

PL-Grid: Innovative Grid Infrastructure for Scientific Research in European Space – Tools and Services

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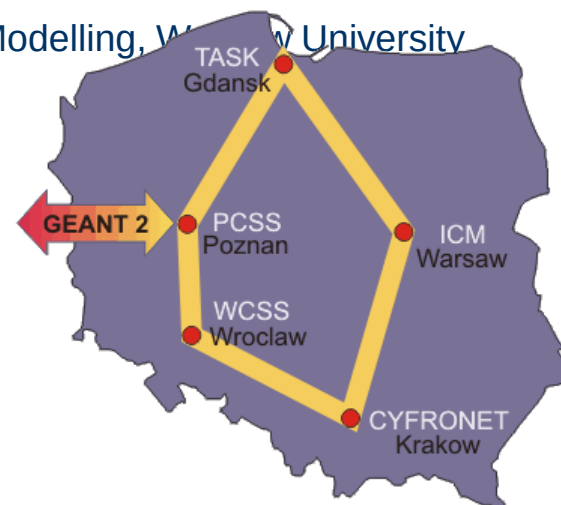
www.plgrid.pl/en

Outline

- ◆ PL-GRID
 - ◆ Basic Facts
 - ◆ Motivation, Consortium and objectives
 - ◆ State of advancement
- ◆ Current results
- ◆ Use in scientific research
- ◆ Summary

PL-Grid Consortium

- ◆ Consortium Creation – January 2007
 - ◆ a response to requirements from Polish scientists and
 - ◆ due to ongoing Grid activities in Europe (EGEE, EGI_DS).
- ◆ Consortium members – make up of 5 Polish supercomputing and networking centres:
 - ◆ Academic Computer Centre CYFRONET AGH, Krakow (coordinator)
 - ◆ Poznan Supercomputing and Networking Centre
 - ◆ Interdisciplinary Centre for Mathematical and Computational Modelling, Warsaw University
 - ◆ Wroclaw Centre for Networking and Supercomputing
 - ◆ Academic Computer Centre, Gdansk
- ◆ PL-Grid Project funded March 2009 by the European Regional Development Fund as part of the Innovative Economy Program
 - ◆ Duration: 1.1.2009 – 31.3.2012
 - ◆ Budget: total 21 m€, from EC 17m€
- ◆ Working Result: First working NGI in Europe in the framework of EGI.eu (since March 31, 2010)



Main Objectives of PL-Grid

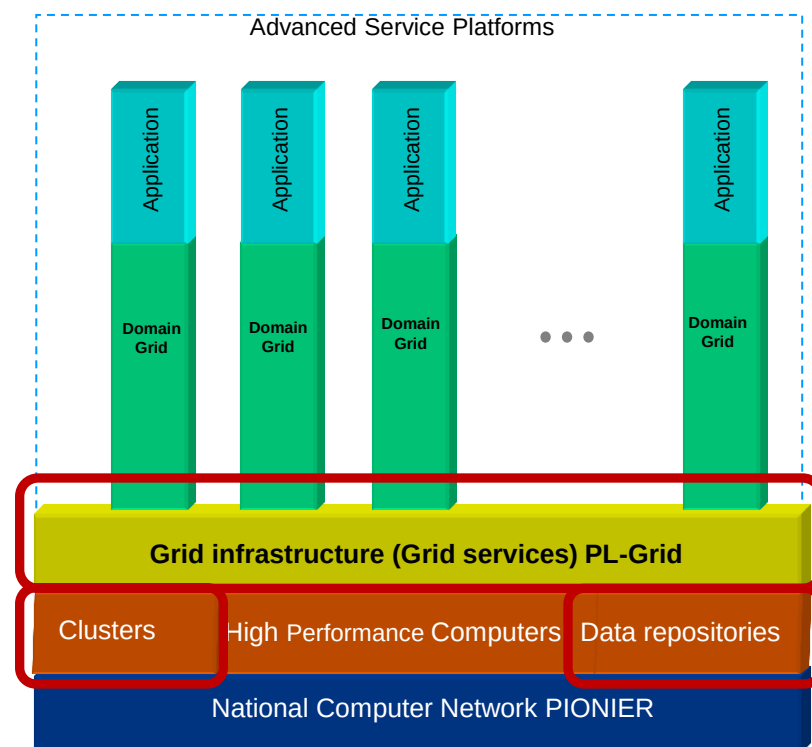
- ◆ Development of a common base infrastructure – compatible and interoperable with international Grids
- ◆ Capacity to construct specialized, domain Grid systems – including services and tools focused on specific types of applications
- ◆ Enabling efficient use of available resources
- ◆ Plans for HPC and Scalability Computing, including clouds environments

Offer for the Users (according to Project)

- ◆ Computing power : 215 Tflops
- ◆ Storage: 2500 Tbytes
- ◆ Operation: 24 x 7 x 365
- ◆ Support from PL-Grid staff on:
 - ◆ using advanced Grid tools
 - ◆ porting legacy codes to Grid environment
 - ◆ designing applications for PL-Grid environment
- ◆ Direct contact with EGI Council and EGI EB

PL-Grid tasks in EGI-InSPIRE

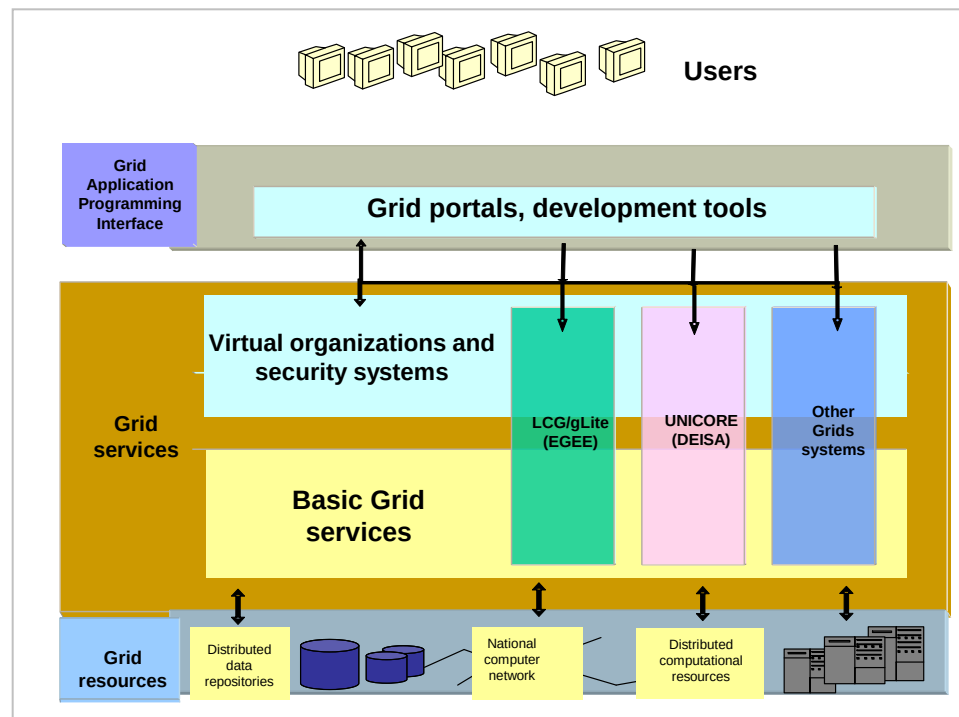
- Global Tasks
- International Tasks (like other NGI)
- Computational Chemistry
- Development of unified middleware via European Middleware Initiative



PL-Grid Building Blocks

PL-Grid software comprises:

- ◆ user tools (portals, systems for applications management and monitoring, result visualization and other purposes, compatible with the lower-layer software used in PL-Grid)
- ◆ software libraries
- ◆ virtual organization systems: certificates, accounting, security, dynamic
- ◆ data management systems: metadata catalogues, replica management, file transfer
- ◆ resource management systems: job management, applications, grid services and infrastructure monitoring, license management, local resource management, monitoring



Three Grid structures are maintained:

- ◆ production
- ◆ research
- ◆ development / testing

Hardware Platform

Partners' Computing Resources

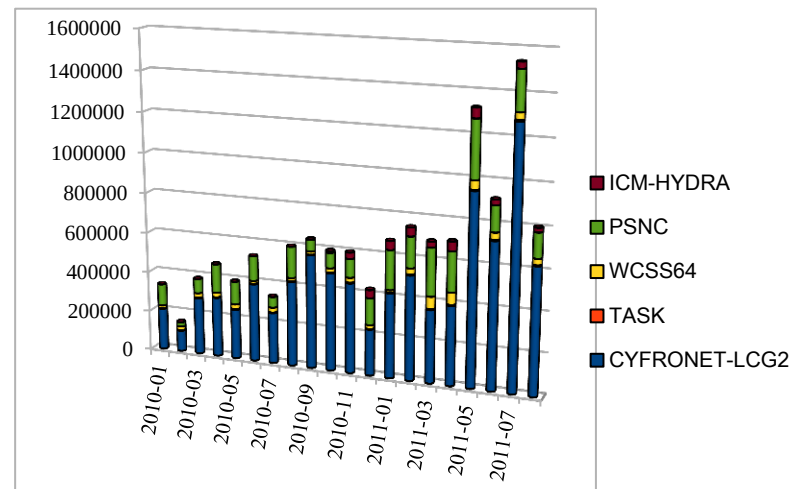
TOP500 – June 2011

Rank	Site	System	Cores	R _{max} (TFlops)	R _{peak} (TFlops)
81	ACK Cyfronet AGH Poland	Cluster Platform 3000 BL2x220, L56xx 2.26 Ghz, Infiniband Hewlett-Packard	11694	104.77	124.42
163	Gdansk University of Technology, CI Task Poland	ACTION Xeon HP BL2x220/BL490 E5345/L5640 Infiniband ACTION	10384	65.59	97.76
194	Wroclaw Centre for Networking and Supercomputing Poland	Cluster Platform 3000 BL2x220, X56xx 2.66 Ghz, Infiniband Hewlett-Packard	6348	57.41	67.54

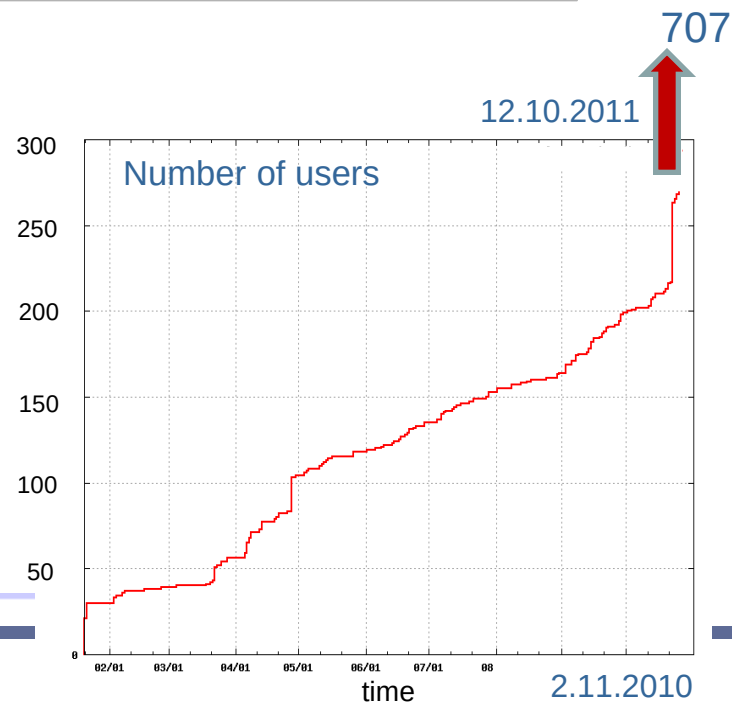
Aggregated Status

- ◆ Total number of cores (static) 26,550
- ◆ Number of registered users 707
- ◆ Number of Helpdesk users 333
 - ◆ Average month number of help request 88
 - ◆ Total number of tickets 1622
- ◆ Number of jobs (9.2011) 2,200,000

Number of jobs/month/partner

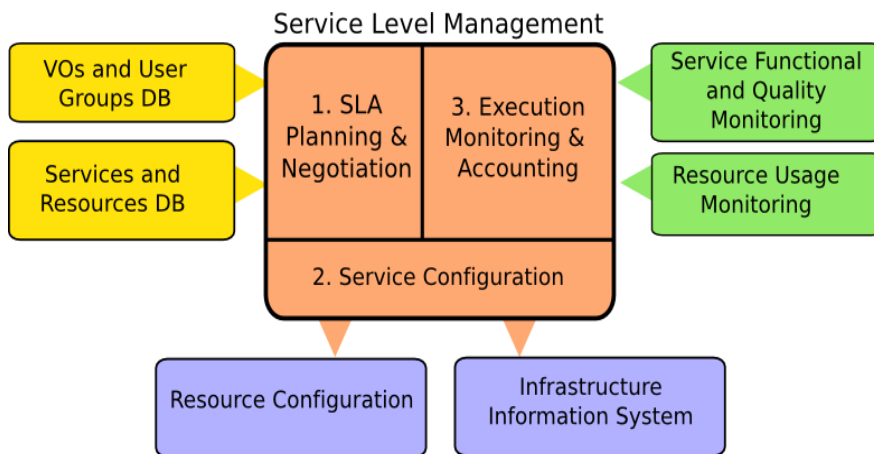


Site	Site Size	Availability		
		July	June	March
CYFRONET-LCG2	8712	95%	98%	98%
PSNC	4720	93%	69%	97%
TASK	8	99%	99%	96%
WARSAW-EGEE	1376	98%	67%	74%
WCSS64	5248	99%	100%	99%



Selected Tools/Software Achievements

- ◆ Providing resources to users with required quality of service
 - ◆ Required = specified in Service Level Agreement
 - ◆ SLA-aware architecture designed according to SLM principles
 - SLA Planning and negotiation
 - Service configuration
 - SLA Execution Monitoring and accounting
- ◆ Resource Allocation-related Operation Model



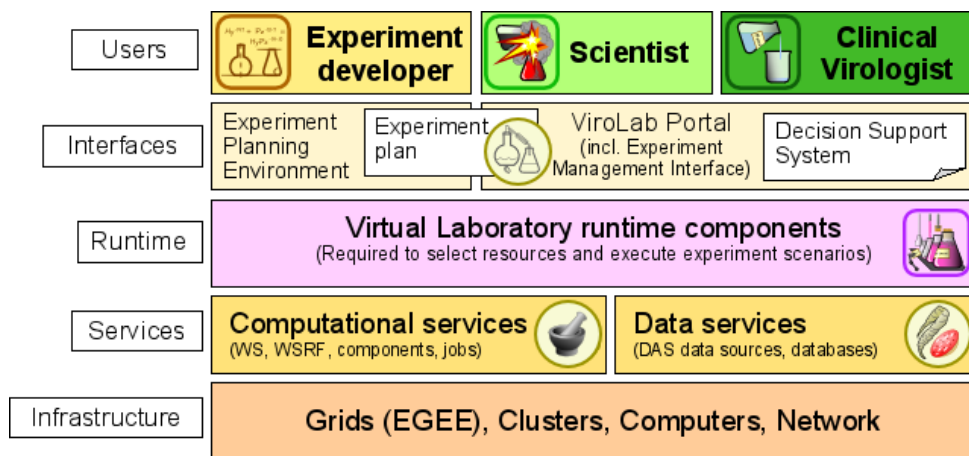
<http://grid.cyfronet.pl/bazaar>

The screenshot displays the Grid Resource Bazaar web interface. The main panel shows a 'New call' form with fields for Date, Title, SLA, and Set. Below this is a 'Log' section with a table of recent calls. To the right, there are two panels: 'Call 426: alice call' and 'SLA 367 for call: alice call'. The 'Call 426' panel shows details like Call name, Responsible person, and Call open date. The 'SLA 367' panel shows details like SLA name, Responsible person, and SLA start date. At the bottom, there are two charts: 'Number of cores/CPU' and 'Storage space [GB]', both showing data over time from 01-08-09 to 31-08-09. The 'List of calls' and 'List of SLAs' tables are also visible at the bottom.

GridSpace2 Experiment Workbench in the PL-Grid Virtual Laboratory – a Web 2.0 interface to experiments

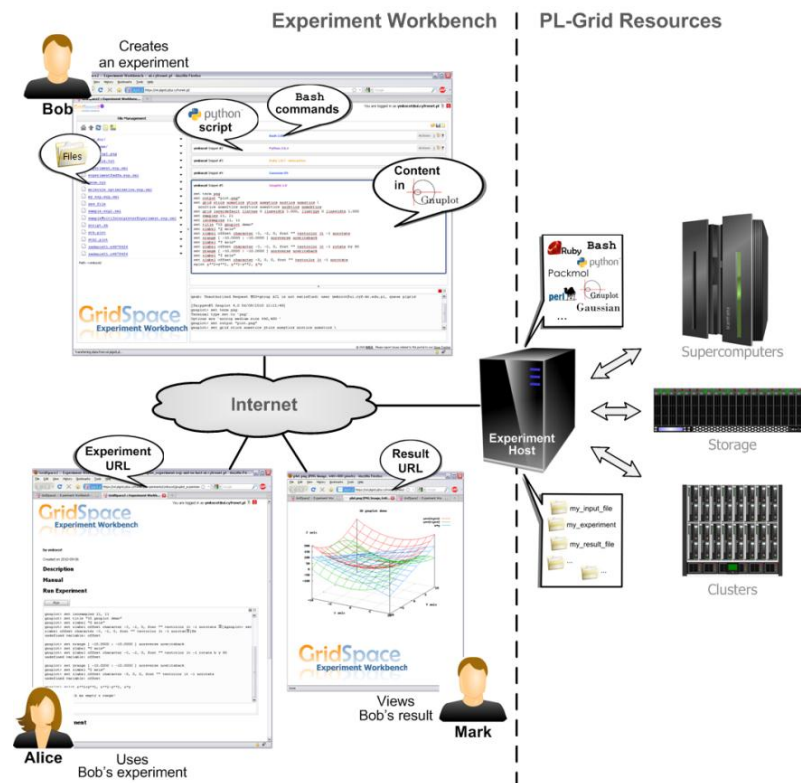
- ◆ Use of distributed computational resources and data repositories
- ◆ High-level tools offered for the user for in-silico experiments

GridSpace



Working with the Experiment Workbench:

- ◆ **Open the workbench** in your browser (<https://wl.plgrid.pl>)
- ◆ **Log into** one of the available servers with your PL-Grid account
- ◆ **Start your usual work.** Your files are already there. Your code snippets may play the role of scripts, bash commands or input to external applications (such as Gaussian or Gnuplot);
- ◆ All the **files** you generate **may be viewed with visualization tools**
- ◆ **Save your work** – the experiment is now visible among your other files
- ◆ **Share the experiment** with other members of your research team



<http://gs2.cyfronet.pl/>
<http://www.virolab.org>

Selected Tools

(3 out of many)

Migrating Desktop Platform:

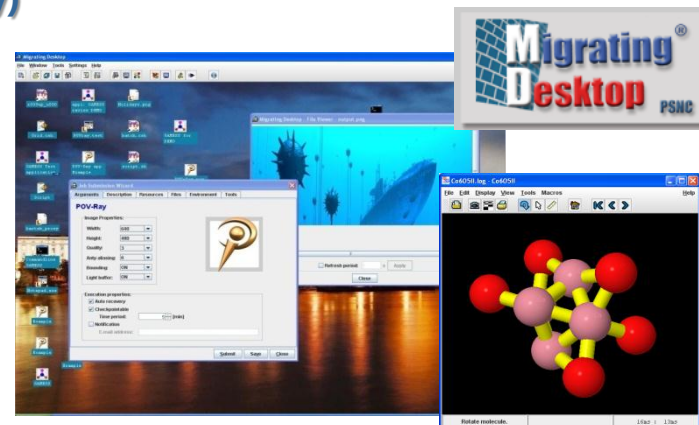
- ◆ Powerful and flexible user interface to Grid resources that gives a transparent user work environment and easy access to resources and network file systems independently of the system version and hardware

Vine Toolkit

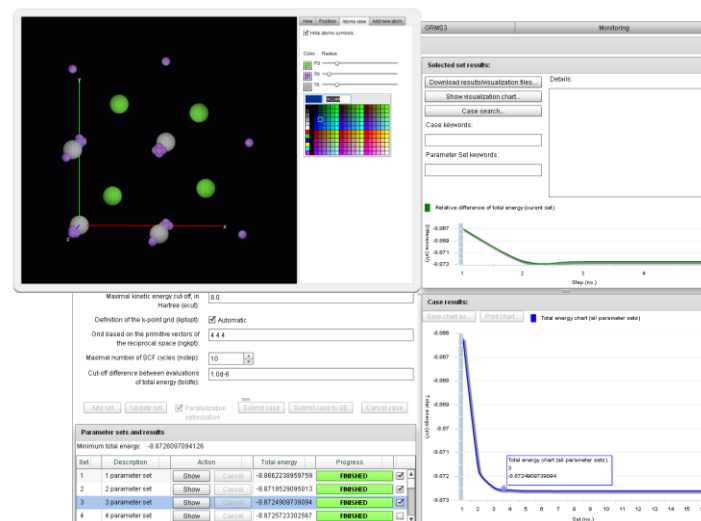
- ◆ Environment to facilitate the development and integration of web-based applications with HPC resources, Grid services and various existing large-scale computing infrastructures managed by Grid middleware, such as gLite, Unicore, Globus, QosCosGrid and GRIA.

FiVO/QStorMan toolkit

- ◆ Provisioning PL-Grid users an appropriate quality of access to storage using non-functional requirements and data localization management



Migrating Desktop main window





QosCosGrid - Distributed Computing Infrastructure



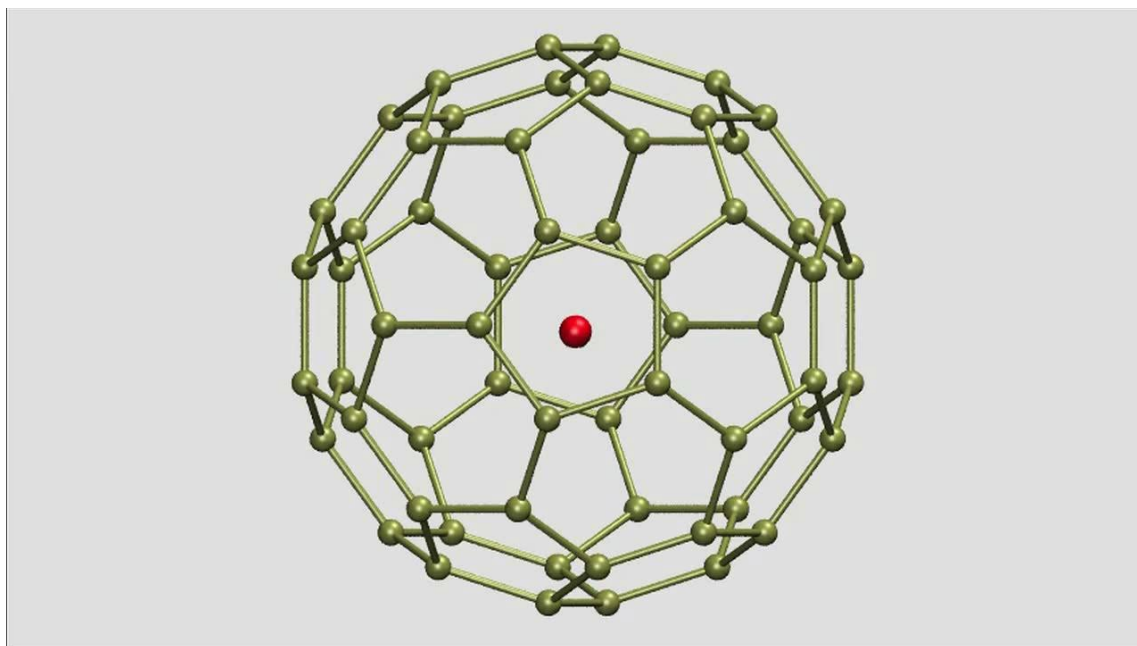
- ◆ QosCosGrid (QCG) has been designed and implemented to meet various specific end-users requirements to offer new and extend capabilities available on existing European e-Infrastructures
- ◆ QosCosGrid is not yet another middleware as it provides many new features:
 - ◆ *Efficiency*: the fastest way to access remotely queuing systems via middleware services (performance benchmarks comparing QCG2.0, gLite 3.2, GT5.0.3, UNICORE 6.4 RC2)
 - ◆ *Applications tools*: many application programming and execution tools have been integrated with QCG, e.g. OpenMPI, ProActive, Eclipse PTP, GridSpace, SAGA, Science Gateways, Kepler wf, Triana, multi-scale tools, mobile apps, etc.
 - ◆ *Advance reservation and co-allocation*: multi-cluster job execution with advanced scheduling and synchronization for new multi-scale simulations, interactive vis jobs, etc.
 - ◆ *Interoperability*: reference implementations of OGF (DRMAA, JSDL, BES, HPC-Profile) and OASIS standards (WS-Brokered Notif, SAML2.0)
 - ◆ *Sustainability*: Roadmap defined till 2015, supported by PSNC and external contributors
- ◆ QosCosGrid has been successfully deployed and is now supported in production on all five supercomputing centers in Poland, deployments in progress in EU
- ◆ QosCosGrid has been successfully registered in the EGI GOCDDB, integrated with the Nagios monitoring tool and accounting systems for 24/7 support
- ◆ QosCosGrid has been recommended for EGI and PRACE to extend existing capabilities - joint taskforce between MAPPER, EGI (MoU signed) and PRACE (after the first evaluation process) driven by PSNC

Selected Use Cases

- ◆ Main fields
 - ◆ Biology
 - ◆ Quantum chemistry
 - ◆ Nanotechnology and material science
 - ◆ High energy physics
 - ◆ astronomy
- ◆ Resource utilisation (2010 example)
 - ◆ Antibiotic simulation – 165 CPU-year
 - ◆ Molecular simulation – 21 CPU-year
 - ◆ Modelling of chemical reactions – 17 CPU-year

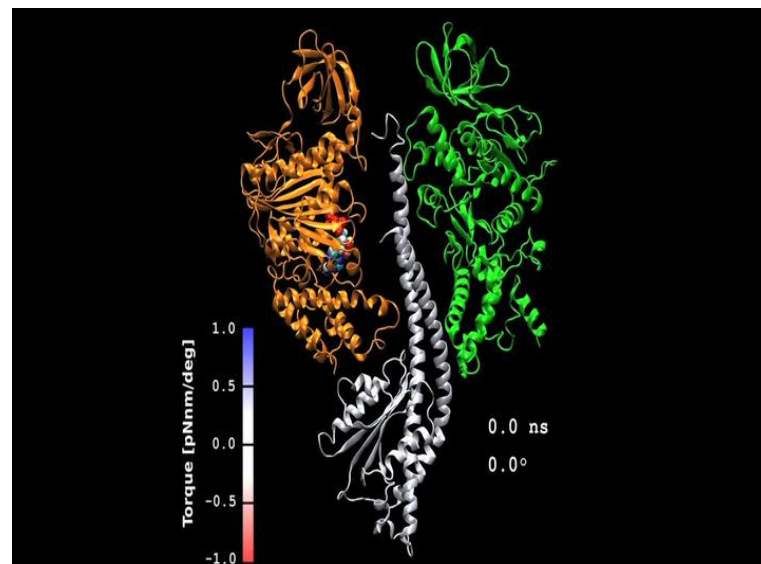
Quantum chemistry

- ◆ Simulation of electronic structure of molecules
- ◆ Example: calculation of electronic structure and oscillations for fulleren C60 – Cu intercation
- ◆ Usage of Turbomole package
 - ◆ Available: ADF and Gaussian



Wide scope of research

- ◆ Protein structures
- ◆ Protein folding
- ◆ DNA research
- ◆ Drug research
- ◆ Electrical phenomena in heart
- ◆ Biopolimers
- ◆ Effects in brain and eye simulation
- ◆ tuberculosis research
- ◆



Antimycosis research

Gdansk University of Technology

165 CPU-year

- Accelerated research according to special Infiniband and software structure (speedup = 5+)

ACK: Jacek Czub, Anna Neumann, PG

Physics

◆ Collaboration with CERN in all LHC experiments

- ◆ Atlas
- ◆ ALICE
- ◆ CMS
- ◆ LHCb



© CERN

◆ Collaboration with nEDM project (12 partners)

- ◆ Neutron electric dipole moment measurements with sensitivity $\sim 10^{-28} \text{ e} \cdot \text{cm}$
- ◆ Polish-European VO with 20TB storage

Astronomy

- ◆ Cherenkov Telescope Array (CTA)
- ◆ Network of detectors 10GeV – 100TeV
- ◆ ESFRI Project



- ◆ Data acquisition by instruments: CANGAROO, H.E.S.S., MAGIC, MILAGRO and VERITAS
- ◆ Data kept by infrastructure and analyzed by our users



ACK: G. Lamana, D. Torres, CTA

Conclusions

- ◆ Innovative tools and approaches are working in the Project at the production level
- ◆ Our tools gaining respect from others EU and US players
- ◆ Heterogeneity of grids is the key
- ◆ We really pay attention to the availability and easiness of the usage our system

The infrastructure will be operable for at least 5 years

- ◆ Further development needed, as identified currently, mainly on Domain Specific Grids

Acknowledgements

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◆ WCSS

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- ◆ Bartłomiej Balcerek

◆ TASK

- ◆ Rafał Tylman
- ◆ Mściśław Nakonieczny

◆ ... and many others....



<http://www.plgrid.pl/en>



Polish Infrastructure
for Supporting Computational Science
in the European Research Space



[Home](#) | [PL-Grid Portal](#) | [Helpdesk online](#)

Start → in English

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News

The article on PL-Grid in the "ISGTW" newsletter

 The article on the PL-Grid project was published in the "ISGTW" newsletter (issue nr 193, from 22 September 2010).

[More...](#)

PL-Grid project at the CGW'10

 The PL-Grid project will be promoted at the exhibition stand held during the CGW'10 in Krakow, Poland, on 11-13 October 2010.

Welcome to the web site of the Polish Grid

Polish Infrastructure for Information Science Support in the European Research Space PL-Grid.

The goal of the project is to provide the Polish scientific community with an IT platform based on Grid computer clusters, enabling e-science research in various fields. This infrastructure will be both compatible and interoperable with existing European and worldwide Grid frameworks. The system will ensure scalability and enable the integration of additional local clusters, belonging to universities, research institutions and technology platforms. We foresee exploitation of PL-Grid by state authorities, crisis management teams and industrial partners.

[Full information...](#)

New materials

PL-Grid movie (9 min. demonstration)

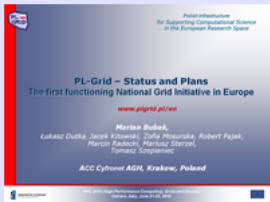


[See the demonstration in a higher resolution ...](#)

PL-Grid leaflet, GridSpace and MD brochures



A talk on PL-Grid given at the HPC 2010 workshop



Search



Events

 **ICT 2010**

Brussels, Belgium,
2010-09-27 - 2010-09-29

 **CGW'10**

Krakow, Poland,
2010-10-11 - 2010-10-13

 **eChallenges e-2010**

Warsaw, Poland,
2010-10-27 - 2010-10-29

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