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Book of abstracts

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Computer Science / 1

Distributed parametric optimization using the Geneva library

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The Geneva library implements parallel and distributed parametric optimization algorithms, capable of running on devices ranging from multi-core systems over clusters all the way to Grids and Clouds. The generic design makes Grid-resources available to user groups that have formerly not been exposed to such environments.

Poster session / 2

Eliminating and preventing Grid Security Vulnerabilities to reduce security risk

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The EGEE Grid Security Vulnerability Group was formed "to incrementally make the Grid more secure and thus provide better availability and sustainability of the deployed infrastructure". The aim is to eliminate vulnerabilities from the Grid and prevent new ones from being introduced, thus reducing the risk of security incidents. This poster alerts users and developers to both the activities of the this group and problems that may be caused by vulnerabilities. It is also intended to inform what they should do to avoid introducing vulnerabilities and report any their find.

High Energy Physics / 4

ATLAS Distributed Computing in Spain and Portugal: from data challenges to real data

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The ATLAS PIC cloud is composed of the Iberian sites: PIC (Tier-1), IFAE, IFIC, UAM, LIP-Lisbon, LIP-Coimbra and NCG-INGRID-PT (Tier-2s) and is finalising preparations for the LHC data taking. To achieve readiness for data taking, all sites has been involved in the ATLAS Distributed Computing activities since early 2006: simulated event production, reprocessing, data and user analysis challenges and cosmic data taking. The evolution of the computing and operations activities from data challenges to the real data is described in this talk giving experiment and site experiences.

Demo Session 1, Welcome Drink / 7

e-NMR: Computational NMR Infrastructure in life science and system biology

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In order to enable the life science community to make full use of the EGEE computing resources we have developed an e-infrastructure named ‘eNMR’ (EU 7th FP, Contract no. 213010).

eNMR deploys and integrates biomolecular NMR applications into a platform, so that EU scientists can easily access it via a standard browser interface and use it at every step of their research process.

The sequence of available web-portals covers all aspects of bio-NMR: data acquisition, processing, analysis, protein/DNA/RNA structure calculation, molecular docking, validation, deposition etc.

High Energy Physics / 8

Response of the ATLAS Spanish Tier2 for the collisions collected in the first run at LHC

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The distributed analysis tests during the STEP09 and UAT exercises were a success for ATLAS and for the sites involved in the ATLAS computing model. The services were exercised at records level with good efficiencies and real users continued to get real work done at the same time.

Sample problems found were :

data access, was troublesome under heavy loads;
pilot factories need to be better organised;
monitoring could be improved

Solutions have ben developed for these problems

Poster session / 9

jGridstart: request, obtain, and install grid user certificates in a friendly way

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The use of X.509 certificates gives flexibility in authentication and authorisation on the grid. The associated key is usually stored on the user's computer. While this is good practice from a security standpoint, managing keys and certificates is far from trivial. jGridstart attempts to bridge this gap by providing a friendly user-interface to guide the user in requesting, renewing, and installing user certificates. It is currently in use at the DutchGrid certification authority.

Infrastructure Tools and Services / 10

A solution to distribute software packages at Grid sites using Squid

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In the current model of Grid computing the software needed by virtual organizations (VO) is stored at the sites in a shared area mounted on NFS and jobs running on the worker nodes access the necessary applications through NFS protocol. An alternative model, based on Squid, is proposed in this article. With this approach, the software packages are pulled from the central VO repository to the sites using http protocol. Squid also takes care of managing the transfers of packages from a central repository at the site to the worker nodes, and optimising network throughput over the LAN.

Security / 11

An Active Security Infrastructure for Grids

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To date, grid security activities have largely focused on prevention mechanisms, i.e., authorization,authentication, and secure communications. Here we present an Active Security Infrastructure (ASI) for grids, the design of which focuses on the areas of detection (e.g. intrusion detection), and reaction, i.e., taking action to prevent, or to recover from, a security incident. The infrastructure is composed of a distributed monitoring and control layer and an analysis layer. Communication between layers is via a grid information system.

Fusion / 12

Montera: a framework for efficient executions of Monte Carlo codes on the Grid

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Monte Carlo codes constitute a powerful tool for scientific computing. Because of their architecture their parallelization is straightforward, and they have been successfully ported to the Grid in multiple occasions. However, there is still a lack of a deep analysis on their optimization for being executed on a distributed environment. To solve this issue we present Montera, a framework that efficiently executes this kind of codes on Grid infrastructures making the most of their particularities.

Poster session / 13

Checking Grid Certificate Profile Compliance

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Digital certificates are used to secure international computation and data storage grids for e-Science projects in EGEE. The International Grid Trust Federation has defined a set of guidelines for digital certificates used for grid authentication. We have designed and implemented a program and test suites to check X.509 certificates against profiles and policies relevant for use on the Grid to assist implementers and users of PKI to reach appropriate trust decisions.

Poster session / 14

Modelling aerosol pollution over Athens, Greece using grid technology

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This scientific work aims at studying aerosol pollution over Athens, through an on-going modeling effort using grid technology. Aerosol predictions by the eulerian model CAMx, will be obtained for different emission scenarios. Focus is given on the role of conventional anthropogenic emissions versus natural emissions (sea-salt and Aeolian dust) on aerosol pollution. Predictions will be evaluated against aerosol measurements by the National Ministry of the Environment.

Security / 15

Encrypted Data Storage

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Biomedical researchers are required to encrypt sensistive patient data before use/storage on Grid Data Management services. The services described enable this operation.

Poster session / 16

gLite Porting to the Play Station 3 using ETICS for electronic High Throughput Screening (eHiTS)

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Since 2003 TCD has invested heavily in middleware porting, constantly engaging with the middlware development groups of the EU DataGrid (EDG), LHC computing Grid (LCG) and EGEE projects. In 2008, TCD ported gLite worker node to Yellow Dog Linux 6 on the Play Station 3, without data management. The node, built in ETICS, and tested in a production environment with gLite WMS job submissions were successfully submitted to it. The decrease in computational performance of porting the eHiTS software to the Grid is too expensive, so porting the Grid to other architectures such as the PS3 is important.

Demo Session 2 / 17

Complex Scientific Workflows exploiting Grid and HPC

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Simulating a full fusion Tokamak requires a range of codes and applications which address different aspects of the plasma and at specific ranges of space and time scales. The computational complexity of all these tools is so high that only paradigms like grid computing or HPC allow to carry out all the simulations. The EUFORIA project enables the European fusion modelling community to exploit Grid and HPC.

In this work we show a complex workflow that uses two applications that run in different computer architectures: grid and HPC.

Demo Session 2 / 18

User-friendly access to computational services with FARO portal for EGEE and ENEA-GRID

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A simple and flexible user access to applications is the final target for any system providing access to computational resources, even more for highly abstract infrastructures as grids and clouds. In this work we present a portal to the EGEE user that allows to submit widely used scientific softwares as jobs to EGEE. The main target of this interface is to hide from the end user low-level details connected with job submission. The expected result of this work is to make the GRID more palatable to other scientific communities, which at the moment are not interested in using this technology.

High Energy Physics / 19

LHCb operations: organizations, procedures, tools and critical services.

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The proliferation of tools for monitoring both activities and the status of the critical services, together with the pressing need for prompt reactions to problems impacting data taking, user analysis and scheduled activities (e.g. MC simulation) brings the need of better organizing the huge amount of information available. The monitoring system for the LHCb Grid Computing relies on many heterogeneous and independent sources of information offering different views for a better understanding of problems while an operations team and defined procedures have been put in place to handle them.

Earth Science / 20

Climate data storage in e-INIS

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We describe the federated national datastore activity of the e-INIS project, aimed at building a sustainable national e-Infrastructure for the Irish academic research community and how the CMIP5 project is using the datastore to meet their storage requirements. The datastore builds upon existing infrastructure and services, including Grid-Ireland, the National Grid Initiiative. Read access to the data is to be offered to international researchers using GeoNetwork and OPeNDAP, requiring that Grid technology be interfaced with community technologies using e-INIS's bridge servers.

Infrastructure Tools and Services / 21

Application Domain Accounting for EGI

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Accounting is a powerful tool for users and VOs to obtain information on grid resources usage. Currently, they can access the accounting portal to display executed jobs. However, grid users and VOs prompt further improvements to enhance the EGEE accounting system and foster cooperative endeavors. One of the most requested features is application-level accounting. Together with COMPCHEM VO the initial requirements are being analyzed. It has suggested to gather extra information on the most executed programs, on the amount of retrieved results (per user/program) and on the used resources.

Astronomy and Astrophysics / 22

Dark energy in the Grid: the PAU survey project

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The PAU survey is intended to study the dark energy and its evidences such as the accelerated expansion of the Universe. With this aim, a large number of galaxies will be catalogued forming a map of the universe in large scale. High volumes of data need to be managed, processed and stored. The facilities of the PIC computing centre and the GRID environment will allow the challenging data management that the PAU survey requires.

Bioinformatics / 23

A Grid Implementation For Genetic Linkage Analysis

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The Genetic Linkage Analysis of SNP markers aims to discover the genetic correlation in monogenic diseases by following their inheritance in families through the generations. The computational cost and memory requirements of the major algorithms in literature make large data sets very hard to be analyzed on a single CPU. The work here presented is a Grid implementation of a data pipeline application for Linkage Analysis, a web based tool for Grid submission, monitoring and retrieval of Linkage challenges with large pedigrees and big markers datasets derived from genotyping chips up to 1M SNPs.

Medical Imaging / 24

Medical image indexing and retrieval in a distributed computing environment

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The problem of indexing and content-based retrieval of medical images in a distributed computing infrastructure is discussed in the paper. It is considered in the context of a national-wide lung screening and diagnosis programme which is currently under development. High-resolution images are drawn from a test database containing results of X-ray chest examination of about 250000 people. The image content indexing and retrieval software is developed using GRID middleware UNICORE and a communication protocol MPI.

Data Management / 26

Deployment and Management of Grid Services for a data intensive complex infrastructure

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Services needed to access scientific data and computational resources in a distributed computing infrastructure are getting more and more complex. Our Atlas Tier2/Tier3 users, and National e-Science and GRID-CSIC initiatives researchers, have different requirements but all need ubiquitous and efficient access to these resources. We will provide details on how we use WLCG and Glite middleware, Storm, Lustre filesystem and our developments within this software to meet our specific necessities, to allow users direct access to the data, and to reach high availability in the provided services.

Novel Architectures and Technologies / 27

Offering GridWay users more power by means of the Amazon public cloud

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We present a mechanism to easily provision public cloud resources for grid users. The extension of the underlying grid infrastructure benefits demanding situations coming from a single user, a group belonging to a Virtual Organization, or even from a institutional requirement. A set of very simple tools allows the GridWay administrator to deploy arbitrary instances and monitor how the enrolment is performed, guaranteeing the usability of the new resources to the specific target community.

EGI Session / 28

EGI InSPIRE HUC SA3 - Services for Heavy User Communities of DCIs

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At this last User Forum of the EGEE project, it is appropriate to consider how services for "heavy users" of Distributed Computing Infrastructures will continue to be provided. The role of the European Grid Initiative (EGI) has been discussed for some time now and a specific activity regarding Service Deployment is foreseen as part of the EGI InSPIRE ("Integrated Sustainable Pan-European Infrastructure for Researchers Everywhere") proposal. This talk explains which communities are targeted by the work that is foreseen and outlines mechanisms whereby its progress can be tracked. Moreover, it examines how the potential benefits – within individual communities, between them (e.g. common tools and services) as well as to the more general DCI community – can be achieved.

Data Management / 29

StoRM, a flexible Storage Resource Manager solution

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StoRM is a high performance and flexible SRM solution for general disk based storage resources that bring in Grid the advantages of high performance storage systems based on cluster file system, such as GPFS from IBM and Lustre from SUN. StoRM can be used in small data centre with low rates of storage management requests and, at the same time, it is capable to grow in terms of storage and workload managed to fulfil requirements from large-scale production sites. The latest version of StoRM satisfies the wish list built with the desiderata of current and future users.

Poster session / 30

The HELIO project.

Dr. COGHLAN, Brian [1]; Dr. KENNY, Eamonn [1]; Dr. QUIGLEY, Geoff [1]; Dr. RYAN, John [1]; Dr. PIERANTONI, Gabriele [1]

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HELIO is a project of the 7th Framework Program that aims at creating a collaborative environment in Heliophysics. As it includes different services that can be computationally intensive and involve large, dispersed volumes of data, HELIO will use a Grid-based system for processing and storage for its most intensive analysis.
The architecture must balance conflicting requirements: to have a powerful, yet easy to use, instrument, to comply with the policies of the back-ends, and to be flexible in orchestrating, locating and co-locating the services.

Scientific Gateways and Portals / 31

An advanced web portal for accessing Grid resources with Virtual Collaboration features.

Mr. BONACCORSO, Fabio [1]; Mr. FAVRETTO, Daniele [1]; Mr. PRICA, Milan [1]; Dr. PUGLIESE, Roberto [1]; Mr. KOUROUSIAS, George [1]; Mr. DEL LINZ, Andrea [1]

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The Virtual Control Room (VCR) is an open source web portal that puts together a rich collaborative environment with the simplified access to the gLite Grid resources. The latest version of the VCR is based on the Gridsphere 3 and Google Web Toolkit (GWT). It uses the DORII Java Common Library for accessing Grid resources, integrates DORII Workflow Management System, presents a much improved Application Manager, introduces tags for user-application mapping and support for robot certificates.

High Energy Physics / 32

The Grid as an Extended Application Service Provider in an Synchrotron Radiation Facility

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The Synchrotron Radiation Facilities (SRF), as large research establishments, have a very important role in Science and a great impact in the community. Due to the data-parallelism of the computational problems in the general field of physical sciences and the very high data volumes in terms of storage, the Grid Computing has been a successful paradigm. But other than their Computational requirements there are additional Grid characteristics and features that can be highly useful. We discuss the Grid utilisation in the SRF ELETTRA.

DCI programming / 33

PROOF on Demand

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PROOF on Demand (PoD) is a set of utilities, which allows starting a PROOF cluster at a user request, on any resource management system. It provides a plug-in based system, to use different job submission frontends, such as LSF or gLite WMS. PoD is fully automated, and no special knowledge is required to start to use it.

Computational Chemistry / 34

A priori modeling of chemical reactions on a grid-based virtual laboratory: towards standard representations of data for molecular chemistry

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We have assembled on the COMPCHEM segment of the EGEE Grid Infrastructure the core of the Grid Empowered Molecular Simulator (GEMS) queueing in a common workflow a suite of - adequately "gridified" - codes for the a priori modeling of elementary chemical processes. The communication between applications from different scientific domains is fostered by the use of common data formats. A test calculation is shown for the benchmark H + H2 reaction.

Demo Session 2 / 35

On demand Grid services for training in Earth Observation

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Current applications involving satellite data need huge computational power and storage capacities. Grid computing technologies that have evolved in the last decade promise to make feasible the creation of an environment, for these kinds of applications, which can handle hundreds of distributed databases, heterogeneous computing resources, and simultaneous users. In this context the recent Grid-based platform GiSHEO offers, for training purposes, satellite image processing services, workflow-based service composition, and user interaction combined with e-learning facilities.

Poster session / 36

Migration of the MAGIC data transfers to a Grid infrastructure

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The MAGIC collaboration is moving from a computing model based on local computer farms to a Grid based model, including the migration of all the services of the official data center. Here we present the recent progress in the adoption of the Grid infrastructure in the MAGIC data center, which relates to the data transfer from the observation site.

Poster session / 37

Running Bag-of-Tasks Applications in EGEE with MaWo

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MaWo is a distributed computing framework which implements a well-known master-worker pattern. It provides a programming interface as well as easy-to-use tools for running Bag-of-Tasks applications across heterogeneous computing resources. MaWo allows the user to seamlessly utilize all available resources including local workstations, clusters and grids among which EGEE is a primary target. The framework significantly reduces the time and effort needed to port an application to grid.

Fusion / 39

Fusion metadata navigation and data delivery services

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The services for user-friendly metadata navigation and data delivery have been developed. The metadata service enables exploring of fusion-specific data storage via a web browser. The data delivery service allows to download a required piece of data from Storage Elements using a link obtained from the metadata service.

Poster session / 40

The APEL CPU Usage Accounting Infrastructure for NGI Grids

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In order to implement and deploy a scalable and flexible distributed CPU usage accounting infrastructure for the NGI Grids, the accounting records transport mechanism of the APEL (Accounting Processor for Event Logs) tool is modified and extended to integrate with ActiveMQ message broker network. The new APEL CPU usage accounting infrastructure supports a robust accounting capability at an NGI level and flexible across VOs accounting records queries.

Poster session / 41

Integration of Nagios plug-in into a data model to improve the Grid stability from the user point of view

Dr. PARDI, Silvio [1]; Dr. APICELLA, Andrea [2]; Dr. CELESTINO, Simone [2]; Prof. MEROLA, Leonardo [2]; Prof. RUSSO, Guido [2]; Dr. PALMIERI, Francesco [2]

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In this work, we propose a new approach to publish and consume monitoring information about Grid sites within a gLite based infrastructure. Starting from a set of tests that are crucial for a Grid site or for a Virtual Organization, we created a data model to represent them in the standard gLite information system. Through the Nagios tool, we have periodically performed sanity checks publishing the results concerning resource monitoring or resource discovery. Preliminary tests have shown the effective benefits provided by this approach in term of successful jobs.

Poster session / 42

Data awareness in gqsub

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gqsub is a user (command line) interface for submitting and monitoring Grid jobs that conforms to the IEEE standard for qsub (and friends).

Recent development has focused around data and data awareness; both in terms of data local to the submission machine, and data elsewhere in a Storage Element.

Medical Imaging / 43

Gwendia workflows for cardiac image analysis

Mr. CARON, Eddy [1]; Mr. CASTA, Christopher [2]; Mr. CLARYSSE, Patrick [3]; Mr. GLATARD, Tristan [3]; Mr. ISNARD, Benjamin [4]; Mr. MAHESHWARI, Ketan [5]; Mr. MONTAGNAT, Johan [5]

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We will present the description of a cardiac image analysis workflow with the new Gwendia language and its enactment on two different grid platforms, namely EGEE (using the MOTEUR workflow engine) and Grid'5000 (using the DIET workflow engine). Technical achievements enabling the execution of the very same workflow on those two grids will be presented. Finally, early application results (both performance and medical imaging) will be reported.

Earth Science / 44

Experiences on porting and running a Climate - Air Quality Modeling System on the Grid

Dr. KATRAGKOU, Eleni [1]; Prof. MELAS, Dimitrios [1]; Prof. ZANIS, Prodromos [2]; Dr. TEGOULIAS, Ioannis [2]; Mr. KOROSOGLOU, Paschalis [3]; Mr. KANELLOPOULOS, Christos [3]

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We present results of regional climate-air quality simulations performed over Europe for the future decade 2091-2100 and the control decade 1991-2000 and briefly discuss the impact of climate change on air quality metrics over Europe throughout the 21st century. In order to meet the increased demands on computational resources the high resolution simulations were performed on the EGEE Grid. Special tools to allow for easy coupling of RegCM3 and CAMx on the underlying resources have been developed and we briefly discuss the benefits and drawbacks of using the Grid for such simulation campaigns.

Medical Imaging / 45

Experience feedback on some scientific gateway components for medical imaging applications

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This presentation summarizes experience acquired at Creatis with some Scientific Gateway components to deploy medical imaging applications on the EGEE grid during the last years. We will detail feedback about various tools that we tested, including pilot-job systems, workflow managers, user front-ends, monitoring components and data management systems. Based on application use-cases ported at the lab, we will discuss advantages and drawbacks of these gateway components and highlight remaining challenges. Finally, an integration of some components in a coherent grid environment will be shown.

Poster session / 46

Experiences with a lightweight GRID infrastructure using AFS

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The Andrews File System (AFS) with certificate-based authentication can be used to provide a system of input and output sandboxes which is simpler and easier to use than the usual tarball. We describe how such a system was set up at Manchester, the experiences of various different users, and the implications for design of Tier3 facilities.

Demo Session 1, Welcome Drink / 47

DrugScreener-G: Towards Grid-enabled Large-Scale Virtual Screening Coming into Handy

Mr. LEE, Sangdo [1]; Mr. LEE, Sehoon [1]; Dr. BRETON, Vincent [2]; Mr. SALZEMANN, Jean [2]; Ms. LUCIA DA COSTA, Ana [3]; Dr. KIM, Jincheol [1]; Prof. HAN, Dongsoo [4]; KIM, Doman [5]; Dr. HWANG, Soonwook [1]

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DrugScreener-G (DSG) is an intuitive and easy-to-use grid-enabled in silico screening tool, aiming to help scientists in drug discovery including biologists and biochemists to conduct a large-scale deployment of virtual screening process on the Grid. With the help of DSG, scientists can easily have access to the PDB database, download and view the 3D structure of target proteins of interest, launch and manage millions of protein-ligand docking simulations on the Grid. To facilitate the analysis of docking results, visualization tools like Jmol and Chimera have been integrated into DSG as well.

Fusion / 48

Numerical reconstruction of fusion-origin carbon structures using refactored GIF portal

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Two developed technologies are shown. The top one is a method for the massive modelling of X-ray propagation in carbon films found in fusion devices as well as numerical reconstruction of such films composition. The basic technology is the strongly re-factored GIF portal that allows the development of high-level logics and user web interface for such grid applications.

Poster session / 49

Supporting 60 e-Science applications from Europe and Latin-America: Best practices and analysis extracted from the EELA-2 project

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Investments to promote e-infrastructures within new scientific communities in several regions of the world have been attracting new research groups interested in porting their applications on the Grid. Such an expansion across many institutions/countries facing different maturity levels of IT infrastructures, network connections and e-science awareness represents new challenges to support a diversity of users/applications. This work aims at presenting a complete picture of all EELA-2 applications as well as to share some best practices and methodologies used to support them.

Bioinformatics / 50

Distributed System Based Strategies for Search, Design and Evaluation of COMBO-FISH probe sets

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A prominent means to detect genetic aberrations is the method of fluorescence in situ hybridization FISH. To avoid labelling large genomic regions by one polynucleotide like in standard FISH, for COMBO-FISH we search for a set of about 30 colocalizing short sequences with the requirement that no more than 4 of these stretches colocalize within 250 kb anywhere else in the genome. The exact search is parallelized and applied to certain subsets motivated by kinetics and stability considerations.

Earth Science / 51

Gridifying the Soil and Water Assessment Tool (SWAT) for the sustainable development of the Black Sea region

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The Soil and Water Assessment Tool (SWAT) is one of the main tools used in the hydrology community. In the EU/FP7 EnviroGRIDS project it is used to study the Black See catchment and to simulate complex scenarios. In several cases, such as the study of the interplay of global and local scenarios, the availability of substantial computing resources in the Grid is important.

Workflow Management / 52

A novel approach to Workflow Management in Grid Environments

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Most workflow management systems in Grid environments provide a push-oriented job distribution strategy, where jobs are explicitly delegated to resources. In those scenarios dedicated resources execute jobs according to the request of a workflow engine or Grid wide scheduler. This approach has various limitations, particularly if human interactions should be integrated in workflows. To support such interactions with the benefit of enabling volunteering approaches, this presentation proposes a pull-based approach, where resources can actively select tasks for execution from a repository.

Poster session / 53

Job management in gLite

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The gLite WMS has been designed and implemented to provide a dependable, robust and reliable service for efficient and transparent distribution and management of end-user requests to high-end resources shared across a production quality Grid.
The WMS comes with a fully-fledged set of added-value features that hide to end users the complexity of such a heterogeneous and ever growing infrastructure and enable, thanks to a flexible, service oriented and general architecture, applications coming from largely different domains

Astronomy and Astrophysics / 54

LOFAR Archive Information System

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The LOFAR radio telescope, consisting of several stations with antennas, will become operational in spring 2010. The signals are collected and correlated by a central supercomputer. The resulting data, several petabytes a year, will be stored in an archive, distributed over a number of partners. The LOFAR Archive Information System plays a crucial role in this long-term archive. It will keep track of the data stored in the archive, and allows for further processing of that data. The information system supports different computing and storage technologies, including the EGEE Grid.

Demo Session 1, Welcome Drink / 55

NeuroLOG: a federated environment for neurosciences supporting multi-centric studies

Mr. GAIGNARD, Alban [1]; Mr. MICHEL, Franck [2]; Mr. JAVIER, Rojas Balderrama [3]; Mr. GODARD, David [4]; Dr. LINGRAND, Diane [3]; Dr. MONTAGNAT, Johan [1]

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The NeuroLOG project develops a distributed environment dedicated to the support of collaborative and multi-centric studies in neurosciences. The NeuroLOG environment leverages grid technologies to deploy a highly secure, large scale data federation and to deliver high throughput neuroimages analysis. It is interfaced to the gLite middleware and takes advantage of the EGEE grid. It integrates in existing site-specific neuro-informatics environments. NeuroLOG clients, deployed on user desktops, provide neurosciences services through a coordinated federation of site servers and grid services.

Computational Chemistry / 56

pKa Calculations of Key Ionizable Protein Residues in Acetylcholinesterase

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One of the most abundant quantities characterising proteins is its isoelectric point, which is directly dependent on the number of charged ionizable residues, on the pKa of all ionizable residues more exactly. In this work, the pKa of buried protein aminoacids are estimated using method based on molecular dynamics called thermodynamic integration. The main scope is to compute pKa in acetylcholinesterase, but the computations on a small protein, thioredoxin, will be also presented as benchmark calculations.

High Energy Physics / 57

LHC ATLAS users analysing data on the Grid

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In this talk we will describe the experience of the experiment ATLAS in commissioning the system (large scale user-analysis exercises in late 2009) and the first experience with real data.
First of all, we will describe the tools to commission and control the sites contributing to user analysis.
We will describe the support structure and the user experience (study of monitoring data and direct feedback from users). We will also show examples of analysis running on new data collected after the first collisions starting December 2009.

Computer Science / 58

An investigation of the effect of clustering-based initialization on Learning Classifier Systems' effectiveness: leveraging the Grid infrastructure

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Strength-based Learning Classifier Systems (LCS) are machine learning systems designed to tackle both sequential and single-step decision tasks by coupling a gradually evolving population of rules with a reinforcement component. ZCS-DM, a Zeroth-level Classifier System for Data Mining, is a novel algorithm in this field, recently shown to be very effective in several benchmark classification problems. In this paper, we evaluate the effect of clustering-based initialization on the algorithm's performance, utilizing the EGEE infrastructure as a robust framework for an efficient parameter sweep.

Computer Science / 59

Grid-enabled parameter initialization for high performance machine learning tasks

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In this work we use the NeuroEvolution of Augmented Topologies (NEAT) methodology, for optimising Echo State Networks (ESNs), in order to achieve high performance in machine learning tasks. The large parameter space of NEAT, the many variations of ESNs and the stochastic nature of evolutionary computation, requiring many evaluations for statistically valid conclusions, promotes the Grid as a viable solution for robustly evaluating the alternatives and deriving significant conclusions.

Computational Chemistry / 60

Porting of Computational Chemistry legacy applications on the EGEE Grid platform: computational aspects and visualization tools

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The work carried out to implement complex computational chemistry suites of codes on distributed systems and, at the same time, to develop appropriate graphical tools for the visual rendering of the outcomes of the calculations on the production EGEE Grid infrastructure available to the COMPCHEM VO, is here presented and discussed with some examples.

Computer Science / 61

Phenomenology of Minority Games in Efficient Regime

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We present a comprehensive study of the utility function of the minority game in its efficient regime. We develop an effective description of the state of the game. For both the step-like payoff function g(x) = sgn(x) and the proportional function g(x)=x, we explicitly represent the game as the Markov process and prove the finiteness of number of states. We also demonstrate boundedness of the utility function. Using these facts we can explain all interesting observable features of the aggregated demand: appearance of strong fluctuations, their periodicity, and existence of preferred levels.

User Support and Services / 62

User Support for Distributed Computing Infrastructures in Europe

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In a worldwide distributed computing infrastructure such as EGEE (Enabling Grids for E-sciencE) one of the challenging tasks is to build and maintain a reliable user support infrastructure. During the last years the GGUS (Global Grid User Support) system has been developed as EGEE's answer to that challenge. GGUS is designed as a centrally coordinated distributed infrastructure that integrates existing tools instead of trying to replace them.
The next challenge will be to adapt the user support infrastructure to the new operations model on which the EGI/NGI infrastructure will be based.

Workflow Management / 63

OpenMOLE: a grid enabled workflow platform

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OpenMOLE is a free and open source workflow engine providing distributed computing facilities, especially suited for scientific research in complex systems. Third-party software packages can be embedded in a workflow that
automatically transfers and processes their input and output (files and data). Embedded software packages are called "tasks". Any task within a workflow can be either executed locally or delegated to distributed computing environments, including the EGEE grid.

Computer Science / 64

Modeling Grid Job Time Properties

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Large-scale analysis of grid job data, consisting of more than 28 million jobs gathered during 20 months from all major EGEE Resource Brokers, provides interesting results regarding the properties of job time parameters. The main parts in a job's life cycle are observed to have different distributions, having also different origins that cause these behaviors. While 'match time' parameter corresponds better to power law distribution,the total job length is well modeled with log-normal distribution. Here we attempt to fit the distributions and give explanation through generative models.

Poster session / 65

Harnessing Heterogeneous Computing Resources for Solving Hard Computational Problems

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The talk presents the BNB-Grid tool aimed at solving hard combinatorial, discrete and global optimization problems in a distributed heterogeneous computing environment. The BNB-Grid can run applications across different service and desktop grid platforms as well as individual workstations and clusters. The BNB-Grid efficiently copes with difficulties arising in such systems: the software diversity, unreliability of nodes and problems with batch (queuing) system. The talk discusses the implementation details and computational results for two challenging problems.

Computational Chemistry / 66

Protein Molecular Dynamics and Free Energy Calculations on the EGEE Production Grid

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Atomistic simulations of large biomolecules such as proteins require extensive computational resources. Dynamical and thermodynamical properties can be obtained either by averaging over very long time trajectories or sampling the phase space by running hundreds of short time trajectories. The latter methods are the most appropriate for high throughput computers such as the Grid distributed computers. Algorithms are presented for calculating vibrational spectra of the active site of cytochrome c oxidase as well as free energy landscapes based on thermodynamic perturbation theory.

Bioinformatics / 67

Estimating the Performance of BLAST runs on the EGEE Grid

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Estimating the response time of large experiments is a key issue for achieving an efficient load balancing and minimizing the failure rate. This requires having a good knowledge of both the application and the infrastructure. This work describes a set of experiments that have conducted to the definition of a performance model that can be used to estimate the response time of the selected resources and to adapt the partition of the load to the dynamic status of the resources.

Infrastructure Tools and Services / 68

Site Status Board: WLCG monitoring from the experiment perspective

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Now that the LHC has started, the experiments require a high standard of reliability and performance on their computing activities. Monitoring these activities is not a trivial task mainly due to two reasons: first of all, asserting the proper behavior of a site depends heavily on the software model of each experiment; secondly, the number of sites taking part in WLCG has increased drastically compared to previous HEP experiments.

Poster session / 69

Gustav : a lightweight approach to CPU accounting

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Gustav is a CPU usage accounting tool developed by INFN, COMETA and the KISTI institute. Gustav collects accounting records from resources and publishes them to a centralised relational database, that can be queried through a web interface. Gustav is characterised by a lightweight architecture, that makes its usage ideal for small sized infrastructures. However, interoperability with more powerful tools, like DGAS or APEL, is accomplished by the adoption of standard format for accounting records.

Poster session / 70

An integrated monitoring system for Grid Data Centers

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We present a monitoring system developed for the Data Centers used for the SCoPE and ATLAS projects in Napoli, Italy. The system is based on a portlet container which gives an integrated view of the Data Center, and allows a graphical-based, hiearchically organized navigation for all the equipments, from the racks to the active components. The system allows monitoring of the whole infrastructure (UPS, cooling, electrical power consumption at single socket level), but also of the network (Gigabit, 10 Gigabit, Infiniband, Fibre Channel) and, of course, of storage and server nodes.

Poster session / 71

MEG - MyProxy Enabled GSISSHD

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MEG allows users to logon to a grid-resource using any SSH-enabled client, so long as they have uploaded a credential to a MyProxy server. MEG accepts the username and password to the credential from the SSH client and retrieves the proxy on behalf of the user, and the uses the proxy to determine if the login can proceed. Resource providers benefit too, as only grid-based authentication mechanisms are needed, so a UI box can be implemented without adding an additional layer of user management.

High Energy Physics / 72

Client/Server Grid applications to manage complex workflows

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Grid Applications adopting a client/server paradigm allow easier enforcement, improvement and optimization of the middlewares. A server allows us to enact specific and complex workflows, in order to centralize application management and hiding Grid complexities to the end users. These features aim to enable Grid to a large and heterogeneous community not only at the infrastructure level, but also at application level. A successful example for the grid server paradigm is presented for CMS and its analysis tool, CRAB.

Astronomy and Astrophysics / 73

Constraints on primordial non-Gaussianity using Planck simulated data: First Results

Dr. LOPEZ CANIEGO ALCARRIA, Marcos [1]; Dr. CURTO, Andres [1]; Dr. MARTÍNEZ-GONZÁLEZ, Enrique [1]

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After the successful porting of the point source detection code and the SZ clusters detection code to the EGEE GRID, we have ported and tested a new application. This application is composed of two codes, one that produces simulations of Planck and another one that looks for non-Gaussianity signatures in these maps using spherical wavelets. These applications are part of an ongoing project being carried out by the Observational Cosmology and Instrumentation Group at the Instituto de Física de Cantabria (CSIC-UC) on different analyses of the Cosmic Microwave Background (CMB).

Computational Chemistry / 74

A multiconfiguration time-dependent Hartree algorithm for non-Born-Oppenheimer calculations

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We have embarked upon a project of performing dynamical calculations treating electrons and nuclei on exactly the same footing,
considering all particles as degrees of freedom of a dynamical system. In that way, the Born-Oppenheimer approximation is circumvented. The very concept of a potential energy surface is abolished and the problems associated with kinetic energy couplings or Berry phase simply vanish. Since an exact treatment of this kind would be prohibitive, we split the various degrees of freedom according to a MCTDH scheme.

Novel Architectures and Technologies / 75

Enabling the use of e-Infrastructures with Microsoft HPC and the Matlab distributed compute server

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Many scientists with smaller scale problems could benefit from e-Infrastructures but are often discouraged by their complexity. These users have little experiences with shell based Linux environments typically offered; instead, they
often use Windows-based platforms and higher level packages like Matlab. In this talk we present a case study from microsystems research, focusing on how the usage of recent technologies like the Microsoft HPC server and the Matlab distributed computing toolbox can improve the productivity of the researchers and allows them to exploit existing e-Infrastructures.

Computational Chemistry / 76

Computational chemistry experiments over a web service-oriented grid

Prof. BARONE, Vincenzo [1]; Dr. BLOINO, Julien [2]; Dr. CASTRIGNANO, Tiziana [3]; Dr. MORELLI, Gianni [3]; Dr. SANNA, Nico [3]

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We will describe the implementation of effective numerical differentiation techniques aimed to obtaining different energy derivatives of quantum chemical energies and properties on a service-oriented grid where the computational workflow is spawned over multiple, geographically distributed, sites. The application porting over the grid and its extension as a web service over local and wide area networks is fully outlined.
A description of the procedures developed for these experiments is given in full detail and the applicability of the methodology to similar problems pointed out.

Regional Activities, International Projects and Collaborations / 77

Disseminating the Grid: An essential guide

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When it comes to dissemination, what works and what doesn't? During EGEE-III, NA2 has coordinated a rich programme of activities through an increasingly wide range of media – press releases, booths, blogs, Twitter and websites to name just a few. This session gathers together best practices based on the lessons learnt with input from collaborating dissemination project, GridTalk. Practical examples and case studies highlight how to deal with the media, make an impact on policy makers, get business leaders interested in the grid and bring new user communities on board.

User Support and Services / 78

Supporting diverse local virtual organisations

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Within ScotGrid-Glasgow, primarily an ATLAS Tier-2 grid site, we are involved in supporting a number of local virtual organisations (VO)'s, including Electrical Engineers, Solid State Physicists (SSP) and Optics all with very specific non-high energy physics requirements (HEP). An account of the main issues and achievements that resulted from working with other groups at our site who sought direct access to a batch system rather than a grid site will be presented. This includes trialling various submission mechanisms and middleware components to achieve the goals of each of the specific VO's

Data Management / 79

Enabling Large Data Transfers Between Web Services

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Despite numerous benefits, many Web Services (WS) face problems with respect to data transport, either because SOAP doesn't offer a scalable way of transporting large data-sets or because orchestration workflows (WF) don't move data around efficiently. In this paper we address both problems with the development of the ProxyWS. This is a WS utilizing protocols offered by the Virtual Resource System(VRS)(Java API used by the VBrowser), to enable other WS to transfer and access large datasets without modifying WS nor the underlying environment.

Regional Activities, International Projects and Collaborations / 80

NDGF approach to serve the non-LHC communities needs: Nordic Material Science VO

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We present the joint NDGF and CSC (Finland) project on setting up and supporting a new Nordic Material Science Virtual Organization inside NDGF (Nordic MS VO). The activities are focused on making the flexible and Nordic MS VO users friendly grid environment available on ARC enabled resources.

Computer Science / 81

Distributed evolutionary optimization framework on the Grid and HEP use case

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This paper describes an optimization framework which utilizes a distributed evolutionary algorithm with the ability of adaptation to the complex physical structure of the grid fabric. The algorithm is divided into several partitions (demes) which are located on physical clusters. This architecture allows simultaneous use of all the available resources, regardless of their geographical location, within one application. The paper also presents an example use case of this technique, which is track reconstruction optimization for COMPASS experiment.

Poster session / 82

Using the EELA-2 grid Infrastructure to Perform HeModynamics Computer Simulations: The HeMoLab Experience

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The main goal of the HeMoLab project is the development of computational models used in the simulation of the Human Cardiovascular System, performed by a general purpose numerical solver that apply distributed computing techniques through the use of the MPI paradigm. This paper describes the main steps of the porting process of SolverGP to gLite environment, covers the main characteristics of gLite, grid tools that have been used in the gridification process, and examples of performance results of computer simulation that were obtained from the application already ported to Grid of the EELA-2.

Demo Session 2 / 83

Interoperabilty among gLite and ARC middleware in training grid infrastructures: GRIDSEED testcase

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GRIDSEED provides a simple tool to setup up a portable fully fledged gLite grid infrastructure based on virtual machines. It exploits the concept of “grid in a box” providing a self-containing grid that could be easily deployed in any existing infrastructure for training and dissemination purposes. In this work we present a recent effort to include ARC middleware in the original GRIDSEED infrastructure
The purpose of the exercise is to provide a training facility where users could learn how two similar grid middleware can interact and have a first knowledge on interoperability issues.

Bioinformatics / 84

Grid assisted structure calculation of large protein systems in solid-state NMR context

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Due to the present experimental limitations of solid-state NMR (ssNMR), 3D structure calculations of proteins using these NMR spectra as a source for structural constraints are demanding in terms of computing power. The application ARIA solid-state NMR is dealing with the automated assignment and structure calculation of large protein
systems in ssNMR context. We are currently adapting and evaluating that structural-biology application to grid computing within the EGEE infrastructure, and to cloud computing infrastructure using the HIPCAL and Eucalyptus systems.

Poster session / 85

grid-CICADA – Efficient Explorer of Conformational Space of Biomolecular Systems

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Knowledge of conformational space is essential in the assessment of dynamical behavior of biomolecules, which is important, for example, in drug design and folding studies. Unfortunately, systematic exploration of conformational space is impossible due to its high complexity. To circumvent this problem, we have developed the program CICADA that tries to rationalize the search in such a space. In this work, we will demonstrate the utilization of a newversion of CICADA in the grid environment during the study of selected middle size biomolecules.

Earth Science / 86

Grid implementation and application of the WRF-ARW prognostic model

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In this work the implementation and deploying of the Advanced Weather Research and Forecasting (WRF-ARW) model on the SEEGRID-SCI grid infrastructure is presented. The goal of porting the model to the grid is to get more accurate and detailed forecast with operational speed-up on high-resolution model grids. The results and the application of the WRF model will be shown through the examples of the operational weather forecast, foehn effects over Banja Luka in Bosna and Hercegovina (BIH) and bora winds simulations over the Adriatic coast in Croatia.

Computer Science / 87

Towards an interoperable representation of the Grid Observatory information: an experiment with Common Base Event

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Reaping the full benefit of the Grid Observatory (GO) initiative requires providing end-users with convenient representation of the traces. The present lack of standardization creates considerable difficulties for developing automated analysis and situation handling solutions. We report an experiment on the representation of internal logs of the gLite WMS with the IBM Common Base Event (CBE) format, categorizing the information of hundred of thousand events to a few generic type situations, with potential applications of the open-source supporting technologies to job monitoring.

Poster session / 88

Stellar energy flux modeling under SYNTSPEC application

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We present the stellar energy flux modeling tool under the SYNTSPEC application. SYNTSPEC is the gridified tool for stellar spectra analysis. It is an example of a data- and compute-intensive application running on the testbed of the EU BalticGrid-II Project (http://www.balticgrid.org), which brings new quality to the research in astrophysics. The multi job application is run within the Gridcom system – the user friendly interface that allows a common (virtual) work of the physically spread scientific group.

Poster session / 89

Performance evaluation of the Estimated Response Time strategy: tools, methods and an experiment

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An extensive body of research focuses on economic and intelligent scheduling models. Conversely, the gLite matchmaking engine adopts an agnostic approach for estimating the waiting time of incoming jobs, derived from the Copernican principle: "this job is not special". An open question is the evaluation of this minimalist strategy. This work reports on the creation of the software tools required for this evaluation, the methodology and criteria, and presents preliminary results using the Grid Observatory logs of the Information System (IS) and PBS scheduler of GRIF/LAL.

Poster session / 90

Visualizing the dynamics of e-science social networks

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Computational grids provide new natural examples of large-scale complex networks emerging from collective behavior. An interesting question is thus whether these networks exhibit properties similar to those of other social networks (SN), or original ones, which would be the specific signature of e-science. As a first step towards answering these questions, we build a scalable interactive visual exploration tool targeted at the spatiotemporal structure of data-access and data-sharing. The primary goal is to help computer science researchers getting intuition about the dynamics of the system.

Earth Science / 91

Bridging the gap between applications geospatial data and the Grid

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CROSS-Fire is a Portuguese NGI funded project aiming to develop a grid-based risk management decision support system for the Civil Protection (CP), using forest fires as the main case study and FireStation (FS) as an application that simulates the fire spread over complex topography.
CROSS-Fire uses EGEE to provide raw technological capability provision, including data management and storage, access to meta-data data bases and HPC and a Geospatial Information Infrastructure based on OCG-SWE Web Services to provide the access and management of remote geospatial data and meteorological data.

Parallel Processing / 92

MPI support and improvements in gLite/EGEE - a report from the MPI Task Force

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The MPI Task Force (MPI-TF) was established in response to calls from the EGEE user communities and site administrators during the MPI session at EGEE09. Improvements in the overall deployment and support of MPI on the EGEE infrastructure were demanded. The objectives of the MPI-TF are to provide solutions which will improve the testing, installation and configuration of MPI-enabled middleware, and to support greater MPI application usage on the Grid. We report on the work performed by the MPI-TF and report on the changes and improvements in MPI support delivered since its establishment.

Computational Chemistry / 93

Ab initio grid chemical software ports – transferring knowledge from EGEE to Polish NGI

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Chemical software, especially with ab initio methods, have been developed over several years of research in the field of numerical methods in chemistry. As the research was performed by many groups of scientists this resulted in a variety of software suites. From this set the commercial packages are of particular interest among the community due to the availability of many computational methods, the fast development of new ones and better user support. To attractthe chemical community to grid computing a set of frequently used software suites have been ported to the grid.

Demo Session 1, Welcome Drink / 94

Grid Web Portal with software plug-ins to chemical software

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New users, especially those accustomed to Graphic User Interfaces (GUI), often face difficulties during the adoption of grid computing for the research. The main source of issues is related to command line interfaces which are hard to adopt by non-experts. To avoid users' disappointment a new web based interface has been proposed. In contrast to existing web-based tools the portal developed facilitates not only job management but primarily can serve as a work environment for chemists. Here, we present the current status of the portal development including several plug-ins to first principles chemistry packages.

Poster session / 95

Trading Computing Resources across gLite and XtreemOS Platforms

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The objective of this work is to present a system that facilitates the commercialization of Grid resources through a Virtual Marketplace of computational resources, where a seller is capable of listing the Grid resources, and buyer can request/bid dynamically for required computing resources for their applications.
This model exploits the benefits of Grid computing, especially the inter-operability and scalability of Grid platforms. Interoperability is achieved by using the OGF SAGA standard on two Grid platforms: XtreemOS, a Linux-based Grid OS, and gLite, a Grid middleware.

Poster session / 96

Monitoring CREAM Jobs in RTM via L&B

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The Real Time Monitor (RTM) is a high-level monitoring tool which aggregates information on grid jobs and presents it in a suitable form. The success of this tool depends on the accuracy of information it is able to receive from lower layers. However, withthe recent increase of the number of jobs submitted directly to Computing Elements (CE) the fraction of jobs seen by RTM decreases. gLite Logging and Bookkeeping service (L), with its recent extension to CREAM jobs, provides the necessary level of abstraction and a glue between different job flavours to allow high-level tools to see full range of grid jobs.

Regional Activities, International Projects and Collaborations / 97

Improvements of the grid infrastructure and services within SEE-GRID

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Enlargement of the grid user community is probably the most important challenge of the grid infrastructure development community. To attract new users, with new applications and needs, the infrastructure should be flexible enough to satisfy their needs and requirements. We present the experience of the development community from the SEE-GRID-SCI project, organized in a Joint Research Activity. The main focus if this JRA was to improve the usability of the infrastructure and Grid services for the end-users from target communities, as well as manageability of the underlying infrastructure.

Poster session / 98

A new middleware component for job monitoring in interactive mode: The SCoPE Experience

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This work aims to extend the standard gLite middleware with a new functionality that enables the final users to interact with their submitted grid-jobs, for monitoring purposes.
The new service is composed by a worker nodes Proxy server, with web-services interface VOMS compliant, easy to deploy and not invasive to respect the standard gLite solution. Through the Proxy, a generic user can connect, from the user interface, to the Worker Node that is taken his job. The tool has been implemented on the SCoPE infrastructure, to support the e-science community of the University of Naples Federico II

Regional Activities, International Projects and Collaborations / 99

EUAsiaGrid – e-Infrastructure Platform for Asian-Pacific Region

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EUAsiaGrid is the EU-funded project aiming to bring together researchers from Asia-Pacific region around the distributed infrastructure being built within in the region. The primary purpose of the project is to support researchers willing to perform scientific discovery though advanced computing. In addition, the project is expected to further facilitate the uptake of e-Infrastructure approach.

Regional Activities, International Projects and Collaborations / 100

Developing e-Infrastructure services for e-Science applications: the EELA-2 experience

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This work aims at presenting the results obtained in the joint research activity of the EELA-2 project. In order to satisfy all heterogeneous applications requirements and to simplify the access to the Grid infrastructure, in the context of this activity, a set of special services has been developed to enhance the functionality of the gLite middleware and provide users with a richer platform. The middleware services developed have widened the number of potential applications taking benefit of the grid e-infrastructure and, moreover, have speeded up the porting process.

Scientific Gateways and Portals / 101

SOMA2 – Open Source Gateway to Molecular Modelling Workflows

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SOMA2 gateway is a WWW-browser operated molecular modeling workflow environment developed and deployed by CSC. The SOMA2 environment allows users to control and combine scientific applications available in the computing system into unique application workflows, which are automatically executed. SOMA2 offers a flexible framework for integrating and executing molecular modeling applications, including molecular data exchange. SOMA2 source code is distributed under the GPL license.

Bioinformatics / 102

Setup and usage of an e-BioScience infrastructure for high throughput DNA sequence analysis

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Current DNA sequencers produce a large amount of data. Because the amount of data is growing and the computation time for analysis is increasing, we initiated a pilot to run applications on the Dutch Grid (Big Grid, part of EGEE). We used the software platform that was developed for medical imaging in the VL-e project (e-BioInfra), and applied it to DNA sequence analysis. With the knowledge gained in this pilot, we now use this platform routinely for computational intensive analyses.

Poster session / 103

ASC: an Adaptive Scheduling Controller

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The deployment, management and TCO of large computing environments always involve huge investments. These systems, once in production, have to meet the needs of users belonging to large and heterogeneous communities: only an efficient and effective use of these systems can repay the investment made. In this context, we report the experience made to design, implement and validate an adaptive scheduling system able to reconfigure itself when a lack in utilization efficiency occurs.

DCI programming / 104

ETICS a success story from research to production

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ETICS is a software build, test and quality certification system which, after four years of development activities and use by the research environment, is now mature to start its way into the commercial software development environment. The experimentation of the use of ETICS also in the commercial environment was part of the challenge since the very beginning. This experimentation has now become a reality thanks also to the project commercial partners like Engineering which is going to offer ETICS as a service to the project managers from its production units.

Poster session / 105

Programming gLite without an UI - a JavaGAT adaptor for gLite

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Programming in the EGEE Grid with gLite currently requires a large toolchain of software, which is installed on UI machines. It is often difficult, if not impossible, to install the full gLite software stack on development machines or on deployment machines, e.g. for web portals.

We present a generic adapter for programming gLite which is independent from the gLite software stack and from UI machines. It can be used on any machine providing the Java Runtime Environment. It provides an API compatible with JavaGAT, the standard for Grid programming.

Demo Session 2 / 106

XtreemOS Grid Operating System

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The XtreemOS operating system provides for Grids what a traditional operating system offers for a single computer: abstraction from the hardware and secure resource sharing between different users. When a user runs an application on XtreemOS, the operating system automatically finds all resources necessary for the execution, configures user's credentials on the selected resources and starts the application. It simplifies the work of users by giving them the illusion of using a traditional computer.
The XtreemOS technology is being developed in the frame of the XtreemOS European IP.

High Energy Physics / 107

CMS Remote Analysis Builder (CRAB) with the ARC grid middleware

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The Compact Muon Solenoid (CMS) is one of the general purpose experiments at the CERN Large Hadron Collider (LHC). For distributing analysis jobs to computational resources scattered across the world, the CMS project has developed the CMS Remote Analysis Builder software (CRAB). Until now CRAB has only supported the gLite and OSG middlewares, but with the help of a new plugin, the CMS analysis jobs can be run on sites running the ARC middleware.

Scientific Gateways and Portals / 108

A Scientific Gateway for Distributed Mining of Biomedical Image Data utilizing Web Services

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Recent advances in biomedical applications like DNA sequencing, microarray data generation, high-throughput, gene-function studies, medical imaging, and electronic medical records, have resulted in the automatic generation of new and vast data repositories. Mining and managing such biomedical data is a complex procedure that requires several processing phases. Especially in the case of biomedical images, proper preprocessing, (e.g., image enhancement, color processing), feature extraction and classification are required.

Computer Science / 109

Evolution of density of interacting agents for the two species irreversible reaction A+B->2A in complex networks

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We use Monte-Carlo simulations to study the dynamics of the irreversible A+B->2A two species reaction on regular lattices, Erdos-Renyi (ER) and scale-free (SF) networks. The problem we study is an analogue to the spread of a virus in computer networks and other epidemiological models, such as information diffusion (i.e. rumor spreading) in social networks, and information propagation among stations in ad hoc mobile networks. We monitor the density of the species with respect to time, which we find to be an exponential function of time in the long time regime.

Poster session / 110

GILDA training infrastructure: present successes and future triumphs

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GILDA is a very successful initiative, led by INFN, aiming to provide a special production-quality Grid infrastructrure (t-Infrastructure) for higher education, training and dissemination purposes. Since its earlier phases, EGEE adopted GILDA as its t-Infrastructure, providing many scientific and humanistic communities with a fully fledged virtual laboratory where to "learn and try". GILDA has officially been adopted as the default t-Infrastructure by other projects such as EELA and EELA-2, EPIKH,EUAsiaGrid, EUChinaGrid, EUMEDGRID/EUMEDGRID-Support, SAGrid, the UNESCO/HP Brain Gain Initiative.

Poster session / 111

A Grid-Enabled Problem Solving Environment for QTL Analysis in R

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There exist a large number of applications in multidisciplinary research environments that require efficient, seamless, and easy-to-use infrastructures to address computationally intensive problems. In this work we present an approach to build Grid-enabled problem solving environments (PSE), that allow end-users to operate within familiar settings and provide transparent access to computational Grid resources.

Demo Session 1, Welcome Drink / 112

Impact of the synthetic seismogram archive for the CMT determination

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The aim of this demo is to show the performance increase provided by an indexed synthetic seismograms archive. It is also an opportunity to identify partners wishing to distribute and consolidate this archive.

Poster session / 113

Earth Science and Astrophysics Applications in Armenia: Present and Perspectives

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The Institute for Informatics and Automation Problems of the National Academy of Sciences of the Republic of Armenia operates, supports and manages the national Grid Infrastructure and Academic Scientific Network of Armenia, which provides all core services to the users and consists of 7 Grid sites located in Yerevan and Ashtarak cities (424 cores). Armenia actively engaged in different international Grid (EU FP7 SEE GRID SCI, ISTC A-1606, ISTC A-1451) and connectivity (EU FP7 BSI) Projects, which make possible to deploy infrastructures and environments in the earth science and astrophysics.

Parallel Processing / 114

Tapas4Grid: a grid tool for performing parametric studies based on complex workflows

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One typical problem to be solved by fusion codes, which is suitable for grid and parallel computing, is the parameter scan. There are several codes whose main purpose is to get results for wide parameter range. So it makes sense to build a tool that allows one to perform this parameter scan in an automated way. We have build and used a new tool suitable for solving this kind of problems: TAPaS. This tool is, in principle, and thanks to its layer based design, suitable for both HPC s and grid computing, although it has only been used on the grid.

Security / 115

Sanctorum: a solution for safe management of digital certificates and passwords in a farm

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Sanctorum is a python tool created to aid sitemanagers to safely manage digital certificates and passwords for hosts in a farm. Motivation for the tool: when releasing a new host certificate, the Italian Certification Authority recommends the site to maintain two backup copies of the private key in a safe place not network reachable. This makes it quite difficult to both respect the CA rule and to efficiently manage the site, especially large ones. The proposed solution makes it possible to manage digital certificates in a comfortable and error free manner while still respecting CA recommendations.

Data Management / 116

Improved Task Scheduling for Distributed Data Analysis Systems

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In this work, we present an evaluation of a late-binding scheduler for HEP distributed analysis, where data is distributed globally with multiple replicas in a non-uniform way. We employ the late-binding technique in order to optimize job placements thereby minimizing the per-job time-to-completion. We evaluate different scheduling and prioritization strategies, and evaluate the approach using a prototype system implemented with the Ganga end-user tool and the DIANE scheduling framework applied to ATLAS distributed analysis.

Demo Session 2 / 117

Using gLibrary with mobile devices: a proof of concept with Apple iPhone

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gLibrary mobile is a native application for the Apple touchscreen devices that allows to access digital libraries, deployed over grid infrastructures, from mobile devices such as the iPhone and the iPod touch. gLibrary mobile is our attempt to offer a mobile client to interact with digital libraries created with the INFN grid digital library solution. It allows to easily browse libraries contents, inspect library items metadata and finally download and view in the device high resolution screen the closest replica of the selected object.

User Support and Services / 118

Lessons learnt from the EGEE Application Porting Support activity

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In its third phase, the EGEE project flagged application porting as a critical service for the successful adoption of grid solutions by new users and new communities and includes “Application Porting Support” among its generic user support activities. The goal of the EGEE Application Porting Support group is to aid developers in effectively porting Virtual Organizations’ (VO) applications to the Grid. The presentation gives an overview of the key activities of this support service, its evolution during the EGEE project, and the lessons learnt by the provision of this service.

Earth Science / 119

Computational Requirement of Meteorological and Crisis Applications

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We present several applications from the domain of meteorology and crisis management that we developed and/or plan to develop. In particular, we present the IMS Model Suite - a complex software system designed to address the needs of accurate forecast of weather and hazardous weather phenomena, environmental pollution assessment, prediction of consequences of nuclear accident and radiological emergency. We discuss the computational requirements and our experiences on how to meet them by grid computing.

Regional Activities, International Projects and Collaborations / 120

The South African National Grid Initiative : From prototype to production

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South Africa is has made significant investments in e-Infrastructure recently. These investments are partly in the form of centralised, centrally-funded initiatives such as the Centre for High-Performance Computing (CHPC) and South African Research Network (SANReN). However, a significant investment has also been made in parallel by universities and national laboratories of computing resources and manpower, dedicated to research support. The South African National Grid is a national federation of these efforts with the goal of deploying a production-quality regional e-Science infrastructure.

User Support and Services / 121

Training in EGEE - creation of a sustainable user service

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EGEE-III Networking Activity 3 (NA3) has the responsibility of coordinating and delivering user training and induction. The activity aims to train a wide variety of users, both those within the EGEE consortium and those from outside the project who make use of the EGEE Grid infrastructure. The presentation will present the evolution of training activities in the EGEE series of projects, provide a summary of its current services and highlight activities that make gLite-related training in Europe a sustainable service

Poster session / 122

Data Mining and Integration of Environmental Applications

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In this paper we presents the data mining and integration of environmental applications in EU IST project ADMIRE. It briefly presents the project ADMIRE and data mining of spatio-temporal data in general. The application, originally targeting flood simulation and prediction is now being extended into the broader context of environmental studies. We describe several interesting scenarios, in which data mining and integration of distributed environmental data can improve our knowledge of the relations between various hydro-meteorological variables.

Poster session / 123

Development plans of the EGEE Operations Portal and dashboard towards and EGI/NGI infrastructure

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The operations portal of EGEE is undergoing a tremendous back-end evolution to wrap-up the 5 years experience gained on daily grid operational needs about procedures and tools developed for and made available to the different EGEE communities.This evolution is crucial to meet the changes to cope with the EGI structural needs and with the NGIs requirements for the regionalisation of the tools where applicable.

Workflow Management / 124

Services for advanced workflow programming on gLite with WS-PGRADE portal

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After the great success of the P-GRADE Portal MTA SZTAKI has created the second generation P-GRADE portal, called WS-PGRADE. WS-PGRADE is a Web based environment for both developers of grid based dataflow applications, and end users who need transparent access to grid based application services. The presentation gives an overview of the application developer functionalities of the WS-PGRADE environment, details the various application patterns that can be realized in the system and executed on cluster based and PC based platforms.

DCI programming / 125

Ganga/DIANE and SAGA for solving complex scientific problems

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An increasingly important requirement for solving complex scientific problems is the simultaneous use of qualitatively different resources, from simple batch nodes to supercomputers. We present a project where Ganga and DIANE user-level middleware tools are used in connection with SAGA, a high-level Grid API, to achieve an improved quality of service when using resources across multiple computing infrastructures, such as EGEE, NDGF, OSG and TeraGrid. We discuss these advances in the context of LQCD simulations in theoretical physics and other applications in the current portfolio.

Poster session / 126

Grid-CSIC project: porting astrophysic applications to Grid

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Two important problems related to astrophysics applications are high computational cost and limited storage. The Grid-CSIC Project promotes the use of Grid infrastructure on the research institutes of Spain. The Institute of Astrophysics of Andalusia (IAA-CSIC) joined this project in order to provide scientific application support in the astrophysics area. Several applications have been implemented by the infrastructure work team.

Parallel Processing / 127

Towards a robust and user-friendly MPI functionality on the EGEE Grid

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An MPI Working Group has been setup with the goal to investigate why so few Grid sites support MPI and why so few people are using it. The Working Group has come up with a recommendation document in which the current issues with MPI on the Grid are analyzed, the reasons for non-usage are investigated and the plans for future expensions are summarized.

Computational Chemistry / 128

MCTDH Quantum Dynamics in EGEE: Advances Made and Improvements needed

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Our communication provides a detailed description of the present performance of grid-Fluss and grid/MCTDH, tools for the direct quantum-mechanical calculation of kinetic coefficients, implemented on the section of the production computing Grid of EGEE accessible to the COMPCHEM virtual organization. The performance and reliability of the method is illustrated by presenting the results of two computational campaigns: the N + N2 reaction and the CH4 + Ni(111) dissociative sticking process.

Infrastructure Tools and Services / 129

Visual GRID Activity Monitoring in the Dashboard Framework

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It is sometimes hard to conceptualise the GRID and visualise its activity. But having a graphical representation of its workings and movements, we can more easily surpass these problems; coupling this with a system that provides accurate measurements of such activities, we obtain a powerful monitoring system that is visually appealing, intuitive to use and of great practical worth.

Our solution is supported on two, interconnected systems: the Google Earth Dashboard monitor provides the high-level, graphical view of the Grid while more detailed information is displayed by Siteview.

User Support and Services / 130

Latest achievements of the MTA SZTAKI Grid Application Support Centre

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The Grid Application Porting Support Centre (GASUC) of MTA SZTAKI has been established in 2007 to support potential users of grids getting their applications to distributed infrastructures. The support team is the leader of the EGEE Application Porting Support Group since 2008 and has been ported about 15 applications since then to various production VOs of the EGEE grid. This presentation will give an overview of the latest applications and tools that the support centre has worked with, developed and operated.

Novel Architectures and Technologies / 131

Grids and Clouds Interoperation: Development of e-Science Applications Data Manager on Grid Application Platform

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The Grid Application Platform(GAP) is a middleware to reduce development efforts of e-Science implementation. The GAP development is stimulated by the systematic framework in which applications can easily well-formulated common components to build up new services and taking advantage of Grid without worrying about new technologies. Cloud technology of data management is of essential importance by its performance and resilience. HDFS is integrated into GAP for the value of a scalable, fault-tolerant distributed file system for an efficient data access services in any stage of an e-Science Apps.

Medical Imaging / 132

Grid-enabled Medical Image Analysis: From Jobs to Workflow-based Service

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Medical image analysis requires large computational effort. The construction of “atlases” specific for each study of a specific brain disease is a good illustration: typically all images need to be aligned (registered) to each other. In this work we explore the Dutch Grid (part of EGEE) to implement a service that automates the construction of such atlases for Diffusion Tensor Imaging (DTI), facilitating usage by neuroimaging researchers. Initial experiments show that the service is robust and valuable for medical imaging research.

Demo Session 2 / 133

LHCb Data Production System based on the DIRAC project

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LHCb is one of the four experiments at the LHC collider are CERN. It has started recently to record the data coming from the real proton-proton collisions. The data processing chain is managed using the tools provided by the DIRAC project. All the operations starting from data transfers from the exprimental area up to the final user analysis distributed in all the LHCb Tier-1 centers are automated.
MC data production is also managed within the same framework. The production controls as well as visualization of the monitoring information are performed through the DIRAC Web Portal.

Security / 135

Improving Grid User's Privacy with gLite Pseudonymity Service

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The Grid computing model provides Grid users a way to use resources that are not usually owned by their parent organizations. The use of Grid resources entails a balance between the resource owner's need to oversee and account for the resource usage and the user's privacy requirements. From the user's point of view, complete anonymity is desirable, but not possible due to requirements like traceability without user intervention. The solution we propose is the concept of a lesser degree of anonymity, pseudonymity: the use of traceable pseudonyms as user identifiers.

Demo Session 1, Welcome Drink / 136

Grid-enabled virtual screening service against the epidemiological disease

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GAP Virtual Screening Service (GVSS), a large-scale in-silico drug virtual screening service, provides a system to speed-up the searching process among all conformations of a compound. Moreover, GVSS is a generic drug discovery framework over gLite by which users can upload their compounds and targets to do grid docking, compare the significance, and verify results by in vitro experiment afterwards. GVSS has proved to provide intensive computing power and effective data management over gLite infrastructure on neglected and emerging diseases, such as Avian Influenza and Dengue Fever.

Demo Session 2 / 138

Molecular Dynamics and Docking Simulations Using Parameter Sweep Workflows

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Carbohydrate recognition is a phenomenon critical to a number of biological functions in humans. Computer programs which can provide insight into such biological recognition processes have significant potential to contribute to biomedical research if the results of the simulation can prove consistent with the outcome of conventional wet laboratory experiments. In order to validate these simulation tools and support their wider take-up by the bio-scientist research community high-level easy to use integrated environments are required to run massively parallel simulation workflows.

Demo Session 1, Welcome Drink / 140

Porting Scientific Application to the EDGeS Service Grid/Desktop Grid Platform

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The EDGeS project connects the g-Lite based EGEE grid to several BOINC and XtremWeb based Desktop Grid system. The EDGeS infrastructure successfully extends EGEE with volunteer and institutional desktop resources to be utilized by master worker or parameter sweep applications. The project has successfully ported several EGEE applications to the combined platform, including the WISDOM meta-middleware for molecular docking simulations, the ISDEP plasma fusion application, or the VisIVO server tool for the visualization of astrophysical data.

Demo Session 1, Welcome Drink / 141

Earthquake Disaster Mitigation on EUAsiaGrid

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Although earthquakes are not predictable at the moment, with the aid of accurate seismic wave propagation analysis, we could simulate the potential hazards at all distances from possible fault sources by understanding the seismic wave velocity structure of the earth and the rupture process during large earthquakes. With the integration ofa strong ground-motion sensor network, an earthquake data center and seismic wave propagation analysis over gLite e-Infrastructure, we could have much better knowledge on the impact and vulnerability of potential earthquake hazards.

Regional Activities, International Projects and Collaborations / 143

Instruments and sensors supported by e-Infrastructure

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The introduction gives the major objectives and the idea of instrument and sensor remote steering, controlling and monitoring. The second part presents the user experiences and requirements following a proposition of the general architectural framework. The way of integrating instrumention with existing e-Infrastructure is especially important for the ESFRI projects, where most are using some equipment for data capturing and computing resources for further simulations.

Poster session / 144

Grid preprocessing application for Environment monitoring in Moldova

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The aim of the EnviMon application is to organize data acquisition and processing for Environment state monitoring. A nation-wide distributed set of sensors are polled from a central station placed at the main site of the State Hydrometeo Service of Moldova (SHMS). The application provides data collection, filtering, storage and processing in order to produce synthetic reports and input that can be used as structured tables for database or input for geoinformation systems maps. .

Earth Science / 145

ES cluster towards ES VRC

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The ES community has actively participated in the EGEE projects as Strategic Discipline Clusters. In the framework of the DCI infrastructure and its related services deployed by the European Grid Initiative (EGI), the ES VRC will gather all ES partners to bring their contribution, i.e. resource and service providers, developers, support teams as well as end-users. This network of support and expertise is constituted within the ES VRC by a kernel of partners with Grid expertise in order to break down the entry barrier and overcome some of the technical difficulties that otherwise exist.

Novel Architectures and Technologies / 147

Managing Healthcare and Medical Information Utilizing Cloud Computing

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Cloud Computing provides functionality for managing information data in a distributed, ubiquitous and pervasive manner supporting several platforms, systems and applications. This work presents the implementation of a mobile system that enables electronic healthcare data storage, update and retrieval using Cloud Computing. The mobile application is developed using Google's Android operating system and provides management of patient health records and medical images (supporting DICOM format and JPEG2000 coding).

DCI programming / 148

Providing uniform and standardised access to European Grid middleware with SAGA

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The Simple API for Grid Applications (SAGA), has demonstrated its ability to provide a simplified and uniform multi-language access layer to heterogeneous grid middleware stacks. SAGA already provides support for Unicore and gLite, and extensions to ARC via OGSA-BES as well as generic DRMAA support are already being developed or planned. First SAGA application integration tests within EGEE have been successful.

Regional Activities, International Projects and Collaborations / 149

Building Scientific Workflows for the Fisheries and Aquaculture Management Community based on Virtual Research Environments

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The management of resources related to the Fisheries and Aquaculture (FARM) domain is complex and involves different scientific activities. The people involved in the domain are distributed worldwide: scientists in the field, regional statistics departments, national governing bodies, etc. Distributed information must be produced, analyzed, processed, shared, and preserved by all multiple actors through a number of scientific workflows. The D4Science-II project provides a number of Virtual Research Environments (VREs) to address the collaboration needs of this community.

Workflow Management / 150

Workflows Description, Enactment and Monitoring through SAGA

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Most existing workflow systems are tightly integrated with middleware, which limit wide scale adoption and may limit efficient execution of workflows. Whereas the use of SAGA enables the use of multiple heterogeneous resources, there exists an initial but somewhat limited support for workflows using the SAGA specification. Thus to reconcile the advantages of the SAGA paradigm with broad usage of workflows as a way of composing applications, this project investigates approaches that extend the SAGA-workflow package (Digedag)to support workflows such as neuroimaging analysis in neugrid.

Novel Architectures and Technologies / 151

EDGeS infrastructure for the EGEE user community

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There is a strong collaboration between EGEE and EDGeS in order to extend the EGEE infrastructure with volunteer and institutional desktop grids (DG) and to support EGEE users to migrate their application to the EDGeS infrastructure. The talk explains to EGEE users how this integrated infrastructure works, what the benefits are and how their applications can be ported and run on this infrastructure. The talk also explains how individual VOs can extend their VO resources with connected DGs. Experiences in related projects (IberCivis, EELA) using EDGeS technology will be presented.

Fusion / 152

Overview of the grid fusion applications and the possible workflows among them

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Grid computing developments have increased substantially in fusion research.
A great variety of applications have been ported to the grid in the frame of EGEE, EELA and EUFORIA projects. These applications belong to different plasma physics domains and different strategies have been used to port them, depending on the nature of the applications. These codes are ready to establish workflows among them in order to produce new relevant physics results that could not be achieved running the applications separately

Poster session / 153

Configuration and optimization for a gLite grid computing farm.

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We will illustrate the optimization work performed on a mid-sized gLite grid-computing farm, testing various solutions, to improve the services offered to both grid and local users. Particular attention was devoted to the storage infrastructure and its configuration trying to improve the overall farm performance, reliability and to minimize the manpower required for its management. Improvements were also pursued by optimizing the configuration of the batch system. Experiences from both LHC users and non LHC ones will be reported.

Poster session / 154

Maintaining Corpus Download Facilities with Changing Technology

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Introduction of federated login using Shibboleth for a linguistic data archive created a problem by making existing local tools for downloading data-sets stop working. To address this problem the use certificate based authentication in combination with a SLCS service was setup. The application domain demanded that special attention was paid to shielding the user from the complexity of working with certificates and making the SLCS handshake as easy as possible. Parallel access to the archive using both Shibboleth and client certificates required careful configuration.

Demo Session 1, Welcome Drink / 155

Cancer Sentinel project: a grid network for distributed medical data management on Cancer.

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The Sentinel project involves several medical actors related to cancer: screening structures, medical laboratories and both regional and national public health authorities.
The project builds upon grid technologies to create a federation of medical data sources related to cancer. The main purpose of the project is to enable secured medical data exchanges between cancer screening structures and cancer analysis (pathology) laboratories. The architecture and tools used to deploy such a network are also relevant to distributed medical images diagnosis, global health and epidemiology.

Bioinformatics / 156

Job submission tool: bioinformatic application porting on the gLite grid Infrastructure.

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The Job Submitting Tool provides a solution for the submission of a large number of jobs to the grid in an unattended way. Indeed the tool is able to manage the grid submission, bookkeeping and resubmission of failed jobs.
It also allows the monitor in real time of the status of each job using the same framework. In this work we will introduce same key new features and application that we have added to this tool. In the work several already executed challenges will be reported together with a logical description

Astronomy and Astrophysics / 157

CTACG - Cherenkov Telescope Array Computing Grid

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Gamma-ray astronomy is one of the most active topics in astroparticle physics involving both particle physicists and astrophysicists leading to the design of new types of research infrastructures. The Cherenkov Telescope Array - CTA - is a proposed new project for ground based gamma-ray astronomy. This communication aims at providing a report of the most relevant activity carried out and in progress within the CTA consortium in EGEE and a view of perspectives and implications of ICT-based infrastructures such as the future EGI for the needs of a project like CTA.

Bioinformatics / 158

Grid-based International Network for Flu Observation

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Since the H1N1 outbreak lately, there has been a worldwide effort to isolate and sequence flu virus genomes. Specimens with a positive result are sequenced and deposited in influenza databases. The present EUAsiaGrid application, called g-INFO (Grid-based International Network for Flu Observation), shows the integration of existing data sources towards a global surveillance network for molecular epidemiology, based on Service Oriented Architecture and Grid technologies. Its relevance is being tested through the current H1N1 outbreak.

Astronomy and Astrophysics / 159

The Grid for Astronomy and Astrophysics in Italy and Europe

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The Astronomical and Astrophysical (A) community is extremely active concerning the use of the EGEE Grid infrastructure in Italy as well as in Europe. We briefly provide a summary of current AA Grid activities and we present selected compute and data intensive applications, which have been recently ported to Grid. Those applications are related either to large international key projects (as Planck ESA satellite) or to small-scale regional scientific activities. In particular, the AA community efforts toward the set up of the Italian NGI will be also presented.

Scientific Gateways and Portals / 160

P-GRADE grid portal family

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Science gateways are important tools to provide user friendly access to various grid systems for various user communities. The most popular way of creating science gateways is the establishment of grid portals through which users can access grid facilities without any grid installation. In many cases science gateway portals completely hide the underlying grid infrastructure and some of them provide high level programming concepts like workflow programming. The P-GRADE portal family belongs to this class of science gateways. It has three main members: P-GRADE, NGS P-GRADE and WS-PGRADE.

Earth Science / 161

Geospatial and Grid infrastructures interoperability in enviroGRIDS

Prof. GORGAN, Dorian [1]; Mrs. RODILA, Denisa [1]; Mr. BACU, Victor [1]; Dr. GIULIANI, Gregory [2]; Dr. RAY, Nicolas [2]; Dr. CHARVAT, Karel [3]; Dr. LEHMAN, Anthony [2]

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EnviroGRIDS (Black Sea Catchment Observation and Assessment System supporting Sustainable Development) is a 4-years FP7 Project aiming to address the subjects of ecologically unsustainable development. The geospatial technologies offer very specialized functionality for Earth Science oriented applications as well as the Grid oriented technology that is able to support distributed and parallel processing. One challenge of the enviroGRIDS project is the interoperability between geospatial and Grid infrastructures by providing the basic and the extended features of the both technologies.

Novel Architectures and Technologies / 162

Parameter sweep job submission to Eucalyptus clouds

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Large parameter sweep applications require large number of resources. Unfortunately the average number of processors in EGEE VOs is between 500-800 processors that is far not enough for large parameter sweep applications. The situation can be improved if jobs of such parameter sweep applications can be distributed to available cloud resources, too. The interconnection of P-GRADE portal with clouds enable this execution scenario. The talk explains how the interconnection of P-GRADE with Eucalyptus has technically been solved and how this new system can be used by the end-user communities.

Novel Architectures and Technologies / 163

A Business-Driven Cloudburst Scheduler for Bag-of-Task Applications

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Opportunistic peer-to-peer (P2P) grid computing infrastructures have been proven to be cheap and effective platforms to run Bag-of-Tasks (BoT) applications. They operate on a best-effort model, which is understandable given their negligible cost. However, for some applications that could benefit from these infrastructures, having some guarantees on the time that takes to complete is an important requirement. In this work we investigate the possibility of combining a P2P grid with a cloud computing provider to provide some quality of service (QoS) guarantees.

Infrastructure Tools and Services / 164

Workflow repository, user specific monitor, and vulnerability analyzer in SEE-GRID

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This talk introduces some high-level services, which extend the gLite-based SEE-GRID infrastructure in order to ease several tasks of end-users, application developers, and grid operators. The Common Workflow Repository Extension (CWRE), and the User/application Specific Grid Infrastructure Monitoring Extension (USGIME) of P-GRADE portal can provide efficient tools for user and application developer communities. With the Grid Site Software Vulnerability Analyzer (GSSVA) the grid operators can inspect the vulnerability/security level of the grid infrastructure with minimized intrusion.

High Energy Physics / 165

Distributed Computing and Data Analysis in the CMS Experiment: the Spanish and Portuguese case

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By the end of 2009, the CMS Experiment at the Large Hadron Collider (LHC) has already started data taking with proton collisions at 450 GeV and 1.2 TeV per beam. CMS has invested a few years to build a robust Distributed Computing system to meet the expected performances in terms of data transfer/archiving, calibration, reconstruction, and analysis. Here, we will focus on the readiness of the Spanish and Portuguese computing centers (PIC [Tier-1], CIEMAT, IFCA, LIP-Lisbon, and NCG-INGRID-PT [Tier-2s]) to first LHC collisions and the measured performance in the Iberian region by April 2010.

Demo Session 1, Welcome Drink / 166

neuGRID - A Grid-Brained Infrastructure to Understand and Defeat Brain Diseases - 3rd Neuroscientific Data Challenge

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Launched early 2008 by the EC Research Infrastructure Unit, the neuGRID project has established a distributed e-Infrastructure interconnecting major clinical research centres in Europe, supplying neuroscientists with the most advanced ICT to defeat Alzheimer's Disease (AD) and neurodegenerative pathologies in general. Based on EGEE gLite, neuGRID has developed a harmonized and powerful environment to design, test and assess new disease markers.

Demo Session 2 / 167

Using Spare Space in Worker Nodes and Desktop Disks to Build a gLite Storage Element

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We present how idle disk space available at desktops and worker nodes in computing elements can be used to implement the file system back-end of a gLite storage element. We developed the BeeFS to federate the distributed disks. Like some special-purpose file systems (eg. GFS), it uses a hybrid architecture that follows a client-server approach for serving metadata and manage file replicas, and a peer-to-peer one for serving data. This allows BeeFS to aggregate the spare space of disks to build a single logical volume on top of which a general purpose POSIX-compliant file system is implemented.

Bioinformatics / 168

A Protein Tertiary Structure Prediction Service in the ProGenGrid System

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Proteins are central to all biological processes: a very important problem in proteomics is the prediction of the three-dimensional (3D) structure of proteins from their amino acid sequence, because this information can be useful for determining the protein function, given by a specific spatial conformation that the protein assumes when it reaches the active state. We have integrated a routinely expert dependent strategy, based on the homology modeling procedure, in an automatic tool that may facilitate the generation of carrier models at low resolution, exploiting the EGEE infrastructure.

Poster session / 169

Earth Science applications of the ES Virtual Research Community

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Earth Science is an all-embracing term for sciences related to the planet earth covering a large user community from academy, industry and organizations. To provide a scientific basis for addressing societal issues is more and more computing resources are neededboth for real and remote time applications. In the framework of the European Grid Initiative, EGI, the ES VRC gathers the partners of 9 Virtual Organizations located in 23 European or associated countries and is linked to EELA2, EUAsia and African partners. Overview of applications and tools are presented.

Demo Session 2 / 170

Applications using Remote Instrumentation in Grid environment - DORII project

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We present here the final results obtained in the context of the EU FP7 project Deployment of Remote Instrumentation Infrastrucutre project. This is one of the EGEE related projects. We present here the oceanographic and coastal observation and modeling using an imaging use case for demonstrating the usage of the remote instrumentation infrastrucure. The remote instrumentation techniques and services has been integrated with grid - glite middleware, giving new possibilities to the scientists. The provided solutions are generic and so could be re-used for different applications.

Poster session / 171

Workflow support for multinode tests of Grid components

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Desktop Grid solutions —such as Internet-based distributed or volunteer computing infrastructures— usually collect non-reliable and vulnerable resources from the donors (desktop PC owners) for some selected, grand challenge projects. In this paper we discuss one of the key issues, the software build, test, and validation procedures for such (and similar) heterogeneous environments, based on the workflow based description of multinode tests and ETICS-2 services.

Bioinformatics / 172

The Nordic BioGrid project – Bioinformatics for the grid

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Life sciences have undergone an immense transformation during the recent years, where advances in genomics, proteomics and other high-throughput techniques produce floods of raw data that need to be stored, analysed and interpreted in various ways. Bioinformatics is crucial by providing tools to efficiently utilize these gold mines of data in order to better understand the roles of proteins and genes and to spark ideas for new experiments.

Novel Architectures and Technologies / 173

Pros and Cons of cloud adoption in the Scientific Data Infrastructures - the D4S-II case

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The D4S project is going to provide as major product the gCube middleware. It is a grid-enabled service oriented middleware enabling the creation and operation of Virtual Research Environments, to serve the management and exploitation of scientific data. As part of the D4S-II project a study on the impact of cloud technology (mainly Virtualisation) and cloud capabilities (on-demand availability and scalability) on the gCube software will be performed. The study will also analyse the impact of cloud technology from a commercial point of view (market positioning, possible exploitation strategies).

Technical Plenary / 174

The computational challenges in Life Sciences

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Life sciences is one of few areas of research where the complexity of the problems grows faster than our ability to deal with them from a computational point of view. Massive genomic projects have yield detail sequence information on all the species of human interest and we are now deriving meta-genomic information of complex ecosystems, including for example the human digestive system. In a near future we might face the pangenomic scenario, where sequence information of all the human beings might be accessible. In parallel, to the genomic revolution, system biology projects are putting all this sequence data in the proper cellular context, building entire networks aimed to explain the chemical complexity of life. The third axis structural genomic projects are increasing the structural knowledge on biological machines opening then the possibility to modulate on their actions and by extension on the entire cellular functioning.

During my talk I will try to draw the exciting, but scaring scenario of the research in biology, trying to outline the main topics were help from computers is needed. I will provide examples of how current computer platforms can help to derive biologically-relevant information and I will emphasize the complexity of the problem from the computational point of view.

Technical Plenary / 175

Addressing Complexity in Emerging Cyber-Ecosystems - Exploring the Role of Autonomics in E-Science

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Significant strategic investments are quickly realizing a pervasive computational cyberinfrastructure that integrates large-scale computing, high-speed networks, massive data archives, instruments, observatories, experiments, and embedded sensors and actuators, and are catalyzing new thinking, paradigms and practices in computational science and engineering – those that are collaborative and information/data-driven. However the ability of scientists to realize this potential is being severely hampered by the complexity of the applications and infrastructure, which together present unprecedented development, configuration and management challenges. Autonomic computing has the potential to fundamentally address these challenges. The goal of autonomic computing is to design and engineer systems and applications that are capable of managing themselves, adapting their resources and operations to workloads and execution context, and anticipating needs, all with minimal involvement of users. In this talk I will explore the role of autonomics in computational science and engineering, both in managing systems and applications as well as in enabling new application formulations. I will then describe specific research efforts aimed at enabling autonomic scientific and engineering applications that can address the challenges of (and benefit from) pervasive cyber-ecosystems.

Technical Plenary / 176

Advanced computing for fusion simulation and modelling

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ITER is the next generation of fusion devices and is intended to demonstrate the scientific and technical feasibility of fusion as a sustainable energy source for the future. To exploit the full potential of the device and to guarantee optimal operation for the device, a high degree of physics modelling and simulation is needed even in the current construction phase of the ITER project. The detailed modelling tools that are needed for an adequate description of the underlying physics cover both a wide range of timescales and spatial orderings and are in general very demanding from a computational point of view. Current modelling activities rely on local or national computational resources and an improved access to computing infrastructures will be instrumental in advancing a pan-European modelling activity for ITER to a very competitive status in relation to the ITER partners.

The EUFORIA project is developing a comprehensive framework and infrastructure for core and edge transport and turbulence simulation, linking grid and High Performance Computing (HPC), to the fusion modelling community.

EUFORIA is enhancing the modelling capabilities for ITER sized plasmas through the adaptation, optimization and integration of a set of critical applications for edge and core transport modelling targeting different computing paradigms as needed (serial and parallel grid computing and HPC). Deployment of both a grid service and a High Performance Computing service have proven essential to the project. A novel aspect is the dynamic coupling and integration of codes and applications running on a set of heterogeneous platforms into a single coupled framework through a workflow engine, a mechanism needed to provide the necessary level of integration between the physics applications. This strongly enhances the integrated modelling capabilities of fusion plasmas and will at the same time provide new computing infrastructures and tools to the fusion community in general.

Current status, lessons learned and future prospects are reviewed in the project.

Technical Plenary / 177

LHC: an Example of a Global Scientific Community

With the advent of large scale scientific instruments, the need for global collaborations in science has arisen. High Energy Physics and LHC in particular has long experience in collaboration on this scale and can serve as a model for other communities which now have to face similar challenges. This talk will give an overview of the need for LHC and the collaborative efforts that have built the accelerator, the experiments and the computing. The computing has benefitted from the e-science infrastructures built in Europe and elsewhere while pushing those infrastructures to unprecedented levels of scale and performance. With the arrival of first data in the LHC experiments, the investments in the computing are paying off in being able to very rapidly analyse the data. The talk will discuss the role of High Energy Physics and CERN in the European and worldwide scientific landscape and how this might develop in the future.

Opening Plenary / 178

The Swedish e-Science Research Centre

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As a result of a strategic research initiative by the Swedish government in the area of e-Science, a consortium of four universities have been able to substantially increase their research activities in the area. The Swedish e-science Research Centre (SeRC) is formed by the universities in Stockholm and Linköping -- KTH, Linköping University (LiU), Stockholm University (SU) and Karolinska Institutet (KI) -- around the two largest high-performance computing (HPC) centres in Sweden: PDC at KTH and NSC at LiU. Research at SeRC is focused on the collaboration between tool makers and tool users, and brings together a core of nationally leading IT research teams with expertise in e-Science method development and leading scientists in selected application areas.

SeRC will provide a platform for increased collaboration between applied and method-oriented groups, with the aim to constitute a visionary e-Science node with a national scope and strong international ties. Work will evolve along three lines: (i) Formation of e-Science Communities that connect application groups with relevant core e-Science groups and computer experts at PDC and NSC, (ii) Research in core e-Science methods such as distributed resources, database technology, numerical analysis, visualization and interaction, mathematical modelling and parallel algorithms, focusing on problems critical for several e-Science communities, (iii) Closer collaboration between PDC and NSC, and a substantial increase in advanced support staff, which will turn the two centres into comprehensive e-Science enablers.

The general structure and scope of SeRC will be presented including examples of collaborative work in some of its communities.

EGI Session - Board None / 179

The EGI-InSPIRE Project: Community Interactions

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The EGI-InSPIRE project has two activities focussed on interactions with the community: External Relations and User Community Coordination. This presentation will provide an overview of the dissemination and policy development tasks that form the basis of the external relations activity in EGI-InSPIRE, and the user community activity that encompasses a support team based at EGI.eu and those located within the community.

EGI Session - Board None / 180

EGI-InSPIRE: Operations

The production grid infrastructure in EGI-INSPIRE is built from resources provided by the participating partners. These are brought together into a secure, integrated, reliable infrastructure by EGI.eu through the federated operations of independent infrastructures. This presentation will provide an overview of the operational infrastructure and the development of the operational tools used to manage it.

EGI Session - Board None / 181

EGI-InSPIRE:Technology

The EGI-InSPIRE project will rely on external software providers to develop the technology that meets the needs of EGI's user and operations community. The EGI.eu staff will work to collect and prioritise requirements across the community from the virtual research communities using the infrastructure and from the operations staff deploying the technology. It is expected that the technology will evolve rapidly during the project, and the technology team will define the functional and performance requirements that need to be achieved by the software providers for their technology to be deployed into production.

Closing Plenary / 182

Cloud Computing at Microsoft and Venus-C

Opening Plenary / 183

Welcome from EGEE Project Director

Opening Plenary / 184

Welcome from Local Organisation

Opening Plenary / 185

Presentation of Uppsala University and history of the building

Opening Plenary / 186

e-Infrastructures as enablers of the "fifth freedom"

Even if the scientific community is often not aware of it, the free movement of knowledge (also known as the "fifth freedom") is anchored in the Lisbon Treaty. Its Article 179 reads "The Union shall have the objective of strengthening its scientific and technological bases by achieving a European research area in which researchers, scientific knowledge and technology circulate freely [...]".

The talk will reflect on the role of e-Infrastructures in enabling the "fifth freedom" and devise some of the challenges ahead.

Closing Plenary / 187

Best demo and poster awards

Closing Plenary / 188

Outlook and farewell

Astronomy and Astrophysics / 189

Final discussion

EEF meeting (Closed) / 190

Introduction

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EEF meeting (Closed) / 191

Review of EEF draft report

EEF meeting (Closed) / 192

Next steps

EEF meeting (Closed) / 193

Preparations for the ESFRI session tomorrow (Tuesday)

EEF meeting (Closed) / 194

AOB

Computational Chemistry / 195

Molecular and material science innovative applications on the grid

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ESFRI session / 196

Introduction

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CESSDA

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Analysis of ESFRI projects e-infrastructure requirements by European e-Infrastructure Forum

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Discussion and next steps

EGI Session / 201

NGIs and VOs Readiness Survey

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EGI Collaboration Board

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