been devised. This tool assists the Grid site administrator with her day-to-day activities. Not only it simplifies the tasks, but it only allows the administrator to perform correct actions.

Analysis:
The Batch Service editor within the g-Eclipse framework allows the administrator of a Grid site to manage her site(s). The editor presents the administrator with a colorcoded representation of the current state of the computing element, queues, and worker nodes as well as their properties. For large sites, the administrator can zoom in/out to view all the elements of the site. Using this editor the administrator can choose from the context menu of the specific item(s) to start/stop/enable/disable/delete queues, enable/disable worker nodes, hold/release/move/delete batch jobs, and initiate wizards to create new queues. If multiple items are selected, then only the actions that can be applied to all the items are available. In addition to the editor there is also a Batch Job view which presents a table of the batch jobs that are currently present on the selected element (worker node, queue) in the editor. The columns in the table present the properties associated with the batch jobs.

Impact:
The novelty of this tool is that it is integrated into a framework where an administrator can perform all her tasks. An administrator can manage her site(operator perspective), write Grid applications (developer perspective), and then test out applications/sites (user perspective). The tool also provides an intuitive the possibility of misconfiguration because the administrator's operations are validated and only valid options are presented. Compared to the usage of CLI or service tailored GUIs the option of an extensible middleware-independent tool is better choice in our opinion. As the tool is part of the g-Eclipse framework, which is an official technology project of the Eclipse project, it is open and transparent for anybody to request features or contribute features to the tool.

Conclusions:
The tool will be used by the local Grid site administrator as a client side tool that remotely interacts with the batch service(s). Currently, the underlying connection method is to SSH into the batch service but in the future gLogin with the administrator's personal certificate will be added. Lessons learned from using the tool are that the batch service commands are not installed in a standard directory and may not be in the system path and the output of a command varies from site-tosite.

Keywords: Batch Service Management Tool

Further information: www.geclipse.eu

114. Configuring and enabling condor for LHC computing Grid

Author: Das, Santanu (Cambridge, UK)

Short overview:
We provide details of the configuration, implementation, and testing of Condor batch system for LCG in multi-cultural environment, where a common cluster is used for different types of jobs. The system is presented as an extension to the default LCG/gLite configuration that provides transparent access for both LCG and local jobs to the common resource. Using Condor and Chirp/Parrot, we have extended the possibilities to use university cluster for LCG/gLite jobs in a very non-privileged way.

Analysis:
Condor is a specialized workload management system for compute-intensive jobs, which can effectively manage a variety of clusters of dedicated compute nodes. Today, there are Grid schedulers, resource managers, and workload management systems available that can provide the functionality of the traditional batch queuing system e.g. Torque/PBS or provide the ability to harness cycles from idle desktop workstations. Condor addresses both of these areas by providing a single tool. In Grid-style computing environment, Condor's "flocking" technology allows multiple Condor compute installations to work together and opens a wide range of possible options for resource sharing. Although Condor, as a batch system, is officially supported by gLite/EGEE, various part of the middleware still limited to the PBS/Torque in terms of transparent integrity. We have extended the support to allow middleware to work seamlessly with Condor and enable interaction with University Compute Clusters.

Impact:
Various “info provider” bits are fixed now, which were previously wrong out of the box. As a result correct info is now being published now. The support is now extended for *sgm jobs to run smoothly as other Torque sites. Now it's also possible to distinguish between the Grid jobs and the local jobs, hence different job environments are provided by the same cluster for the jobs from a number of different communities. WN tar-ball installation on other remote machines (e.g. University cluster) is even easier now without any root access. As a result, now it's possible to use existing group/university cluster for Grid jobs when it's not in use. So, a site can use more non-dedicated resources withing investing money for extra hardware.

Conclusions:
We are continuously developing the configuration so that it takes minimum effort to setup. Pushing jobs to university cluster is presently in testing. We plan to deploy WN software at CamGrid (a campus wide cluster) system and the departmental machines and the goal is to demonstrate the possibilities to use non-dedicated resources. Tests so far under SL3/SL4 and as a next step we will be on other distro.

Keywords: Batch System

115. European space agency astronomy projects using Grid technology: XMM-Newton and integral

Author: Alvarez, Ruben (European Space Agency)
Co-authors: Arviset, Christophe (European Space Agency); Gabriel, Carlos (European Space Agency); Ibarra, Aitor (European Space Agency); Belanger, Guillaume (European Space Agency); Tapiador, Daniel (European Space Agency)

Short overview:
The European Space Agency astronomy projects XMM-Newton and Integral have started to use Grid technology for two main purposes: result enhancement and as collaborative platform to cooperate with other Astronomy institutions. Three cases in total are presented: 1) Scientific Analysis through Web Services in the Grid; 2) XMM mosaic construction; 3) Integral bulk processing. Cases 1) and 2) are for XMM-Newton and 3) is for Integral. Both current status and future development are shown.

Analysis:
With the introduction of Grid technologies in the European Space Astronomy Center (ESAC) and once the astronomers are getting used to them, new possibilities both for result enhancement and for collaboration with other Astronomy institutes have started to be explored. Here we present some examples of such usage, showing the current status and also the immediate future development: a) The Remote Interface for Science Analysis (RISA), which makes it possible to run SAS, the XMM-Newton data reduction software, through fully configurable web service workflows, enabling observers to access and analyse data making use of all of the existing SAS functionalities. The workflows run primarily but not exclusively on the ESAC Grid, directly connected to the XMM-Newton Science Archive. b) The production of mosaics on the Grid from XMM-Newton data. c) The gain in processing time when processing Integral data on the Grid are the three examples presented of current usage of Grid at ESA.

Impact:
The impact of the cases where an enhancement of the results was pursued by looking for processing power and speed have started to show up: the production of XMM mosaics is now possible in a sensible time scale and the Integral data can be now processed also in a reasonable amount of time. On the other side, by developing RISA on the Grid, we are offering all the astronomy community with a powerful tool to process XMM-Newton data. Users will only need a web browser to process data, no other local installation of HW or SW will be needed to process XMM-Newton data. This case also includes collaboration with other Grids: IFCA, Cantabria, Spain and INFN, Trieste, Italy.

Conclusions:
Enhancement of results by using the Grid and usage of Grid as a collaborative way to obtain those results are now being achieved at the European Space Agency for astronomy projects. The aim is now to offer the Grid to more rojects and to reinforce the collaboration with other institutes.

Keywords: Web Services, workflows, astronomy, XMM-Newton, Integral, bulk reprocessing

Further information: http://www.sciops.esa.int/egw

116. Early failure detection: a method and some applications

Authors: Germain-Renaud, Cecile (LRI & LAL/IN2P3, France); Krenek, Ales (Masaryk Univeristy)

Short overview:
Both Grid middleware services and applications face failures, and the more widely deployed they are, the higher is the price for not detecting the failures early (lost jobs, wasted resources,etc.). Automated detection, diagnosis, and ultimately management, of software/hardware problems define autonomic dependability. This work report on a generic mechanism for autonomic detection of EGEE failures involving abrupt changes in the behaviour of quantities of interest, and on some applications.

Analysis:
The complexity of the hardware/software components and the intricacy of their interactions, defeat attempts to build fault models only from a-priori knowledge. A black-box approach, where we observe the events to spot outliers, is appealing by its simplicity, and large body of experience in quality control. The general challenge is to detect anomalies as soon as possible. Much better solutions than simple thresholding are routinely used in e.g. clinical trials and the supervision of production lines. In the case of abrupt changes, the Page-Hinkley statistics provides a provably efficient method, which minimizes the time to detection for a prescribed false alarm rate. We have applied this method to quantities (e.g. number of arrived and served jobs per unit of time) that are easily computed from the output of existing services. The main result is that we are able to efficiently detect failures of very different origins (e.g. some software bugs, blackholes) without human tuning.

Impact:
Fast and reliable detection of failures can both raise alarms bringing operator intervention, as well as trigger automatic reaction, e.g. avoid job submission to blackhole sites. The proposed method is quite general, and can be applied at various points in the middleware, including the site level, or by end-user software. Nonetheless, gLite Logging and Bookkeeping service, which concentrates information on the job processing, would be the most effective target. The approach of affecting job scheduling by LB-computed statistics had been used before. Experimental validation and comparison is thus desirable: a significant dataset of “challenge examples” should be available. Examples tagged by system administrators are rare. The Job Provenance (archive of LB data and more) provides the required information from two aspects: easy access to filtered L data, and valuable information for calibrating and evaluating failure detection methods wrt. known and well-understood past events.

Conclusions:
The implementation of the statistics per-se is fairly straightforward. The codes for exploiting the test on archived data, including both the extraction of the quantities of interest and the test itself, will be released through the Grid Observatory, in order to demonstrate the performance and scalability levels required for the production environment. Full integration into gLite raises the usual technical issues, and appropriate tools (triggering alarms etc.) remain to be developed.

Keywords: Fault detection, Statistics

117. The porting of a Grid software for virtual eye surgery from globus 4 to gLite

Author: Bosa, Karoly Jozsef (JKU/RISC)
Co-authors: Schreiner, Wolfgang (JKU/RISC)

Short overview:
"Grid-Enabled SEE++" is a Grid-based simulation software that supports the diagnosis and treatment of certain eye motility disorders (strabismus). The overall goal is to to develop an efficient Grid-based tool for "Evidence Based Medicine", which supports the surgeons in choosing optimal surgery techniques for the treatments of different syndromes of strabismus. In the current poster demonstration, we propose to report our experiences regarding the porting of this application to gLite.

Analysis:
In Globus Toolkit 4, we developed a parallel version of the simulation of the Hess- Lancaster test (typical medical examination). By this, we speeded up this simulation by a factor of 14-17. Furthermore, we reported the prototype implementation of a medical database component for "Grid-Enabled SEE++". Our next steps concentrate on developing a distributed Grid-enabled database system. Finally, we designed a so called Grid-based Pathology Fitting algorithm, which would be able to determinate (or at least estimate) automatically the pathological reason of a patient's strabismus. Since the outcome of this algorithm strongly depends on the initial estimation for the pathological case, we propose to exploit the Grid in the following way:
- by searching in the Grid-based SEE++ medical databases for similar pathological cases and
- by starting concurrent pathology fitting processes with these cases as the starting points of the optimizations (parameter study).

Impact:
Since we met with some limitations of Globus 4, we also designed and developed a version of "Grid-Enabled SEE++" compatible with gLite. We use some kind of server jobs (as executers for parallel Hess calculations) started via the WMProxy. To return the allocated port numbers, we investigated the interactive job submission feature of gLite. We may exchange the access layer developed earlier for the SEE++ medical databases to an AMGA-based solution. Pathology Fitting is proposed to execute on gLite as parametric jobs. Each job will be started with different initial parameters founded in the SEE++ medical databases. We plan to apply the R-GMA information system as well, such that our system will be able to discover automatically the available databases and the executer jobs on the Grid. An important security concept is the managing of the Virtual Organizations, because we have to be sure that the published medical data will be hosted only by certain trusted Grid nodes.

Conclusions:
The fact that "Grid-Enabled SEE++" is an interactive application with many finegrained jobs (the users change the eye parameters by a manual trial and error before each simulation) may make the software an interesting testcase for gLite. In this updated poster demonstration, we intend to focus on the differences between initial (but in some senses already more sophisticated) gLite version and the Globus version of our software system and to report on some comparative benchmark results.

Keywords: Medical Imaging, "Grid-Enabled SEE++"

118. Testing 65536 parallel pseudo-random number streams

Author: Reuillon, Romain (LIMOS)
Co-author: Hill, David (LIMOS)

Short overview:
Some Monte Carlo simulations execute many independent replications to converge. They should therefore be considered as killer applications for the Grid infrastructure. However distributing stochastic simulations requires many independent high-quality pseudo-random number streams. We have run a statistical test battery on the EGEE Grid in order to test 65535 streams generated by a recent parallel pseudo-random generator: the parametric Mersenne Twister.

Analysis:
Monte Carlo simulations are typical Grid applications, they are considered as naturally parallel because many replications of the same experiment can be distributed on multiple execution units to reduce the global simulation time. However, one needs to take care of the underlying random number streams and ensure that the generated streams do not show intra or inter-correlations. TestU01 is a well known stringent sequential statistical tests battery that aims to detect defaults on pseudo-random number sequences. Matsumoto designed a parallel version of a very good and famous pseudo-random generation algorithm called Mersenne Twister. With a parameterization technique, we have generated independent parallel Mersenne Twisters that have to be tested for statistical deficiencies using TestU01. The best generators can then be safely used in parallel for nuclear medicine Monte Carlo simulations.

Impact:
We have generated 2^16 parameters for the Mersenne Twister parameterization algorithm. This leads to 65536 different Mersenne Twisters which have to be tested separately, knowing that the full test battery can take more than 24 hours on nowadays processors. In order to dispatch this computing load, we have then used the DistMe software framework to generate jobs for the runtime management software package called Ganga. Each job is testing one of the generators. We have run this huge set of jobs in separated Ganga instances to accelerate the job submissions. Each job ran during 8 hours (for a total of 60 CPU years), we could not achieve this kind of task without a computing Grid. Such independent random streams are crucial in parallel Monte Carlo simulations for nuclear medicine.

Conclusions:
We have tested 65536 independent pseudo-random number streams. To achieve this work, we have installed our test battery on 54 tagged computing elements (CE – VO BIOMED). The scheduling of jobs has been entirely done by resource brokers. The output text files, weighing each around 100 KB, were collected using the output sandboxes. The next step is to test cross-correlations between the different pseudo-random number streams. The amount of work is growing exponentially with the number of streams.

Keywords: Statistical tests, parallel pseudo-random numbers, Mersenne Twister, parameterization, Monte Carlo.

119. EDGeS: integrating EGEE with desktop Grids

Authors: R.Lovas, P.Kacsuk (MTA SZTAKI); O.Lodygensky (CNRS LAL IN2P3)
Co-authors: M.Cardenas Montes (CETA-CIEMAT); F.Gilles (INRIA); T.Kiss (Univ. of Westminster); I.Kelley, (Univ. of Cardiff); F.Araujo (Univ.of Coimbra); A.Emmen(Stichting AlmereGrid); M.Van Leewen (Fundecyt)

Short overview:
EDGeS (a new FP7 project) will interconnect Service Grids (SG) with Desktop Grid (DG) systems. The primary SG in the project will be the EGEE infrastructure and the primary DGs will be BOINC and XtremWeb. EDGeS will investigate how such an integrated SG-DG infrastructure can be established, how applications can be adapted and developed for such an infrastructure, and how the execution of those applications can be controlled and managed on the new integrated SG-DG infrastructure.

Analysis:
For the EGEE users, having the option to enhance jobs with the ability to seamlessly migrate them to a DG environment will open up new possibilities and enable more widespread and frequent use of data challenge problems that require massive resources. Large DGs far outstrip the performance of even the largest supercomputers, and although DGs are certainly not intended, nor suited, for every application, especially those that are tightly coupled and require inter-processor communication, they have proven to be very beneficial for a wide range of applications, including many that are currently being run on expensive supercomputers and clusters. E.g. most parameter sweep applications of EGEE can easily be migrated into the connected DGs. The EGEE-DG Bridge will provide a mechanism to migrate these applications to a Desktop Grid environment when needed, thereby freeing up resources for use by tightly coupled MPI applications that require low latency inter-processor communication.

Impact:
Currently the SG and DG infrastructure provider communities are completely separated. Although some preliminary experiments have been conducted between CERN and IN2P3 to try to make interoperable the EGEE Grid and XtremWeb these experiments were in initial status and in practice the two communities have been developing and maintaining their infrastructure completely independently. As a result, their infrastructure, their user communities and their resource providers have been completely separated, too. This project will lead to a real turning point in the relationship of these communities. As a result of EDGeS a combined e-infrastructure will be established with the following advantage: large number of desktop resources can be reached by the EGEE user community through public and local DG systems connected directly to EGEE. It is not only the scale that makes this vision very attractive but also its sustainability by involving home, school, city and company based computers.

Conclusions:
EDGeS will create a production EGEE->DG and a DG->EGEE bridge. DG systems require validated applications that can be 100% trusted by PC donors and hence EDGeS will provide an application validation service and a repository of validated applications. EGEE users can run the validated applications not only on EGEE but also on the connected DGs. Six DGs will be connected with more than 100.000 PCs: two new DGs devoted to EGEE, Extremadura DG, SZTAKI DG, AlmereGrid, Westminster DG, IN2P3 DG.
Keywords: service Grids, desktop Grids, volunteer Internet computing, application validation

Further information: www.lpds.sztaki.hu/edges

120. GridAE a Grid-based framework for artificial evolution applications

Author: Sener, Cevat and Ketenci, Ahmet (Middle East Technical University)
Co-authors: Sahin, Erol and Sivri, Umit (Middle East Technical University)

Short overview:
Artificial Evolution (AE) is an approach, inspired from the famous theory of evolutions of Darwin, which can generate solutions for complex optimization problems. The approach relies on computing the "fitness" (quality) of a population of candidate solutions, and employed in many areas such as engineering, computer graphics, medical imaging. However, one limiting factor is the high cost of "fitness computation" of solution candidates, requiring it to run on federation of computational resources.

Analysis:
The candidate solutions found in AE are used to generate "offsprings" based on their fitness values; fitter candidates generating more offsprings into the next generation. This makes the entire computational requirements tend to be proportional to that of evaluating a single individual. Hence, the fitness evaluations of candidate solutions need to be spread over a large number of processors to make the whole process viable. The development of GridAE (supported under the SEE-GRID2 project) aims to create a Grid-based framework for AE applications by porting the idea and experience of our earlier study, Parallelized Evolution System (developed as a part of our Swarm-bots project to be run on clusters), onto the Grid. This framework should create a transparent interface for the AE user (similar to BEAGLE or GAlib), which would manage the execution of the evolution on the Grid, to be achieved both as a command line interface and a GUI through a portlet on the TRGrid P-GRADE portal.

Impact:
The GridAE framework employs the master-worker paradigm with the modules below: Interface to Framework (IF) interacts with the user. Currently, the command-line version is in use, and its portlet version (to be included in the TR-Grid portal) is under development. Job Manager (JM) is the application initiator running on a gLite UI host. It starts up master and worker jobs, monitors them to achieve fault tolerance, and controls the iteration of the evolution process. Instant Messaging (IM) service layer has been developed on top of gLite SE through lcg_utils calls to LCG File Catalogue. It provides messaging, using temporary files, among the master and workers running within an AE application. Each of the worker modules calculates a series of fitness values belonging to a group of individuals using the user-defined fitness function. Master module finds the best solutions, out of the ones provided by the workers, using the user supplied parameters for selection, crossover and mutation.

Conclusions:
We are now testing and debugging the framework on the multi-Grid-sites using sample applications on robotics. We have achieved the messaging requirements among the master and workers by adding the IM layer on the SE services. The main difficulty was due to some malfunctioning sites, which has been attacked by adding monitoring function to our job manager module to achieve fault-tolerance. Currently, its command-line interface is in use, and also a portlet is under development to provide a GUI.

Keywords: Artifical Evolution, Messaging, Robotics, Application Framework, Master-Slave

Further information: Application Home: "http://Gridae.ceng.metu.edu.tr/"

121. Grid enabled applications for modeling, simulation and optimization

Authors: G.Neagu, N.Andrei, and V.Sima, (ICI Bucharest); V.Cristea, (UPB, NCIT); C.Nae (INCAS Bucharest, Subsonic Wind Tunnel Laboratory); R.Potolea (UTCN); D. Petcu (WUT)
Co-authors: A.Stanciu (ICI Bucharest); F.Pop (UPB, NCIT); V.Pricop (INCAS Bucharest); A.Suciu (UTCN); D.Zaharie (WUT)

Short overview:
The applications have been ported to Grid infrastructure within the project "GridMOSI-Grid technology based virtual organization for high performance modeling, simulation and optimization" funded by the Romanian Research of Excellence Programme. The project aims at setting up the first national VO providing the research and academic community with access to advanced MOSI solutions in different domains according to the scientific expertise of partner organizations.

Analysis:
The candidate applications to be ported on Grid were selected based on the following criteria: mature implementation in classic mode, extensive memory and/or computational requirements, Grid as innovative approach for the given MOSI domain, expected user community in research and academic area, potential interest from industry. The list of selected applications includes: GridModRed - Model Order Reduction, GridIdent - System Identification, CGALLP and BIBFR – Unconstrained optimization based on conjugate gradient algorithms and Related high performance library (developed by ICI Bucharest), OPT-GT and MFCC - Optimizer based on Grid Technology and Application cluster for CFD-FEM oriented simulation (INCAS Bucharest), DEMO/G - Distributed Evolutionary Multiobjective Optimization on Grid (WUT), CryptoGrid - Cryptographic and Cryptanalitic Algorithms for the Grid (UTCN), DIOGENES - Application oriented task scheduling using genetic algorithms (UPB).

Impact:
The GridMOSI infrastructure includes 5 sites with counting for about 130 kSI2k computing power and 9 TB of memory. One of them is active in the EGEE infrastructure, while all the other are in preparation to join this infrastructure during EGEE II project. All of them support the GridMOSI VO. Applications are running either in Cluster mode (GridModRed, GridIdent , CGALLP, OPT-GT and MFCC) or in both Cluster and Grid modes (DEMO/G, CryptoGrid), taking advantage of DIOGENES capabilities to optimize job scheduling based on the information coming from information and monitoring services available in the GridMOSI infrastructure. The project portal provides access to the web based user interface (currently under implementation for each application), which facilitates the selection of execution conditions, depending on application specificity: class of algorithms and their execution mode, architectural variant, requested Grid resources.

Conclusions:
The main challenges of the project are to improve the visibility and accessibility of selected MOSI solutions, to coagulate a user community from both academia and industry, to gradually enlarge the VO offer by attracting new solution providers, to improve the potential for international cooperation. Current applications are in the final stage of their porting to Grid. Main difficulties have been related with the limited experience, low network speed that limits the performance level.

Keywords: VO, advanced system modeling and optimization, CFD, application scheduling, cryptography

Further information: www.Gridmosi.ro (site under development, first draft of Romanian version available)

122. Service-oriented applications development support in gLite

Author: Goranova, Radoslava (University of Sofia, Bulgaria)
Co-author: Dimitrov, Vladimir (University of Sofia, Bulgaria)

Short overview:
Service-Oriented Architecture (SOA) is an architecture within which all functions are defined as independent services with well-defined invokable interfaces, which can be called in defined sequences to form processes. gLite is by idea service-oriented Grid middleware, but do not provide the whole set ot tools for development of end-to-end processes.

Analysis:
Basic characteristics of service-oriented architectures are self-describing interfaces in platform-independent XML documents and interoperability between different systems and programming languages. gLite provides a lot of Grid services but very few of them have self-describing interfaces with endpoints and WSDL documents. The lack of WSDL files for main gLite Grid services make them very hard to use in service-oriented Grid application. And moreover, the end user often needs more complex functionality, which can be achieved as composition of Grid services or Grid processes.

Impact:
The evolution of gLite to SOA support will permit development of SOA based Grid applications and something more – deployment of SOA based application to Grid environment. One of the most important tools for SOA based applications is process orchestrator tool. After some consideration of available tools for such purpose in Grid middleware we decide to use Oracle BPEL PM. The tool is installed on SLC 4.5 operating system. An example process was developed as composition of gLite Grid services.

Conclusions:
Integration of process orchestration tool in Grid middleware will facilitate the deployment of Grid application in Grid middleware and will better the possibilities for more effective use of Grid through portals.

Keywords: Grid, service-oriented architecture, process management, Grid processes

Further information:
http://www.mff.cuni.cz/veda/konference/wds/contents/pdf07/WDS07_113_i2_Goranova.pdf

123. Smart adaptative identifier for a medical data retrievement system

Author: De Vlieger, Paul (ERIM / LPC)
Co-author: Boire, Jean-Yves (ERIM INSERM ERI 14)

Short overview:
At the time where we talk in Europe about a system to ease patients' access to all their medical history, this issue causes a lot of difficulties. Actually patients who want to build it need to manually visit all medical centres they ever consult. However, the main problems lie on security: for that, hospitals and all other medical structures adopted a high protectionist policy by keeping inside their own buildings all patient data. The Grid technology can help us to overcome this problem.

Analysis:
Grids provide a lot of possibilities in terms of data storage and exchange. By using the telemedecine application developed at LPC Clermont-Ferrand we plan to add some functionality to manage patient data throughout medical centres. To get back all data around Europe concerning a patient we need to be able to identify these data ownership while certifying that alone, it must be impossible to regain the patient id by using data encryption technologies. For that we decided to consider the patient as the center of the medical data retrieval system. The idea is to store a scalable and dynamic identification number, stored in the patient' smart card and this identifier should be the key to regain all data regarding this patient. Each part of this identifier matches an accurate medical act in the patient life. So the data retrieval system consists in an analysis of these parts, a download of associated data and a decryption.

Impact:
The two parts: patient «number» and act key will be sufficient to retrieve the associated data. So for each kind of medical act, we would be able to find everything we want wherever they are located just with the data inside the patient smart card. Finally the goal is to ease the patient access to their medical historic. Due to the high secure behaviour inside medical structures, it's completely impossible to get out data form these structures. Of course a centralized server isn't the good way to follow. The main advantage of the Grid is its capability to overcome the problem of accessing distributed data. We can use this technology to offer a high level abstraction of data management. The user should ask for a request and the Grid sends this one to all concerned databases inside several locations. After that, we can use the computation power of the Grid to put forward a bridge between data management and medical imaging treatment especially for high-cpu-time consuming 3D algorithms.

Conclusions:
Everything needs to be done, and for the beginning, we plan to test this method inside a small test structure: the ERIM, located at the Clermont-Ferrand hospital can directly access to both Grid and hospital network. If we obtain a well-structured tool we plan to spread it inside several locations to test it in a real-case application. After that, everybody knows that the crucial point is located in the hospital and medical structures management.

Keywords: medical history, distributed databases, data encryption, smart identifier

124. Evaluation of EGEE-Grid security

Author: Fouossong, Dorine (IN2P3-LPC)
Co-authors: Breton, Vincent (IN2P3-LPC); Reichstadt, Pierre Louis (IN2P3-LPC); Liauzu, Stephane (IN2P3-LPC)

Short overview:
AUVERGRID is developing an activity in the field of security management which aims at answering the question of many Grid users and administrators: «How much can I trust EGEE security features and services?". Our goal is to provide a formal response to site security managers, and Grid users.

Analysis:
Our first goal is an evaluation of the overall security. Using the Grid introduces in the information system of a laboratory or a company new infrastructure and processes that have to be taken into account in the management. This is especially true in the security management, where relevant subsystem should be introduced in the trust chain. The trust chain is the subset of the information system that is "secure" in terms of the security strategy plan of this specific firm. The everyday work of the security manager is to deploy and maintain that trust chain. A good management strategy in our terms should follow the Deming Wheel: plan, do, check, act. Our work is mainly concerned by the third point which is "check" as it evaluates the security level of the new trust chain (modified to take in account the EGEE-Grid resources). Thus, this activity should contribute significantly to the security risk management of the EGEE-Grid environment.

Impact:
This activity is complementary to the other activity dealing with security in EGEE. In fact, EGEE Grid Security provides the basis for Grid security (operational management tools and security infrastructure), and ISSEG focuses on practical expertise on the deployment of integrated site security; our activity, as described above, aims at providing assessment. The activity will produce feedback for those projects. Finally, the ISMS (Information Security Management System) deployment task will be made simpler to security manager who are dealing with EGEE-Grid.

Conclusions:
The approach is pragmatic because it focuses on results and is iterative. We work on both technical and organisational sides by checking the vulnerability risk assessment of software and auditing operational guidelines for the use of the Grid. Achievement of security objectives is measured against the standard ISO27000s. That will lead us to get a formal estimation of the level of maturity for integrated security one could expect from EGEE resources.

Keywords: Grid security, security risk mitigation, authenticity, secure access, authorization

125. The Dutch Grid

Authors: Dr. Bouwhuis, Maurice (SARA); Dr. Jansen, Machiel (SARA); Mr. Van Beek, Pieter (SARA)

Short overview:
This paper will describe the distributed infrastructure called the Dutch Life Science Grid and the applications using it.

Analysis:
Today's Life Scientists need to have advanced High Performance Computing facilities at their disposal. For that reason, and commissioned by the Dutch BioInformatics Centre (NBIC) and the Dutch Grid infrastructure project (BiGGrid), SARA places, maintains and supports small but powerful computer clusters at the local sites of academic medical hospitals and universities. These clusters are interconnected by high speed network connections and can be used simultaneously by the use of GLITE Grid middleware. A number of Use Cases have been formulated and development of a number of biological applications running on this infrastructure is in progress. Among the areas which are involved are metabolomics, proteomics and micro array analysis. The use cases describe several biological pipelines which will be realized by Grid and web services, interconnected by workflow descriptions.

Impact:
For some scientific disciplines, such as high energy physics and quantum chemistry, High Performance Computing (HPC) is part of the standard toolkit. For other scientific disciplines, for example the Life Sciences, this is not yet fully the case. In addition to Grid access the Duch Life Science Grid offers the life scienctist standard batch-type access to a single cluster's compute and storage facilities in order to make the use of it as low threshold as possible and facilitate easy debugging of applications. In a sister project the NBIC provides the hosting institutes with scientific programmers to Griddify the life scientists's applications.

Conclusions:
The Dutch Life Science Grid is in operation and is being used by Dutch Life Scientists. It currently consists of Grid nodes at five locations. Over the coming 18 months another 10 locations will be added to this.

Keywords: Grid facilities, Life Science,

126. Development and adaptation of a Web-enabled in silico oncology application in Grid environment

Authors: T.Athanaileas, A.Menychtas, G.Kousiouris, D.Dionysiou, G.Stamatakos (NTUA)
Co-authors: D.Kaklamani, T.Varvarigou, N.Uzunoglu (NTUA)

Short overview:
A Grid-enabled simulation tool for large scale in silico oncology simulations has been developed. In silico oncology aims at mathematically describing and computationally simulating the multiscale biological mechanisms that constitute the phenomenon of cancer and its response to therapeutic techniques. The application has been ported to EGEE infrastructure and a web based interface has been implemented for providing a user-friendly environment and additional QoS and management functionalities.

Analysis:
This tool was developed following a multi-tier architectural approach in order to provide access to the core Grid services through a state of the art web interface. Initially the in silico oncology source code was modified to facilitate the execution of simulations to Grid nodes using parameter files that are automatically created from the end users using the tool. Additionally, Grid specific wrapper-scripts were developed for setting up the simulation and for gathering useful statistics for the QoS mechanisms. The end users exploiting these mechanisms' functionalities were able to create dynamically simulation specific JDL files based on the user requirements and on the status of the Grid infrastructure. Finally a web portal was designed and developed that simplified the access to the Grid resources and automated the job submission and monitoring. This portal enabled additional services to the framework, such as user management and job scheduling based on QoS criteria.

Impact:
Exploitation of the vast resources provided by a Grid may lead to a better understanding of the biological and clinical behavior of cancer and especially solid tumours. Furthermore, computer simulation may be employed in order to optimize treatment of cancer, by conducting a number of simulations for different therapeutic schemes based on the individual data of a patient. As the number of possible therapeutic schemes and consequently the number of simulations increases, the time required for evaluating and comparing the effects of the different schemes may become forbiddingly high. Exploiting Grid computing is a very attractive solution, as the resources provided in a Grid infrastructure may be efficiently used to reduce overall required execution time in a handy, cost-effective and efficient manner. Additionally, this framework guaranteed high level of QoS for the end users utilizing the experience of the past job submissions and the status of the Grid infrastructure.

Conclusions:
This tool provides a web-based, user-friendly interface with added functionality, for performing parameter-sweep simulations on the resources provided by the EGEE infrastructure. The vast resources available in the Grid enable the evaluation and comparison of different therapeutic schemes, while the access to these resources was considerably simplified through the web portal. The tool has been utilized in order to perform comparative simulations for a large number of radiotherapy schemes.

Keywords: In silico oncology, Grid portal, HellasGrid, EGEE, Grid-app, QoS

Further information: http://www.gsrt.gr/default.asp?V_ITEM_ID=4318

127. Workflow meta-scheduler for Grid environments

Authors: Pop, Florin (University "Politehnica" of Bucharest); Cristea, Valentin (University "Politehnica" of Bucharest)

Short overview:
Based on the analysis of DAG scheduling methods, we proposed an algorithm for workflow scheduling in Grid environments that respects the total scheduling time, the schedule length and load balancing. It provides efficient resource utilization by minimizing the idle time on the processing elements. Experimental results are provided to support the performance evaluation of the algorithm and compare them with other scheduling strategies. The algorithm has been integrated in the DIOGENES scheduler.

Analysis:
Based on our contribution to the 2nd EGEE User Forum, we extend the DIOGENES (DIstributed Optimal GENEtic algorithm for Grid application Scheduling) project that provides a solution to the Grid scheduling problem at application level. The extension consists of a new algorithm that aims to achieve a distributed, faulttolerant, scalable and efficient method for dependable task (DAG) assignment in Grid environments. Several metrics including scheduling time, scheduling length and load balancing are used to highlight improved behavior of our proposal as compared with other existing scheduling strategies (HLFET – Highest Level First with Estimated Times, ETF – Earlier Time First, MCP – Modified Critical Path). The scheduling priority is represented by the ALAP (As Late As Possible) parameter. The improvements are made in the node sorting step: defining additional criteria for nodes with the same ALAP and use of descendant prediction to improve the critical path.

Impact:
The proposed algorithm is useful in heterogeneous environments in which the optimization of task workflow scheduling leads to performance improvement. The algorithm has a quadratic polynomial time complexity. Example applications that generate workflows can be found in many application domains. In particular, for satellite image processing, some tasks that process an image segment (a region or a spectral band) could send their output (associated with attributes such as the resolution used in processing) to other tasks in a flow, or could create, configure and submit new tasks. For these applications, the integration of the proposed algorithm in DIOGENES meta-scheduler, which uses an agent framework for management and communication, offers access to different clusters in Grid and intercommunication between different VOs. The scheduler doesn't control the clusters/resources directly. We can consider it closer to Grid applications and consider user requirements as optimization criteria.

Conclusions:
The proposed algorithm provides improvements of critical path based on using a heuristic prediction. The impact of the algorithm is directly visible in integration with an existing Grid meta-scheduler, DIOGENES used in national and international projects (MedioGRID, SEE-GRID). The future plans for extensions refer to coallocation of resources in scheduling process for a set of tasks with dependencies, and to the prediction the Grid status for building an advance reservation mechanism.

Keywords: Grid scheduling, DAG scheduling, Task Dependencies, Workflow Applications, Optimization, Heuristics.

Further information: http://diogenes.Grid.pub.ro

128. Advantages of pre-production WLCG/EGEE services for VOs and users

Authors: N.Thackray and A.Retico (CERN); C.Fernandez Sanchez, E.Freire Garcia, A.Simon Garcia, J.Lopez Cacheiro (CESGA)

Short overview:
The benefits that the Pre-Production Service (PPS) can offer to VOs and new users will be shown. Current PPS processes will be described so they have a better understanding of the PPS environment. PPS offers a proper place where VOs can test their applications and check their compatibility with upcoming middleware releases. PPS could help VOs improve their applications and at the same time, VOs would be helping PPS to produce better tested middleware releases that would go into Production (PROD)

Analysis:
Currently a well-defined set of procedures is followed in PPS, beginning with the pre-deployment activity and finishing with the approval of a new middleware release that can go into PROD. The PPS Coordination Team takes care of supervising all these steps, mainly trying to spot possible bugs in the middleware before it goes into PROD. Unfortunately, VO contribution in this part of the deployment is currently very limited and the PPS team does not have a full feedback from these important groups. One of the problems is that PPS is not very well-known for many VOs and users and this situation should change. When a VO has a new application or there is an upcoming middleware upgrade, they should be aware that they can test it in PPS, helping to discover possible problems before going into PROD. Indeed, PPS sites have a great quantity of free resources that can and should be used. Finally, VO and users should remember that PROD is a critical service not to be used for testing purposes.

Impact:
The PPS team tries to find all possible bugs that could be encountered in upcoming middleware versions before these versions are submitted to PROD. This is a critical process in the middleware release cycle because the fact that the final software released to Production works correctly depends on the effort made in PPS in order to find all possible failures. Regarding VO's software, at this moment it is only tested in PROD sites (with all the risks that this entails). Applications are not tested against upcoming middleware versions before they are actually deployed into PROD. This means that problems are usually detected too late. If VOs and users start to test their applications in PPS they check their compatibility with new middleware before it is actually released to PROD. At the same time they would be helping to discover possible bugs in the middleware that could be corrected before it is released. At the end everybody will benefit from a better production environment.

Conclusions:
PPS could be the proper place where VO can test their applications and check in advance the compatibility with new middleware releases; helping at the same time with their work to discover bugs in the middleware before it is deployed to production. As well PPS could be a good place for VOs to deploy new versions of their applications or even new services before they are moved to the production environment. We hope that after seeing the poster more VOs and users will be interested in using PPS.

Keywords: Pre-Production service, PPS coordination team, PPS pre-deployment team

Further information: http://egee-pre-production-service.web.cern.ch/egee-pre-production-service

129. Decentralized access to medical images in research and enterprise PACS applications

Author: Kukhanek, Tomas (CESNET)
Co-author: Sarek, Milan (CESNET)

Short overview:
The aim of this paper is to introduce the pilot project of enterprise PACS (Picture Archiving and Communication System) in the Czech Republic which is deployed next to the existing Metropolitan PACS MeDiMed (Metropolitan Digital Imaging System in Medicine) using the service oriented architecture (SOA) style and Grid technologies for distributed systems. This project follows the idea to build decentralized system used to exchange medial images.

Analysis:
A significant activity in the classic distributed solution with computer servers and long-term storage devices of high capacity is the MeDiMed project (Metropolitan Digital Imaging System in Medicine), where the Masaryk University in Brno cooperates with a range of university and city hospitals. To be interconnected they take advantage of the CESNET2 high speed computer network. The goal of the MeDiMed project is to create shared outsourced medical multimedia data archiving and communication center (Metropolitan PACS). The presented pilot project is a parallel project next to MeDiMed. It provides an interface able to operate in DICOM standard (Digital Imaging and Communications in Medicine). It allows interchange medical images with modalities (e.g. medical devices or software application) and with existing PACS (e.g. with the mentioned MeDiMed).

Impact:
The pilot project uses the Globus MEDICUS project as a test DICOM interface build upon the OGSA Globus Toolkit - opensource Grid implementation. This integration provides replication service and failure recovery and allows to integrate federalized authorization. The main services of the pilot project follow SOA principles to allow flexible evolution of these services. These follow the idea to enhance the existing Metropolitan PACS using the new concepts and allowing key features of reliability the access to the data.

Conclusions:
The pilot project is now deployed to the high speed CESNET2 network as a site-level service. The interconnection is being treated between existing Metropolitan PACS in Brno and Central Military Hospital in Prague. There is planned other distribution of the Grid nodes of the pilot project into the Central Military Hospital in Prague and into the First Medical Faculty of Charles University in Prague.

Keywords: PACS, DICOM, medical imaging Grid

Further information: http://medicus.cesnet.cz

130. Interaction of a 3D finite-difference application for computing synthetic waveforms with the Grid infrastructure

Authors: Skarlatoudis, Andreas (Geophysical Laboratory, Univ. Thessaloniki); Korosoglou, Paschalis (Grid Operations Centre, A.U.Th.); Kanellopoulos, Christos (Grid Operations Centre, A.U.Th.); Papazachos, Constantinos (Geophysical Laboratory, Univ. Thessaloniki)

Short overview:
Thessaloniki is lying across Thermaikos gulf in the Northern part of Greece. Its moderate earthquake activity is controlled by a significant number of active faults, striking in close distances from the city (Papazachos et al, 2001). The city's geographical position and financial importance imposes the need for a thorough and complete study of the structure and the expected ground motions.

Analysis:
The aim of this study is to shed some light into the ground motion properties of Thessaloniki in 3 dimensions. Using a computer code that implements a 3D - 4th order staggered-Grid velocity-stress finite-difference (FD) scheme (Moczo et al., 2002) full 3-dimensional synthetics of ground motion have been computed. The studying Grid covers an area of 63 km2 with a depth of 12 km, which is translated in approximately 47x108 nodes. The execution of the 3D FD code is very demanding in terms of CPU power and computer memory and for the previous Grid the memory demands reach the 20 GB and the time of computations is approximately 30 hours in a 4-processor machine.

Impact:
The Grid infrastructure could significantly contribute in minimizing the execution time of the code and eliminating the high cost investment for number crunching machines, which can be prohibitive for small working groups. So far we have developed a workflow on top of basic gLite utilities and have performed a series of test runs using coarse models to check that our results on the Grid match the ones obtained from other computational infrastructures. The evolution of the present work involves computation of synthetic waveforms for a larger studying area and for higher accuracy on the computational domain. Our imminent target is thus to successfully run computational models that require approximately 70-80 GB of accumulative computer memory and ~100 CPUs. The result from this first phase of test runs will determine our next steps and whether we will attempt to run even higher precision models.

Conclusions:
The final goal is to obtain 3D synthetic waveforms that will be representative of the expected ground motion for the city of Thessaloniki and if possible to minimize uncertainties in the available structural models.

Keywords: Earth Sciences, seismology

131. GEOSCOPE applications on EGEE

Authors: Weissenbach, David (CNRS); Clevede, Eric (CNRS); Stutzmann, Eleonore (CNRS)

Short overview:
The French worldwide network of digital seismological stations GEOSCOPE has collected during the past 20 years hundreds GB of seismological data. Several applications using this dataset have been running on EGEE over the last year, also allowing to register the dataset in EGEE catalogues for a more convenient and scalable access for future applications.

Analysis:
For now, applications dealing with seismic noise (signal collected between earthquakes, more than 99% of the data) or major earthquakes are taking advantage of the Grid facilities:

- average seismic noise level per day over the past years is computed
- polarized noise and source determination also over the past years

Although much more demanding on CPU time, this was achieved faster than the corresponding raw noise calculation as GEOSCOPE data was already transferred on EGEE. - source and mechanism determination for large earthquakes. It is still one of ESR's most successful application on EGEE as hundreds hours of computing time are completed during a very short period, delivering the results almost right after the data is available.

Impact:
It is yet the first time that seismic noise is thoroughly determined over a long period. Coming articles will detail the various incomes. Earthquake source mechanism is determined almost for every major event (magnitude over 6.8) and reported through the GEOSCOPE web site.

Conclusions:
Any production using GEOSCOPE dataset as input will be much faster since it is directly available on EGEE and needn't to be obtained from the GEOSCOPE data center which is unable to scale to a rate even far below Grid possibilities. Seismic noise is going to be computed as averages over 2 hours periods (day averages were produced up to now).

Keywords: earth sciences, seismology

Further information: http://geoscope.ipgp.jussieu.fr

132. Implementation of geospatial services in gLite: the RISICO case study

Authors: Angelini, Valerio (CNR-IMAA); Mazzetti, Paolo (CNR-IMAA); Nativi, Stefano (CNR-IMAA)
Co-authors: Dal Pra, Stefano (INFN); D'Andrea, Mirko (CIMA Foundation)

Short overview:
The CYCLOPS project is a FP6 SSA which aims to bring together two important Communities: GMES and Grid, focusing on the operative sector of European Civil Protection (CP). Recently RISICO, a pre-existent Civil Protection application for forest fires risk assessment, has been successfully ported to gLite. As a further step we discuss which benefits could be granted to the CP application, implementing an intermediate layer of geospatial web-services between the CP environment and gLite.

Analysis:
RISICO presently runs in gLite accessing input data stored in a SE using various proprietary formats. Our aim is to integrate this application with a framework of standard geospatial web services to gain more flexibility. In this case the data will be stored in standard formats (GRIB) and will be accessed through standard interfaces. The workflow will be as follows:
-The CP user selects an area in which the model should be run, selects the input data URIs and indicates an appropriate priority for the action;
-A Web Processing Service (WPS) receives the request,evaluates the input size and the priority, and then activates various independent data access services (WCS/WFS) which split the input data;
-When the various inputs have been set up, the WPS spawns and distributes an adequate number of jobs on the Grid. These are responsible for the execution of the core algorithm;
-When all the jobs have correctly run, the WPS takes care of merging the results and publishes them to the CP user.

Impact:
With this new approach, new use cases could be easily implemented with a limited effort:
a) in case of an emergency the CP could easily choose to increase the priority of the run, telling the WPS to submit the algorithm on a greater quantity of WN to get the results in a shorter time. Alternatively WPS could run the algorithm on a specific region with a better resolution;
b) the same algorithm could be run using data accessed through standard interfaces from different data providers on the same region for increased availability and for comparison purposes.
c) in future scenarios different algorithms accessible trough the standard WPS interface could be run on the same data inputs for output comparison and integration.

Conclusions:
A prototype of RISICO that makes use of the Grid enabled WPS and WCS services is under development. This project is going to be part of the OGC-OGF interoperability initiative.

Keywords: civil protection, geospatial services, interoperability, forest fires, risk assessment, workflows, GMES

133. Astronomy and astrophysics applications on EGEE from Paris, Grenoble, Lyon and Strasbourg observatories

Authors: Lecubin, julien; Dubernet, Marie-Lise; Le-Petit, Franck; Le-Sidaner, Pierre; Berthier.
Co-authors: Roueff, Evelyne; Roy, Fabrice; Schaaf, Andre; Semelin, Shih, Albert; Slezak, Eric; Sol, Helene; Spielfiedel, Annie; Stehle, chantal; Taburet, sylvestre; Thuillot, william ; Valiron, pierre; Valls-Gabaud, David; Wiesenfeld, Laurent (LAOG); Wozniak, Herve; Alimi, Jean-Michel; Balanca, Christian; Combes, Francoise; Chilingarian, Igor; Corasaniti, Pier-Stefano; Di Matter, Paola; Faure, alexandre; Feautrier, Nicole; Fouchard, Marc; Frouard, julien; Godard, Benjamin ; Lainey, Valery; Le Bourlot, Jacques; Lenain, Jean-Philippe; Lesaffre, Pierre; Menard, Francois; Razera, Yann; Revaz, Yves

Short overview:
We present the french project for Astronomy and Astrophysics in the cluster A of EGEE III. The scientific interests cover a broad range of hot topics as simulations in cosmology and galaxies evolutions (HORIZON project), simulations for celestial mechanics, atomic and molecular computations, models for the interstellar medium for Herschel/ALMA observations, data-processing with workflows, design study of the Cherenkov Telescop Array for high energy astrophysics.

Analysis:
Numerical simulations, data analysis, as well as design study for new instruments and telescops, often require important computing time. If is not uncommon that the analysis of a single observation requires to run a huge number of times the same simulation code to explore the parameters space. On the other hand, the same reduction pipeline has to be used several times for data reduction of a set of observations. On the other hand, the physics introduced in simulation codes may be limited due to computing time restrictions. By sharing computing facilities thanks to Grid technology, we can expect to work faster and to go further in the detail of the physics of simulations

Impact:
A applications require the deployment of codes on the Grid on the fly and in a transparent way. The sharing of computing facilities between different institutes thanks to Grid technology as EGEE will allow the A community to work in a more efficient way, to share codes and to facilitate collaborations. Thanks to EGEE, the A applications will allow to have a fast return of space and ground missions such as Herschel/ALMA, to more detail the physics in numerical simulations. As examples this concerns the exploitation of the theory in the virtual observatory, collaborative projects such as HORIZON, scientific preparation and exploitation of observational space and ground missions such as HERSCHEL/ALMA and design study of new instruments as CTA

Conclusions:
The Astronomy and Astrophysics community is beginning to adapt simulations and reduction pipelines for Grid technology. If we have not yet experience with EGEE, we have experience on two other systems: Grid'5000 (HORIZON collaboration) and CIMENT (Astrochemistry and Radiative transfer), the Grenoble regional Grid. CNRS researchers in Grenoble have been involved in the specifications and testing of CIGRI, and have demonstrated its ability to tackle large campaigns of millions of jobs.

Keywords: Astronomy, Astrophysics, High energy physics, Cosmology

134. EGEETomo: 3D electron tomography on EGEE. A user-friendly and fault-tolerant Grid application

Authors: Bilbao-Castro, J.R. (Dept. Computer Architecture and Electronics, University of Almería, 04120, Almería, Spain); Garcia, I. (Dept. Computer Architecture and Electronics, University of Almería, 04120, Almería, Spain); Fernandez, J.J. (Dept. Computer Architecture and Electronics, University of Almería, 04120, Almería, Spain)

Short overview:
EGEETomo is a new, easy-to-use Grid application for performing three-dimensional tomographic reconstructions on the EGEE Grid. Special emphasis has been put on making this application user-friendly and fault-tolerant. User-friendly applications are not usually the norm on Grid applications, which can make non-trained users to avoid adopting new technologies like the Grid. Also, the unstable nature of the Grid makes fault-tolerance implementation a must-have on Grid applications.

Analysis:
3D Electron Tomography is a key imaging technique when studying large biological complexes like cells organelles or even whole cells structures. Projection images of the specimen are taken through electron microscopes. Nevertheless, technical limitations reduce the number and quality of the projections that can be obtained from the specimen under study. Because of this, the commonly used reconstruction algorithms, like WBP, which are relatively fast, present some limitations in terms of the reconstruction quality they provide. On the other hand, the iterative reconstruction techniques provide better reconstruction quality but at a much higher computational cost. Fortunately, the whole reconstruction task can be divided into smaller, independent, reconstruction subtasks. This makes the Grid a perfect place to run tomographic reconstructions, with hundred of long-lasting independent tasks. Nevertheless, making such application usable implies making it user-friendly and fault-tolerant.

Impact:
Previous works have shown that EGEE Grid platform is well suited to perform reconstruction tomographies. Nevertheless, command-line interfaces as well as the need to closely monitor Grid tasks status, prevents the Grid to be broadly used by non Grid-trained users. This fact motivated this work as an improvement on Grid usability for the tomographic reconstruction application. This was done through three main points; (a) user interaction through a GUI hides the Grid commands complexity and shows the information in a very readeable, interactive way, (b) fault tolerance: The Grid is huge, different points of the Grid fail at some time making our jobs to fail and our stored data to temporarily be inaccessible. Data replication as well as jobs monitoring is vital, and (c) automatic process: Since the moment the user enters needed data and pushes the go-ahead button, the whole process will run automatically, detecting and solving problems through fault-tolerance techines.

Conclusions:
Preliminary tests have shown that the application performs well in an unstable environment like a big Grid. Graphical user interface provides a fast learning curve for new users while completely hides the Grid complexity. The user interaction with the Grid is limited to entering the proxy password at the beginning of the session. Grid applications should not be limited to using the Grid to do something but doing it in a confortable and fault-tolerant way.

Keywords: 3D Reconstruction, Iterative Reconstruction Algorithms, Grid Usability, Fault- Tolerance

Further information: http://bioinformatics.oxfordjournals.org/cgi/content/abstract/btm459v1

135. A full stokes model for large scale ice dynamics simulations

Author: Zwinger, Thomas (CSC - Scientific Computing Ltd.)
Co-authors: Raback, Peter (CSC - Scientific Computing Ltd.); Grohn, Matti (CSC – Scientific Computing Ltd.); Lyly, Mikko (CSC - Scientific Computing Ltd.)

Short overview:
Current state-of-the-art ice sheet models apply scaled equations, such that even computations of large ice masses fit in a single work station. Nevertheless, this scaling prohibits correct numerical treatment of ice-domes, ice streams and ice margins with a possible transition to ice-shelves. In order to address these shortcomings the Open Source (OS) FEM software Elmer has been adapted to simulate the dynamics of ice on high resolution meshes and introduced to the EGEE environment.

Analysis:
In contrary to scaled equations, Elmer applies Full Stokes (FS) simulations, where horizontal scales of the mesh are of similar size than vertical, leading to a scale-up of the problem size by a factor 100. Models earlier run on a single workstation consequently occupy 100 and more processors if FS is applied, demanding parallel computations on clusters or Grid environments. The main focus of the work presented here is to make the needed modules for FS ice-dynamics modeling within Elmer available on the EGEE environment. With the increased capacity of the EGEE infrastructure, we attempt to obtain an enhanced resolution down to a horizontal scale in the size of a few kilometers, resulting in computations containing millions of degrees of freedom. At these scales, details such as ice streams, which were below the resolution of a standard SIA run can be investigated. This provides an enhanced insight into the mechanics and thermodynamics of ice sheets.

Impact:
First tests on the EGEE environment applied to the complete Greenland Ice Sheet (GIS), which proved to work on a coarse computational mesh, are scheduled for end 2007. The EGEE environment provides a reliable and economic platform to perform production runs on high ressolution meshes that are needed for instance for computationally extensive sensitivity studies.

Conclusions:
The OS FEM code Elmer has been ported to the EGEE environment. Currently models for using the code as a tool for high-resolution ice-dynamics simulations are being developed and tested within the environment. In close future they will provide a tool to investigate ice dynamics of continental ice sheets with resolutions down to sub-kilometer scale omitting the limitations introduced by codes applying scaled equations, as has also been demanded in the IPCC report on climate change.

Keywords: Finite Element, Geophysics, Glaciology, Ice Sheets

136. The WLCG common computing readiness challenge: CCRC`08

Authors: Mendez Lorenzo, Patricia (CERN IT/GD); Sciaba, Andrea (CERN IT); Campana, Simone (CERN IT); Santinelli, Roberto (CERN IT); Lamanna, Massimo (CERN IT); Lanciotti, Elisa (CERN IT); DI Girolamo, Alessandro (CERN IT); Magini, Nicolo (CERN IT); Miccio, Enzo (CERN IT); Shiers, Jamie (CERN IT); Renshall, Harry (CERN IT)

Short overview:
The World's biggest machine - the Large Hadron Collider (LHC) at CERN, Geneva, Switzerland- will enter operation in 2008. Using the Grid infrastructure provided mostly by EGEE and OSG, the WLCG project has been chosen to provide the computational and storage resources needs for the 4 experiments of the LHC. The goal of the Common Computing Readiness Challenge (CCRC'08) is to demonstrate that these computing facilities can be used to satisfy the needs of the experiments

Analysis:
The LHC machine will produce some 15PB of data per year. The management and the analysis of these data rely on a worldwide production Grid service involving hundreds of sites from EGEE and collaborating Grids. One significant challenge remains: to demonstrate that these computing facilities can be used to satisfy simultaneously the needs of the 4 major experiments of the LHC at full 2008 rates. During the CCRC`08 we will demonstrate precisely this. Given the importance of the challenge, two phases are foreseen: an initial run in February, when not all sites will have their full 2008 resources in place and a second period in May, when the full 2008 capacity is required to be in place

Impact:
The challenge will stress all aspects of the experiments' offline computing production and batch analysis systems. Furthermore, it will require the effort of teams spread around the entire planet, working closely in harmony. As such, it will bring together a gamut of activities, most of which have been extensively tested, but not neccessary at the full 2008 scale, not for all experiments and for all activities simultaneously. To achieve these goals, the infrastructure developed within EGEE over the past years will be exploited to the full. The results of this challenge will demonstrate the readiness of the Grid infrastructure provided by EGEE during a real data taking approach. In addition, state-of-art techniques for the design, implementation of highly reliable and resilient services, equally relevant to other application domains, are required

Conclusions:
The stress of the services under a real condition approach will allow to the WLCG to understand better the computational and storage needs in real conditions using already the Grid infrastructure that will be provided to the 4 experiments. A draft Schedule including the agreement of key services and goals, the setup of an integration plan, the review of metrics, tools for testing and monitoring, before the integration in February 2008 are the major plans to cover in a short time

Keywords: WLCG, LHC experiments, Grid services, EGEE resources, Challenge, real data taking

Further information: https://twiki.cern.ch/twiki/bin/view/LCG/LCGServiceChallenges

137. Fair Grid scheduling

Author: Medernach, Emmanuel (LPC - Clermont, France)

Short overview:
Computing Grids allow sharing of distributed resources such as CPU or storage to the service of many scientific communities. Users submit irregular bursts of jobs. This irregular usage of the Grid allows an efficient sharing of resources because unused resources can be collected this way. Jobs are mono-processors and arrive on-line to clusters. Jobs on a cluster are independents; they could be run in any order. Pre-emption is not used Because of memory and communication costs.

Analysis:
Jobs durations vary a lot among groups or users depending of the kind of applications. For instance a group dedicated to test the middleware have 90% of their jobs of duration less than 5 minutes. Biomed jobs have a quarter of jobs running less than 2 minutes, another quarter between 2 minutes and 8 hours, another quarter between 8h and one day and the last quarter between one day and 3 days. Other groups have many jobs running up to 3 days. Each site have to schedule jobs coming from the Grid in an efficient and fair way. Site needs sometimes to be able to justify part of resources granted to groups or users. Consequences of unfairness are possible leaving of groups or users. These differences in the way jobs are scheduled could lead to unfair treatment of users or groups. We propose to take fairness into account when dealing with multi-users scheduling problems and to seek how scheduling could be improved in order to be fair.

Impact:
As in load balancing resources may be badly distributed at the expense of everyone. The objective is not to starve users but on the contrary to maximize fairness between users. How to measure the quality of a schedule with respect to fairness? One criterion is evaluated for all users, this leads to a vector of evaluation indexed by users. We have to compare these vectors with an order expressing fairness. An order is fair is and only if it is symmetrical and if it is decreasing if 2 values are changed so that their minimum decrease. For instance [5, 3, 2, 8] is less fair than [5, 4, 2, 6] because of the second user. By maximizing such order, it is impossible to increase a user without decreasing another user who has less than the first one. Such order is the Leximin ordering and cannot Be represented with a scalar function. This means that we cannot always obtain fair solutions when maximizing a scalar function in a multi-user setting.

Conclusions:
Multi-user scheduling is a NP-hard problem as soon as we have only one machine with 2 users and release dates. For the moment, we have studied fair on-line storage allocations and described an algorithm able to list all possible solutions. We still have to study the online case with unknown duration in order to propose algorithm suitable for the Grid.

Keywords: Grid scheduling, Fairness, Workflows

Further information: http://clrwww.in2p3.fr/ www.isima.fr/limos/

138. Be elegant on the Grid

Authors: Pugliese, Roberto (ELETTRA); Currri (ELETTRA); Del Cano (ELETTRA); Del Linz (ELETTRA)

Short overview:
ELETTRA is a multidisciplinary Synchrotron Light Laboratory in the AREA Science Park of Trieste. ELETTRA is open to researchers in diverse basic and applied fields. The laboratory is equipped with ultra-bright light sources in the spectral range from UV to X-rays and offers a stimulating and competitive environment to researchers from all over the world.

Analysis:
ELETTRA is now building a new light source FERMI@Elettra which is a single-pass FEL user-facility covering the wavelength range from 100 nm (12 eV) to 10 nm (124 eV). The advent of femtosecond lasers has revolutionized many areas of science from solid state physics to biology. This new research frontier of ultra-fast VUV and X-ray science drives the development of a novel source for the generation of femtosecond pulses. ELETTRA is a large data producer. As a partner of EGEE, ELETTRA is representing the new community of light sources. In this work we describe the use case of initiating this new community to the eInfrastructure and in particular the case of Elegant, an application program used to design the new light source FERMI@Elettra.

Impact:
Being this a new community a special care has to be put on making the path easier to the Grid newcomer. In order to meet this requirement we selected carefully a set of key applications to be ported and deployed a Grid portal called Virtual Control Room (VCR). The first application selected was Elegant which is the typical application with high throughput computing requirements and which greatly benefits the possibility to run parametric jobs. Users log in the portal which hides the complex details of the Grid. The portal first provides all the information needed to use the Grid and then simplifies access to all the resources in the VO and in particular the WMS and the LFC. The user just submits the job and downloads and visualizes the results.

Conclusions:
The received feedback by the users of Elegant was enthusiastic. The experience gained will be reused in porting the rest of key applications and will pave the way to the involvement of the other light sources in the Grid world.

Keywords: Synchrotron, Light Sources, Simulations, Grid Portals

Further information: http://www.elettra.trieste.it, https://ligths-vcr.Grid.elettra.trieste.it

139. Charon GUI - feature rich interface to distinct Grid niches

Author: Kmunicek, Jan (CESNET)
Co-authors: Plsek, Vitezslav (CESNET); Kuba, Martin (CESNET)

Short overview:
Here we present a graphical user interface to Charon Extension Layer system – well established framework for computational jobs and application programs management within the generic Grid environment. Charon GUI offers simple and intuitive interface to predefined set of options required for seamless research work in Grid environment in graphical, highly useable and reliable way.

Analysis:
Charon GUI is Java-based application currently running at specific server that functions as a dedicated frontend/user interface to individual virtual organization on EGEE or national Grid environment. The one and only prerequisite on the server side is to have Java Runtime Environment installed. Charon GUI displays on a remote X-server that can be either Linux OS or MS Windows with X-Window emulator. The full list of Charon GUI features includes key Charon Extension Layer functionality (job submission, monitoring, results retrieval as well as exploration of available application modules) enhanced by the graphical representation. Charon GUI functions as a laboratory book to keep track of end user's research projects and computational jobs allowing full project and/or jobs manipulation. Secondly, the exhaustive job overview and filtering functionality is ready to provide overview of the individual research project progress.

Impact:
The development of graghical frontend to all Charon Extension Layer system commands has been shown as a next logical step towards end users satisfaction to provide easy yet powerful way of utilization various Grid resources available worldwide. As the Charon GUI retains the simplicity and usability of the original, command line based Charon Extension Layer system and simultaneously includes a set of new, highly anticipated features, Charon GUI seems to be a potential candidate to influence the direction of Grid resources utilization in a day-to-day research.

Conclusions:
Charon GUI has been developed to provide interactive frontend towards distinct Grid niches and is ready for production release. The modular base of Charon system allows extensibility of Charon GUI too. The further planned development concerning Charon GUI will focus especially on the preparation of remote client version simultaneously with extension of supported Grid environments.

Keywords: Charon Extension Layer system, application portfolio, job management, Java, graphical user interface

Further information:
http://troll.chemi.muni.cz/whitezone/development/charon/wiki/index.php/Introduction

140. The Grid application platform: development and applications

Authors: Lee, Hurng-Chun (ASGC); Wei-Long, Ueng (ASGC)
Co-authors: Shi-Chung, Chiu (ASGC); Eric, Yen (ASGC); Simon, Lin (ASGC)

Short overview:
Grid Application Platform (GAP) is a light-weight framework for developing problem solving applications on the Grid, while reducing efforts of application integration and adapting new technologies in the future. Layered architecture was deployed to make the system easy to scale, manage and reuse, by three frameworks from bottom to the top. Compared to the traditional Grid services, it provides a simpler way for both users and developer to use the Grid and create Grid application.

Analysis:
GAP is developed with the following aspects. It is easy to use for not only the endusers but also the Grid application developers. GAP provides higher level of Java API which maps the problem domain model to programming domain model. GAP is easy to evolve for adapting new IT technologies as well, and the accommodation is transparent to both developers and users. The GAP abstracts the difference of Grid middleware with an unified interface and could be extended to adapt new middleware. The GAP is light-weight in terms of the deployment effort and the system overhead. Its goal is to provide problem domain models for Grid application and prevent developers from reinventing the wheels.

Impact:
In the collaboration of the EGEE WISDOM project, the docking services for Avian Flu drug analysis was implemented as an application of the GAP framework. The service has been promoted to wider auto-docking research groups of Taiwan and Asia Pacific Region through the collaboration of the 2nd Grid challenge of the avian flu drug analysis on the EGEE Grid infrastructure. It provides biologists a simplified way to run largescale docking simulations on the Grid directly from their desktop and also the possibility to integrate the Grid-enabled docking simulation service with the existing tools that has been used in the daily work.

Conclusions:
At present, GAP is going to be integrated with more practical Grid applications such as the digital archive application, earthquake data center services and so on. Application usability would be improved by the aid of GAP based on the experiences of Avian Flu Drug Analysis System. In the future, the flexibility to integrate existing tools, the improvement of user interface, and the reusability of client API are the focus for advancement.

Keywords: Grid Applications, Grid Services, Service-Oriented Architecture, Drug analysis, Avian flu

Further information: http://www.twGrid.org/Application/Bioinformatics/AvainFlu-GAP/

141. The experiment dashboard for medical applications

Authors: Andreeva, Julia (CERN); Boulebiar, Kamel (Informatics Institute, University of Amsterdam); Saiz, Pablo (CERN); Sidorova, Irina (CERN) ; Templon, Jeff (NIKHEF) ; Cirstoiu, Catalin (CERN) ; Da Rocha, Ricardo (CERN) ; Gaidioz, Benjamin (CERN) ; Herrala, Juha (CERN) ; Kan, Andrevan (NIKHEF) ; Lamanna, Massimo (CERN) ; Maier, Gerhild (CERN) ; Olabarriaga, Silvia D. (Academic Medical Center, University of Amsterdam)

Short overview:
The Experiment Dashboard is a monitoring system initially developed for the LHC experiments to provide the view of the Grid infrastructure from the perspective of the LHC virtual organization. The poster describes the first experience of the deployment and usage of the system outside the LHC community, for monitoring of medical applications on the Grid.

Analysis:
Functional magnetic resonance imaging (fMRI) is a popular tool used in neuroscience research to study brain function. The Virtual Lab for fMRI (VL-fMRI) is developed as one of the activities of the ``Medical Diagnosis and Imaging'' subprogram of the Virtual Laboratory for e-Sciences Project. VL-fMRI has taken steps to enable data management and analysis tasks for fMRI studies on the Grid infrastructure. Since spring 2006 the Experiment Dashboard is used for job processing monitoring of the VL-fMRI activities. The Experiment Dashboard provides an easy way to users to follow their jobs on the distributed infrastructure. Furthermore, the system allows to detect problems or inefficiencies of Grid sites or services and to understand the underlying problem. This functionality is important for site administrators and VO support teams.

Impact:
fMRI studies are data intensive, since large amounts of data are stored, analyzed and manipulated. They require high throughput computation on demand for real-time image analysis and for large-scale studies. Collaboration and distributed computing are essential, in particular for multi-center studies, where data is distributed. Using the Grid infrastructure is a natural choice in order to satisfy the requirements mentioned above. On the other hand the fMRI users (in particular psychologists, psychiatrists, radiologists, etc.) typically have limited background in computing and therefore need a user-friendly environment, which would enable the preparation, submission and monitoring of their jobs on the Grid. The Experiment Dashboard is providing the job monitoring functionality for the fMRI users and VO supporters.

Conclusions:
The first experience of using the Experiment Dashboard by the VL-fMRI community was positive. It was proven that the system, initially developed for the High Energy Physics community, is flexible enough and provides the necessary functionality to be easily adapted to the needs of users of completely different fields.

Keywords: monitoring, medical applications, functional magnetic resonance imaging

Further information: URL to the VLEMED dashboard: http://opkamer.nikhef.nl/

142. A network monitoring framework in the SCoPE project

Author: Pardi, Silvio (Dipartimento di Scienze Fisiche - Università degli Studi di Napoli Federico II - Italia); Serio, Fulvio (Dipartimento di Scienze Fisiche – Università degli Studi di Napoli Federico II - Italia); Russo, Guido (Dipartimento di Scienze Fisiche - Università degli Studi di Napoli Federico II - Italia); Ciuffoletti, Augusto (Univ. di Pisa - Largo B. Pontecorvo - Pisa)

Short overview:
The SCoPE project aims to create a metropolitan Grid infrastructure, gLite based, among the departments of the University of Naples Federico II. In this environment we have implemented and deployed GlueDomains, a network monitoring framework, in order to provide the measurements needed to support the network aware meta-scheduling algorithms and the QoS of the network services. In this work we show as the use of network measurement can improve the performances in the general purpose Grid.

Analysis:
The network reliability appears to be a crucial factor to guarantee the distributed services availability and the proper system functioning of a Grid infrastructure. The network performances can affect dramatically the job computation time in those applications that processing bulk of dataset and is obviously crucial during data replication activities. Currently in the main Grid deployments, the network resource is considered as pure facility and the middleware components act agnostically to respect the network parameters, so that the Grid infrastructure working globally below the best effort threshold, if we considered the Grid, in the first approximation, as an integration of computational, storage and network resources. In this work we present GlueDomain, a network monitoring framework created to support the middleware services by offering a set of measurement useful for general operations, bandwidth performance previsions and our deploy in the SCoPE infrastructure.

Impact:
The impact of the GlueDomains deployment is to optimize the use of the network resources and to provide a growing of the general performances during the data transfer operations. The metropolitan wide implementation of a network measurement system, also offer the opportunity to study and to test the cooscheduling algorithms and to understand how the use of the network parameters can improve the performance of the "best effort" based Grid systems. The the SCoPE framework allows having an excellent and complete testbed platform in which deploy and evaluate the new Grid services. The expected impacts due to the diffusion of this experience will be related to the progress of the know-how about the potentiality to use the network measurements in more large environments.

Conclusions:
The GlueDomains Framework has been deployed in the main sites of the SCoPE infrastructure and the measurements are in used by users and developpers for monitoring the network reliability and to test some network aware cooscheduling algoritms. Some new measurement tools are ready to be added to the framework. In the immediate future we plan to allarge the testbed and add new measurements tools to the environment with the feedback of the users and developers.

Keywords: Network, Monitoring, QoS, Metropolitan Grid

Further information: http://www.scope.unina.it

143. AIDA: Atlas graphical Interface for Distributed Analysis

Authors: Lampoudis, Christos (Aristotle University of Thessaloniki - Department of Physics); Houiris, Anastasios (Aristotle University of Thessaloniki - Department of Physics); Sampsonidis, Dimitrios (Aristotle University of Thessaloniki - Department of Physics)
Co-authors: Petridou, Charikleia (Aristotle University of Thessaloniki - Department of Physics); Christidi, Ilektra (Aristotle University of Thessaloniki - Department of Physics); Kanellopoulos, Christos (Aristotle University Grid Operations Center); Korosoglou, Paschalis (Aristotle University Grid Operations Center); Zilaskos, Dimitrios (Aristotle University Grid Operations Center)

Short overview:
Analyzing data from the LHC experiments will have to deal with data and computer resources distributed along numerous locations around the globe, with different access methods. AIDA is a graphical User Interface for the data analysis of the ATLAS experiment using the Grid infrastructure. The main objective in the development of AIDA is to make the creation, submission and output retrieval of Grid jobs as easy as possible.

Analysis:
AIDA specifically addresses the needs of the ATLAS high energy physics experiment, performing large scale data processing on globally distributed resources. AIDA is an easy-to-use strong tool implemented in java. User faces a single Graphical User Interface, instead of having a set of different applications. In such a way, the application offers the opportunity to avoid the complexity of Grid's command line interaction. This tool assists the user in all steps of a job's life cycle, starting from job creation, data set mining, multiple job submission, job monitoring and result collection.

Impact:
AIDA does not use its own Grid services, but those in common use. Prior to the job submission action, user must track the desirable data set and identify all available remote resources (storage/computer elements). AIDA gives this opportunity since it comprises the basic LCG and DQ2 commands. In such a way the user avoids any 'command line' interactions. Since AIDA is running from the user's pc, it is more convenient comparing with similar applications such as GANGA which runs the user interface on the Grid UI. Specifically in the case of the ATLAS experiment, the data – processing applications include simulations, reconstruction and physics analysis based on the Gaudi/ATHENA framework. This provides core services, such as message logging, histogram creation and allows run-time configuration via option files. At it is last phase of development, AIDA already demonstrated reliability and effectiveness in the case of ATHENA reconstruction data analysis work (ZZ4l decay channel).

Conclusions:
All that the user requires to run the AIDA GUI is an internet connection and the Java Runtime Environment 1.6 (JRE 1.6) installed on a pc. Trial users showed a very positive response to AIDA. Further development may allow the application to expand it's usage in other Grid user communities.

Keywords: GRID gui, ATLAS, ATHENA, job submission.

Further information: http://skiathos.physics.auth.gr/atlas/AIDA/

144. A parallel data mining application for gene ontology term prediction

Author: Psomopoulos, Fotis (Aristotle University of Thessaloniki)
Co-authors: Gkekas, Christos (Aristotle University of Thessaloniki); Mitkas, Pericles (Aristotle University of Thessaloniki)

Short overview:
Protein classification is one of the most commonly discussed problems in bioinformatics. One of the latest tools for protein function annotation is the Gene Ontology (GO) project which provides a controlled vocabulary to describe gene and gene product attributes in organisms. Although there are several cases of automated annotation, the bulk of the annotation process is performed by human curators. We present a parrallel algorithm for GO term prediction, deployed over the EGEE Grid environment.

Analysis:
Gene ontology can be thought of as a database of expert-based terms. The application presented utilizes the motifs that exist in already annotated protein sequences in order to model the corresponding GO terms. The input data set is created in a semiautomatic way, using the unique (UNIPROT) code of each protein and the InterProScan tool so that all available sequence databases (such as PRODOM, PFAM etc) will be taken under consideration. For each GO term that appears in the original protein set, a new training set is created, which contains all the protein sequences that have been annotated with the specific GO term. Based on the motifs present in the new data sets, a finite state automaton model is created for each GO term. In order to predict the annotation of an unknown protein, its motif sequence is run through each GO model thus producing similarity scores for every term. Results have shown that the algorithm is both efficient and accurate in predicting the correct GO term.

Impact:
The methodology has been implemented so that it can be used both as a standalone and as a Grid-based application. The algorithm however is by design an embarrassingly parallel one allowing for multiple models to be trained simultaneously, thus making the Grid the ideal environment for execution. In fact, it has been shown experimentally that the time to process the entire dataset on a single processor is prohibitively long. In an MPI-enabled application the utilization of the clusters available over the Grid provides a significant reduction of the processing time. The Grid also enables the seamless integration of the training process with the actual model evaluation, by allowing the concurrent retraining of GO models from different input sources or experts and the use of the existing ones.

Conclusions:
The initial dataset is stored and replicated as a single compressed file on multiple storage elements (SEs). The application was executed on available clusters using from 4 to 32 processors in different experiment configurations. In all cases a significant speedup was observed. Overall, the utilization of the Grid as the application platform has provided both a reduction in processing time and a seamless environment for running simultaneously different experiments.

Keywords: Bioinformatics, Protein Classification, Data Mining, Parallel Algorithms, Gene Ontology

145. Numerical modeling of electrodynamic aggregation of magnetized dust in electric discharges

Authors: Kukushkin, Alexander (RRC "Kurchatov Inst."); Marusov, Nikolay (RRC "Kurchatov Inst.")
Co-authors: Minashin, P.V. (Moscow Engineering Physics Institute, Russia); Neverov, V.S. (2Moscow Engineering Physics Institute); Cherepanov, K.V. (RRC "Kurchatov Inst.")

Short overview:
The present work is aimed at developing the numerical modeling approaches to describing a new branch of dusty plasma physics. The problem covers a wide range of research and application fields: erosion of plasma facing components and dust-tritium codeposition in nuclear fusion devices, controlled assembling of nanodust-based networks for creating new nanomaterials, structuring of astrophysical objects (dust clouds, planetary rings, etc.).

Analysis:
We examine the hypothesis for a fractal condensed matter composed of magnetized nanodust capable of forming a skeleton of filamentary structures observed in various laboratory electric discharges, severe weather phenomena and space, suggested for explaining the unexpected longevity of these filaments and their unexpected (sometimes transverse) direction with respect to that of main electric current. A 3-D numerical model of many-body system of basic blocks (magnetized, electrically conducting thin rods) managed to describe the following processes:

- self-assembling of a quasi-linear filament from a random ensemble of basic blocks and the capability of such filaments to close the electric circuit
- self-assembling of coaxial tubular skeleton in a system of initially-linear electric current filaments, composed of above basic blocks and linked to the biased electrodes
- the trend towards self-similarity of structuring during these self-assembling processes

Impact:
Application of Grid technology to solving the inverse problem of reconstructing the electrodynamic parameters of basic blocks (i.e. elementary dust particles) allows the substantial decrease of total computation time (e.g., by two orders of magnitude for the case of modelling the electrodynamic self-assembling of coaxial tubular skeleton in a system of ~1000 magnetic dipoles, which are initially arranged as 50-100 linear electric current filaments).

Conclusions:
Resources of Russian Fusion_RDIG virtual organization were used for these studies. Computation of a single variant takes about 6 hours and produces about 200 MB data set. While modeling the full process from the chaotic initial conditions to the final state for over 100 variants it was produced about 20 GB of data. After each omputation the 3D dynamics of the system is visualized using the same worker node.

Keywords: Numerical Modeling, Magnetized Dust, Electirc Discharge, Nuclear Fusion, Astrophysics

Further information: http://uni-skeletons.narod.ru/English-main.htm

146. Enhancement and breast hierarchical segmentation on digital mammograms

Author: Aliu, Azir (SEEU)
Co-author: Kon-Popovska, Margita (professor)

Short overview:
Computer use by clinicians in digital mammography image screening has advantages over traditional methods: enhancing the appearance of the images and highlighting suspicious areas. In this paper, we present our own algorithm that hierarchically segments the digital mammograms. It consists of two phases: the pre-processing and the processing phase of hierarchical mammograms segmentation. Grid infrastructure capabilities were explored in order to improve the algorithm's implementation.

Analysis:
Our algorithm enhances the results of digital mammogram processing. For image enhancements and appearance improvement, noise or error elimination, or to highlight certain image features, the algorithm uses density measures based on a normalized breast representation, method of image equalization and Kuvahara filter. This first phase is designed to have a very high sensitivity; the large number of false positives is acceptable, since they will be removed in the second phase. In the second phase moments are used for image description and as its intensity distribution shape indication. This phase automatically generates the boundary values and segments the mammograms hierarchically. Using the Grid improved both the image processing and mammogram segmentation. We hope that Grid infrastructure can be used clinically for early detection of subtle signs of breast cancer, including calcifications and speculated masses.

Impact:
Breast cancer as a medical condition, and mammograms as images, are extremely complex with many dimensions of variability across the population. X-ray mammography is the most reliable method available at present for the detection of breast cancer in screening programs, although it still does not detect all cancers. The proposed algorithm for digital image processing could be used in a breast cancer screening center in many possible scenarios. The system could be used to pre-screen mammograms and select those areas that need more attention for analysis. The results are expected to improve the accuracy of early breast cancer mammography diagnosis, reduce patient mortality, and reduce health care costs. Therefore it is important to split the mammograms into interesting regions in order to put into focus a technique when we search for abnormalities.

Conclusions:
The results obtained at clinics for radiology in our country have shown a general good use. Future enhancements will be done while trying to increase the collaborative work between local health care organizations in sharing and diagnosing mammogram images, aiding early breast cancer detection. The Grid infrastructure provides good platform for this work, and we will focus our efforts to enhance the methods, to consolidate the algorithms and to use the Grid for image processing.

Keywords: Digital mammography, Grid infrastructure, Computer-aided detection, algorithm

147. ArchaeoGrid, a laboratory for the past on e-infrastructures

Authors: Pelfer, G (CSDC, Florence, Italy); Pelfer, Pier Giovanni (Dept. of Physics, University of Florence / INFN)
Co-authors: Cecchini, R (INFN); Politi, A (CNR)

Short overview:
The ArchaeoGrid project is proposed as a Laboratory for the Past on e-Infrastructures for the reconstruction, management and access of Archaeological Heritage, focused on combination of analysis tools and data from many human and natural sciences in a multidisciplinary and interdisciplinary approach and related to innovative methods. The ArchaeoGrid applications are in the fields of Archaeological Research and of Archaeological Heritage Management and Economical Exploitation.

Analysis:
A primary goal of ArchaeoGrid as simulation engine is the development of simulation of integrated human-in-natural-systems models, which are treated as complex hypotheses, tested against the archaeological record and used for reconstructing the ancient societies history integrated with the Earth history. In our study cases archaeological and non archaeological data are multivariate geospatial and temporal data. Grid technology has been developed for general sharing of computational resources but has not been designed for the specialty of geospatial data. In order to make Grid technology applicable to geospatial data, it needs integrate the technologies for the geospatial data with the Grid technology. Grid service-oriented geospatial standards, compliant to Grid framework, are developed for giving to the researchers the possibility to build up their models, to execute them and to have back the desired geospatial products.

Impact:
The ArchaeoGrid system has a complex structure that needs the availability of services for the access, analysis, visualization of archaeological data and results and for the final narration by production of some digital document, where text, data and results are simultaneously accessible independently from their geographic distribution. With geospatial Grid services, ArchaeoGrid needs the integration on the e-Infrastructure with Virtual Laboratory services, with Digital Library services and with Multi-Agent System Platform services integrated with Archaeological GIS. The interoperability and accessibility with other Grids (Earth Sciences Grid, Bio- Medical Grid, etc.) is also useful for sharing data and methods of analysis.

Conclusions:
ArchaeoGrid applications are installed and run on GILDA t-Infrastructure and on EUMEDGrid e-Infrastructure. The installation of ArchaeoGrid System on new e-Infrastructures and the extension of ArchaeoGrid Community to new researcher groups will be the goal in the near future.

Keywords: Archaeology, GIS, MAS (Multi-Agent System), Digital Library, Virtual Reality

148. Organising scientific data by dataflow optimisation on the petascale

Author: Lassnig, Mario (CERN & University of Innsbruck, Austria)

Short overview:
Scientific applications on the Grid are in most cases heavily data-dependent. Therefore, improving scheduling decisions based on the co-allocation of data and jobs becomes a primary issue. Hence, it is crucial to analyse the behaviour of existing data management systems in order to provide accurate information for decision-making middlewares in a scalable way. We show current research issues in understanding the behaviour of data management systems on the petascale to improve Grid performance.

Analysis:
We analyse the Distributed Data Management system Don Quijote 2 (DQ2) of the High- Energy Physics experiment ATLAS at CERN. ATLAS presents unprecedented data transfer and data storage requirements on the petascale and DQ2 was built to fulfill these requirements. DQ2 is built upon the EGEE infrastructure, while seamlessly enabling interoperability with the American OSG and the Scandinavian NorduGrid infrastructures. Thus it serves as a relevant production-quality system to analyse aspects of dataflow behaviour in the petascale. Controlled data transfers are analysed using the central DQ2 bookkeeping service and an external monitoring dashboard, provided by ARDA. However monitoring dynamic data transfers of jobs and enduser data transfers cannot happen centrally because there is no single point of reference. Therefore we provide opportunistic clients tools for all scientists to access, query and modify data. Those tools report the needed usage information in a non-intrusive, scalable way.

Impact:
We characterise three areas for improvement of dataflow. First, controlled data transfers issued by experiment operators or Gridsite operators. This is constant data export from the experiment to distributed computing facilities, mostly defined by experiment computing models. Second, dynamic data transfers issued by jobs on a Gridsite. Those production jobs may need to access data that is only available on remote sites. Third, uncontrolled data transfers issued by end-users; scientists fetching data for direct analysis. We argue that on the petascale complete replication of files is not a suitable option anymore as there is too much data and that erratic and unpredictable data movements are the norm. Furthermore it is important to value the relevance of certain data with respect to time to find useful data on the Grid. Our model derives those usage patterns implicitly. Therefore global data movement and usage patterns on data must be taken into account when doing job/data co-allocation.

Conclusions:
The objective of reasonable organisation of scientific data on the Grid is not a new one. Already, many approaches especially in file replication show good improvements. We argue though that once we approach petascale, low-level file reorganisation is not sufficient anymore and a global view of Grid dataflow must be taken into account. We provide a preliminary model and its accompanying tools to understand erratic and unpredictable dataflows and show their usefulness in the production EGEE Grid.

Keywords: Data Management, Dataflow, Grid Behaviour, Petascale

Further information: http://www.dps.uibk.ac.at/

List of institutions

A

ACC CYFRONET AGH (Academic Computer Centre Cyfronet Akademie Gorniczo-Hutniczej), Poland

Aitek S.p.A., Italy

Aristotle University of Thessaloniki, Greece

ASGC (Academia Sinica Grid Computing Centre), Taipei, Taiwan

Athens University of Economics and Business, Greece

B

BCCS/UIB, Norway

BIFI (Institute for Biocomputation and Physics of Complex Systems), Zaragoza, Spain

Brunel University, London, UK

C

Cass Business School, London, UK

CDC – Center for Disease Control, USA

CDS - Observatoire de Strasbourg, France

CEA - (Commissariat A L'Energie Atomique), France

Centre de Physique des Particules de Marseille, France

Centre Jean Perrin, France

CERN (European Organization for Nuclear Research), Geneva, Switzerland

CESGA (Fundacion Centro Tecnologico De Supercomputacion), Spain

CESNET (Czech Republic's National Research and Education Network), Prague, Czech Republic

CETA (Center for Electromagnetic Theory and Applications), USA

CIEMAT (Centro De Investigacion Energeticas, Medioambientales Y Technologicas), Spain

CIMA Foundation, Italy

CIMENT, France

CLMC (Computational Learning and Motor Control), USA

CNAF, Italy

CNR (National Research Center), Italy

IMAA (Institute of Methodologies for Environmental Analysis), Italy

ISTI (Institute of Science and Technology), USA

ITB (Institute for Biomedical Technologies), Italy

CNRS (Centre National de la Recherche Scientifique), Paris, France

COMETA Consortium, Italy

CRAL, France

CREATIS LRMN, France

CRS4, Italy

CS, France

CSC - Scientific Computing Ltd, Finland

CSDC, Florence, Italy

D

DKRZ (Deutsches Klimarechenzentrum) GmbH, Hamburg, Germany

DutchSpace, Netherlands

E

ELETTRA, Italy

ENEA FIM, 00044 Frascati, Roma, Italy

ENS-Lyon, France

ERIM, France

ESA (European Space Agency), Italy

EU-IndiaGrid team, India

Euro-Mediterranean Centre for Climate Change, Italy

F

FhG,Germany

FNAL, USA

Foundation for Research and Technology-Hellas, Greece

FZK (Forschungszentrum Karlsruhe), Germany

Fraunhofer Institute for Algorithms and Scientific Computing, Germany

Fundecyt, Spain

G

GCRAS – Geophysical Center, Russian Academy of Sciences, Russia

GEPI - Galaxies Etoiles Physique et Instrumentation, France

Grid Operations Centre, A.U.Th, Greece

GRNET, Greece

GUP, Austria

H

High Performance Computing Center Stuttgart, Germany

Ho Chi Minh City Institute of Information Technology, Vietnam

I

IBCP (Institute de Biologie et Chimie des Proteins), France

ICI Bucharest, Romania

ICTP - International Centre for Theoretical Physics, Italy

IMCCE - L'Institut de Mecanique Celeste et de Calcul des Éphemerides, France

IMPB RAS, Russia

Imperial College London, UK

IN2P3 LPC Clermont-Ferrand, France

INAF, Italy

INCAS Bucharest, Romania

INFN, Istituto Nazionale di Fisica Nucleare, Italy

INRA Clermont-Ferrand, France

INRA URGI, France

INRIA, France

INSERM, UMR S 525, Faculté de Médicine Pitié-Salpêtrière, Paris, France

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Institute of Electronic Structure and Lasers, Greece

Institut of Information Systems, RRC "Kurchatov Inst., Russia

Institut Pierre Simon Laplace, France

Institute of Informatics, Slovakia

Institute of Informatics, University of Amsterdam, Netherlands

Institute of Molecular Physiology and Genetics, Slovakia

Institute of Physics, ASCR, Prague, Czech Republic

Instituto de Fisica de Cantabria, CSIC-UC, Santander, Spain

IPGP, France

IPP - BAS, Sofia, Bulgaria

IPSL, Paris, France

IR & T engineering s.r.l, Italy

Istituto di Tecnologie Biomediche, CNR, Italy

Istituto per le Applicazioni del Calcolo, CNR, Italy

ISUFI Settore Nanoscienze e Grid Computing, Italy

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J

JKU/RISC, Russia

K

Kapteyn Astronomical Institute, Netherlands

KARLSRUHE, Germany

KISTI, Korea

Koninklijk Nederlands Meteorologisch Instituut, Netherlands

L

LAL IN2P3, France

LAOG - Laboratoire d'Astrophysique de Grenomble, France

LERMA, France

LIFL - UMR 8022 CNRS, France

LIG - MOAIS project, France

LIG Laboratory, France

LIMOS, Clermont, France

LPC - Clermont, France

LUTH, France

M

MAAT GKnowledge, Spain

Masaryk Univeristy, Czech Republic

Microsoft Research, USA

Middle East Technical University, Turkey

Mimos Berhad, Malaysia

Moscow Engineering Physics Institute, Russia

MTA SZTAKI, Hungary

N

National Institut of Agrobiological Sciences, Japan

National Institute for Aerospace Research, Romania

National Institute for R in Informatic, Czech Republic

National Research Council - Institute of Biomedical Technologies, Italy

NEC Laboratories Europe, Germany

NERI, Roskilde, Denmark

NeSC – National e-Science Center, UK

NICE srl, Italy

NIKHEF, Netherlands

NTUA – National Technical University of Athens, Greece

Nuclear Fusion Inst., RRC Kurchatov Inst., Russia

O

Observatoire de Nice, France

P

Politecnico Bari, Italy

Poznan Supercomputing and Networking Center, Poland

Pune University, India

R

RAL - Rutherford Appleton Laboratory, UK

Royal Institute of Technology (KTH), Sweden

RRC "Kurchatov Inst, Russia

Russian Academy of Sciences Institut, Russia

S

SARA, Netherlands

SCAI, USA

SEEU, Macedonia

SIEMENS AG, Germany

Slovak Academy of Sciences, Slovakia

SPACI Consortium - Southern Partnership for Advanced Computational Infrastructures, Italy

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T

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U

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Univesity Milano Bicocca, Italy

UNSA, France

UPB, NCIT, Romania

UPV - Universidad Politécnica de Valencia, Italy

UTCN, Computer Science Department, Romania

UvA, Netherlands

W

WUT - West University of Timisoara, Romania

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