
Domain-oriented services and resources of Polish Infrastructure for Supporting Computational Science in the European Research Space

# PLGrid PLUS Project
## Status and Current Achievements

Jacek Kitowski, Łukasz Dutka, Tomasz Szepieniec and Mariusz Sterzel

ACK Cyfronet AGH, Kraków, Poland
PL-Grid Consortium

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# Polish e-Infrastructure for Supporting Domain-Oriented Computational Science in European Research Space

Jacek Kitowski

ACK Cyfronet AGH, Krakow, Poland
PL-Grid Consortium

CeBIT Hannover, Poland, March 6, 2013

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY

# Outline

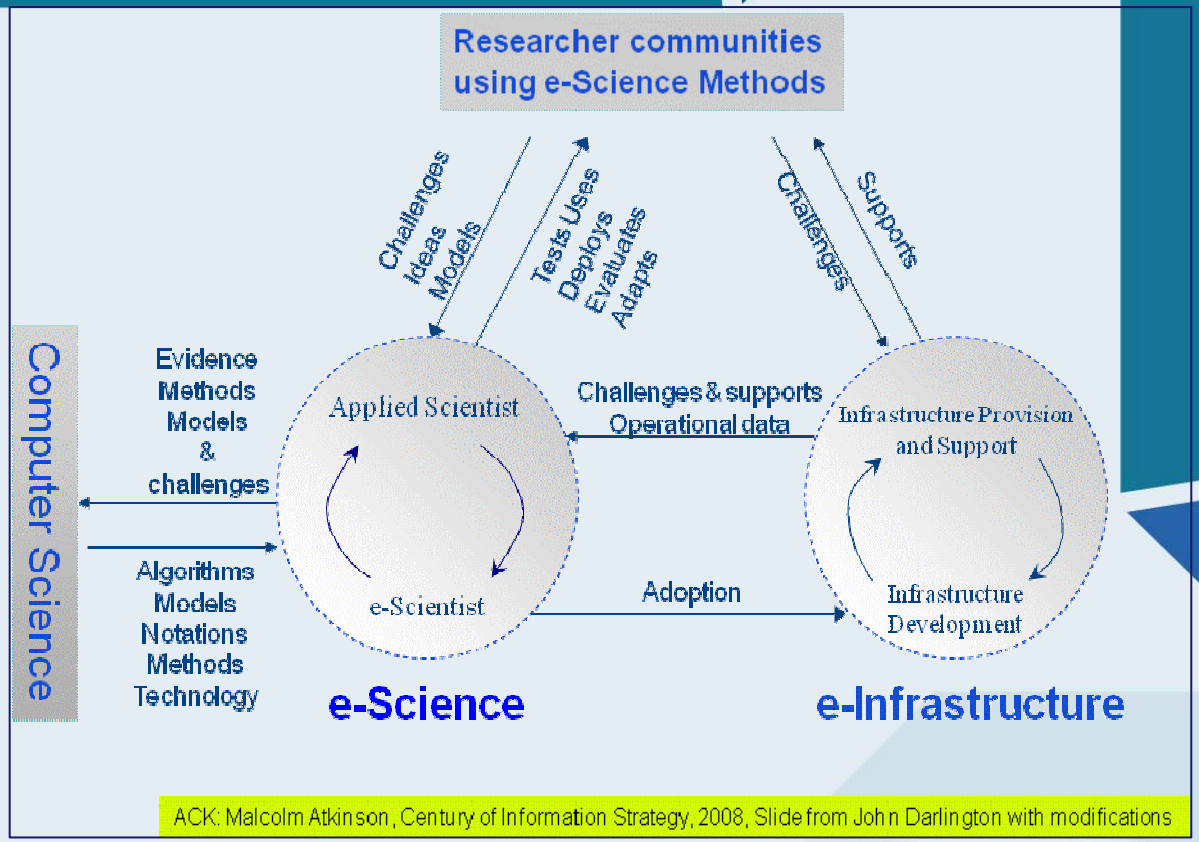
- Motivation Reminder
- PL-Grid and PLGrid Plus Projects – basic facts
- Current Achievements
- Domain-specific solutions and services
- Conclusions

# Outline

- Motivation
- Consortium PL-Grid
- E-Infrastructure Development
- PL-Grid and PLGrid Plus Projects – basic facts
- Current Achievements
- Domain-specific solutions and services
- Conclusions

# Motivation Summary

- World progress in Big Science:
  - Theory
  - Experiment
  - Simulation
- Experiments in silico
  - Advanced, distributed computing
  - Multiscale and multidisciplinary, extreme space-time scales
  - Development n computer /computational sciences required
  - User interaction
  - Big international collaboration
  - E-Science and e-Infrastructure interaction
  - Data mining and aggregation of data for knowledge acquisition




- Computational Science problems addressed:
  - Simulation algoritms and environments
  - 4th paradigm
  - Big Data
  - Data Farming

# Computational Science

## High Performance Computing

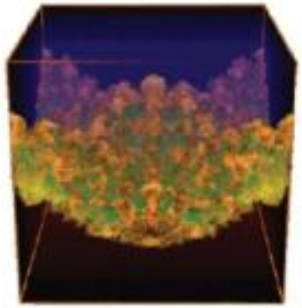
- Computational Science (one of definitions by K. Wilson*):
  - ...”
  - a precise mathematical statement,
  - being intractable by traditional methods
  - with a significant scope
  - requires in depth knowledge of science, engineering and the arts...”

- *„Computational science is about using computers to analyze scientific problems.*
  - *it is distinct from computer science, which is the study of computers and computation, and...*
  - *it is different from theory and experiment (...) in that it seeks to gain understanding principally through*
  - *the analysis of mathematical models (on)*
  - *high performance computers.“*

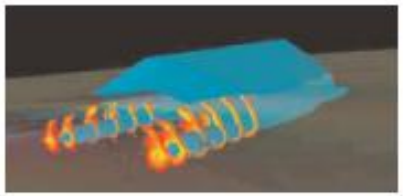
*K.G. Wilson, Basic issues for Computational Science, ICTP, 1986

# Grand Challenges

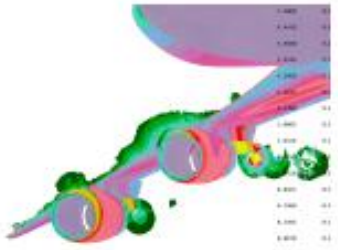
## Applications of High-End Computing:
### *Big Problems with Big Impacts*



Nuclear Stockpile Stewardship



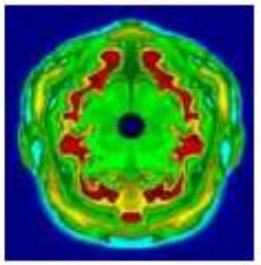
Ship Design



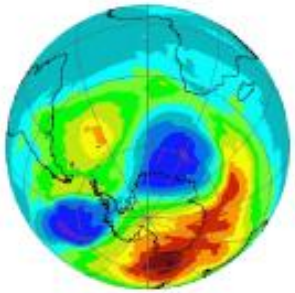
Aeronautics

Weather Prediction

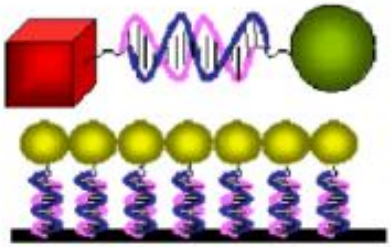
Cryptanalysis



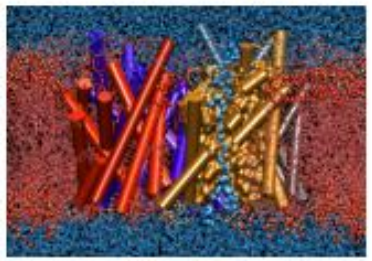
Astrophysical Simulation



Climate Modeling



Nano-Science



Biology

HEC – September 22, 2004

4

*ally broad*
*by*

Modelling, Simulation, Analysis

# Motivation Summary
## Consortium PL-Grid

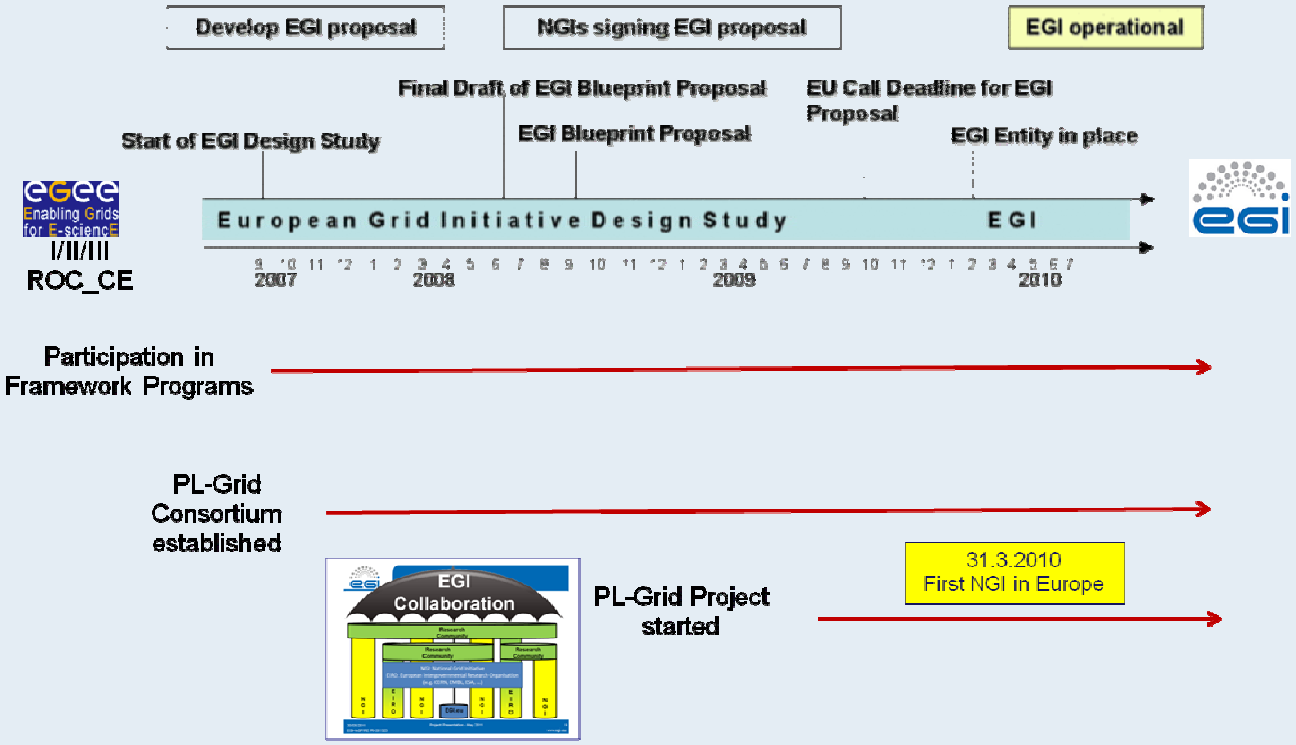
- Rationale behind Consortium
  - Polish scientific communities (top-level publications)
  - Experience by participation in international and national projects
  - Computational resources already available
  - European/Worldwide integration activities
  - Top-level record of ROC_CE in EGEE I/II/III
  - Pionier National Network Infrastructure available


- PL-Grid Consortium created (Jan. 2007)
  - Consortium members – make up of 5 Polish supercomputing and networking centres
  - with goal:
  - Significant extension of amount of computing resources provided to the Polish scientific community
  - based on Projects
  - funded by the European Regional Development Fund as part of the Innovative Economy Program

# PL-Grid Consortium

## Projects

- PL-Grid Project (1.1.2009 – 31.3.2012)
  - Budget: total 21 M€, from EC 17M€




- PLGrid PLUS Project (12.10.2011 – 31.3.2015)
  - Budget: total ca.18 M€, from the EC: ca.15 M€

# First Step: PL-Grid Project

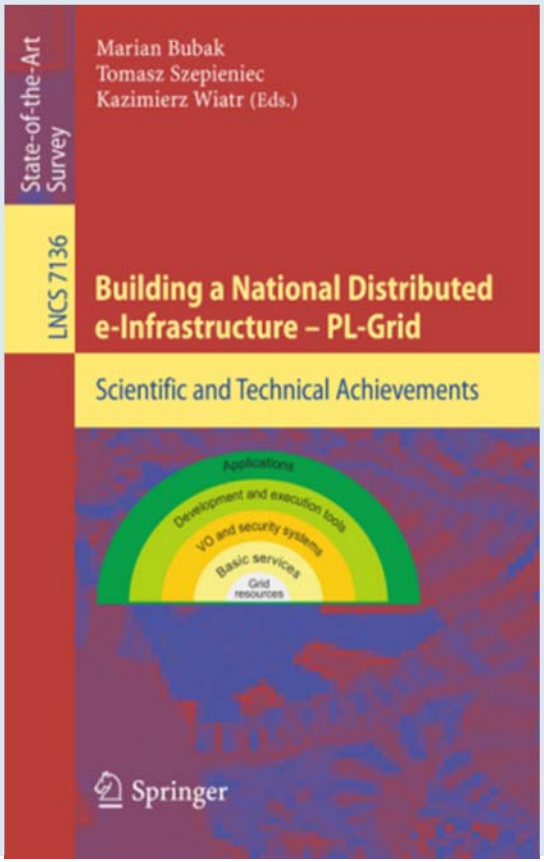
## Polish Infrastructure for Supporting Computational Science in the European Research Space

- Significant extension of
- computing resources
- basic middleware

provided to the Polish scientific community

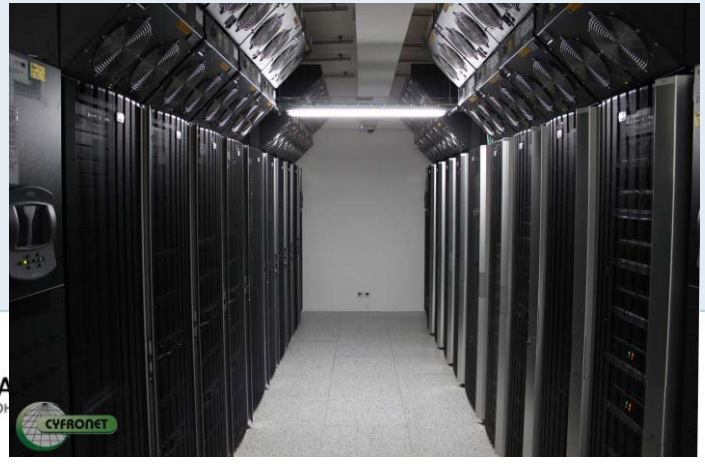
- Outcome:
  - Common base infrastructure
    – National Grid Infrastructure (NGI_PL)
    – internationally compatible
  - Potential capacity to construct specialized, domain Grid systems
  - Resources: 230 Tflops, 3600 TB
    users: 1000+
    jobs/month: 500,000-1,500,000
  - innovative grid services and end-user tools like Efficient Resource Allocation, Experimental Workbench and Grid Middleware
  - Scientific Software Packages
  - User support: helpdesk system, broad training offer

- Publication of the book (Springer 2012) with PL-Grid achievements
- Content: 26 papers



# TOP500 Nov.2011 Polish Sites

| Rank | Site | System | Cores | Rmax TFlop/s | Rpeak TFlop/s |
|---|---|---|---|---|---|
| 88 | **Cyfronet** | **Zeus** - Cluster Platform 3000 BL 2x220, Xeon X5650 6C 2.66 GHz, Infiniband, HP | 15264 | 128.8 | 162.4 |
| 279 | **Gdansk CI Task** | **Galera Plus** - ACTION Xeon HP BL2x220/BL490 E5345/L5640 Infiniband, ACTION | 10384 | 65.6 | 97.8 |
| 296 | **ICM Warsaw** | **Boreas** - Power 775, POWER7 8C 3.84 GHz, Custom, IBM | 2560 | 64.3 | 78.6 |
| 298 | **PCSS** | **Rackable** C1103-G15, Opteron 6234 12C 2.40 GHz, Infiniband QDR, SGI | 5640 | 63.9 | 136.4 |
| 348 | Grupa Allegro | Cluster Platform 3000 BL 2x220, Xeon L5420 4C 2.50 GHz, Gigabit Ethernet, HP | 10748 | 59.1 | 107.5 |
| 360 | **WCSS** | **Supernova** - Cluster Platform 3000 BL2x220, X56xx 2.66 Ghz, Infiniband, HP | 6348 | 57.4 | 67.5 |

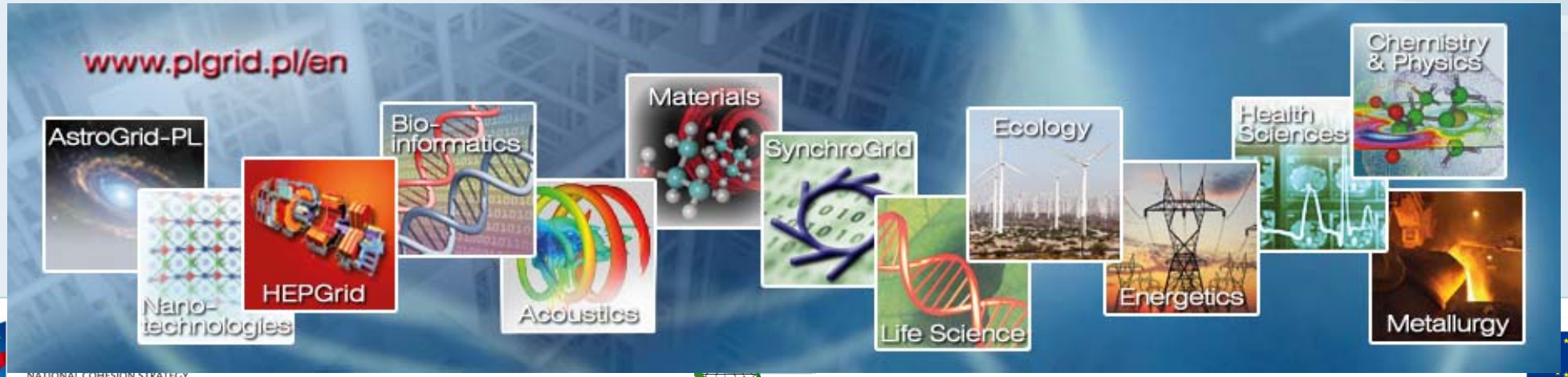


# Second Step: PLGrid PLUS Project

## Domain-oriented services and resources of Polish Infrastructure for Supporting Computational Science in the European Research Space

- Significant extension in line with European solutions of
- Preparation of specific computing environments, i.e., solutions, services and extended infrastructure (including software), tailored to the needs of different groups of scientists.
- Necessary IT services
- Computing and software resources

- These domain-specific solutions are created for identified 13 groups of users representing strategic areas and important topics for the Polish and international science
- astronomy, high energy physics, nanotechnologies,
- bioinformatics, acoustics, material science, synchrotron radiation, life science,
- ecology, power systems, health, chemistry and physics, metallurgy



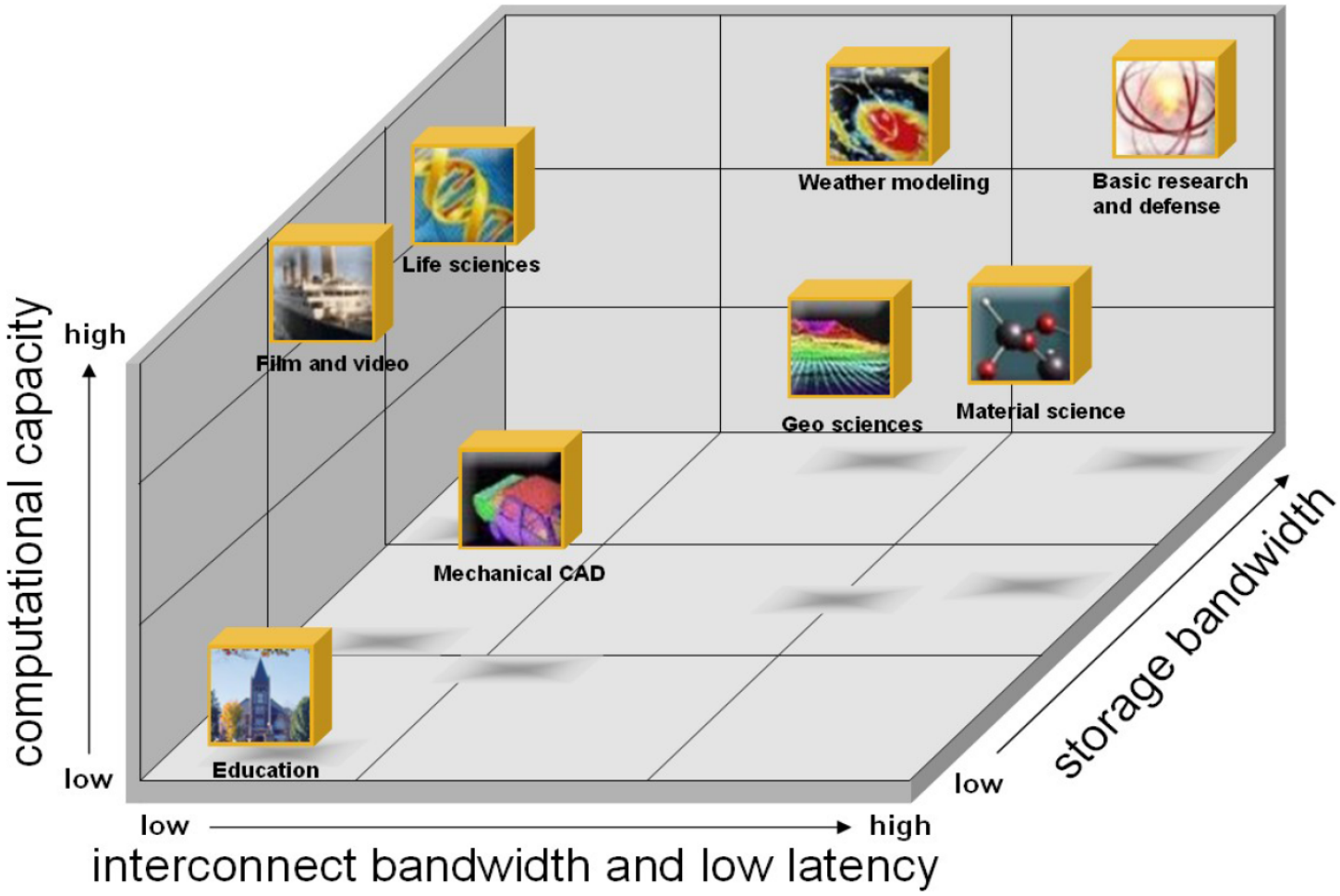
# PLGrid PLUS

## Activities in Domain Grids in general

- Integration Services
  - National and International levels
  - Dedicated Portals and Environments
  - Unification of distributed Databases
  - Virtual Laboratories
  - Remote Visualization
  - Service value = utility + warranty
  - SLA management
- Computing Intensive Solutions
  - Specific Computing Environments
  - Adoption of suitable algorithms and solutions
  - Workflows
  - Cloud computing
  - Porting Scientific Packages
- Data Intensive Computing
  - Access to distributed Scientific Databases
  - Organization of Scientific Databases
  - Data discovery, process, visualization, validation….
  - 4th Paradigm of scientific research
- Instruments in Grid
  - Remote Transparent Access to instruments
  - Sensor networks
- Organizational
  - Organizational backbone
  - Professional support for specific disciplines and topics

# Diversity of Requirements

## HPC Technical Market Segmentation



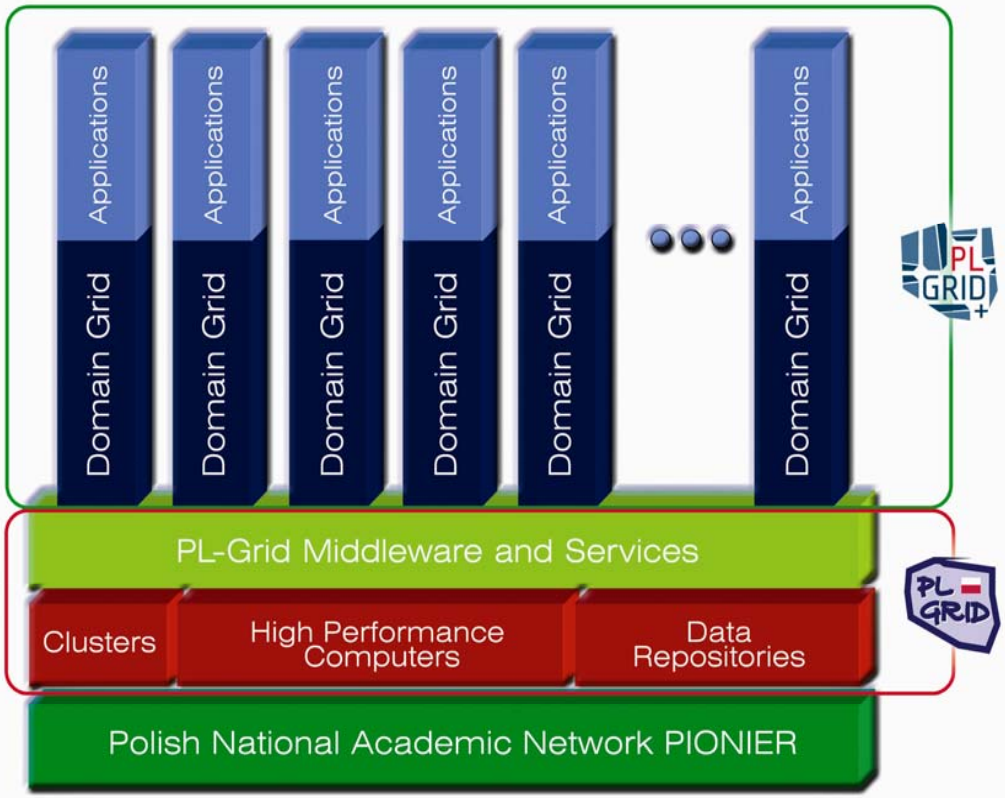

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY
CYFRONET
ACK: HP

# PLGrid PLUS

www.plgrid.pl/plus

## Project tasks and expected outcome

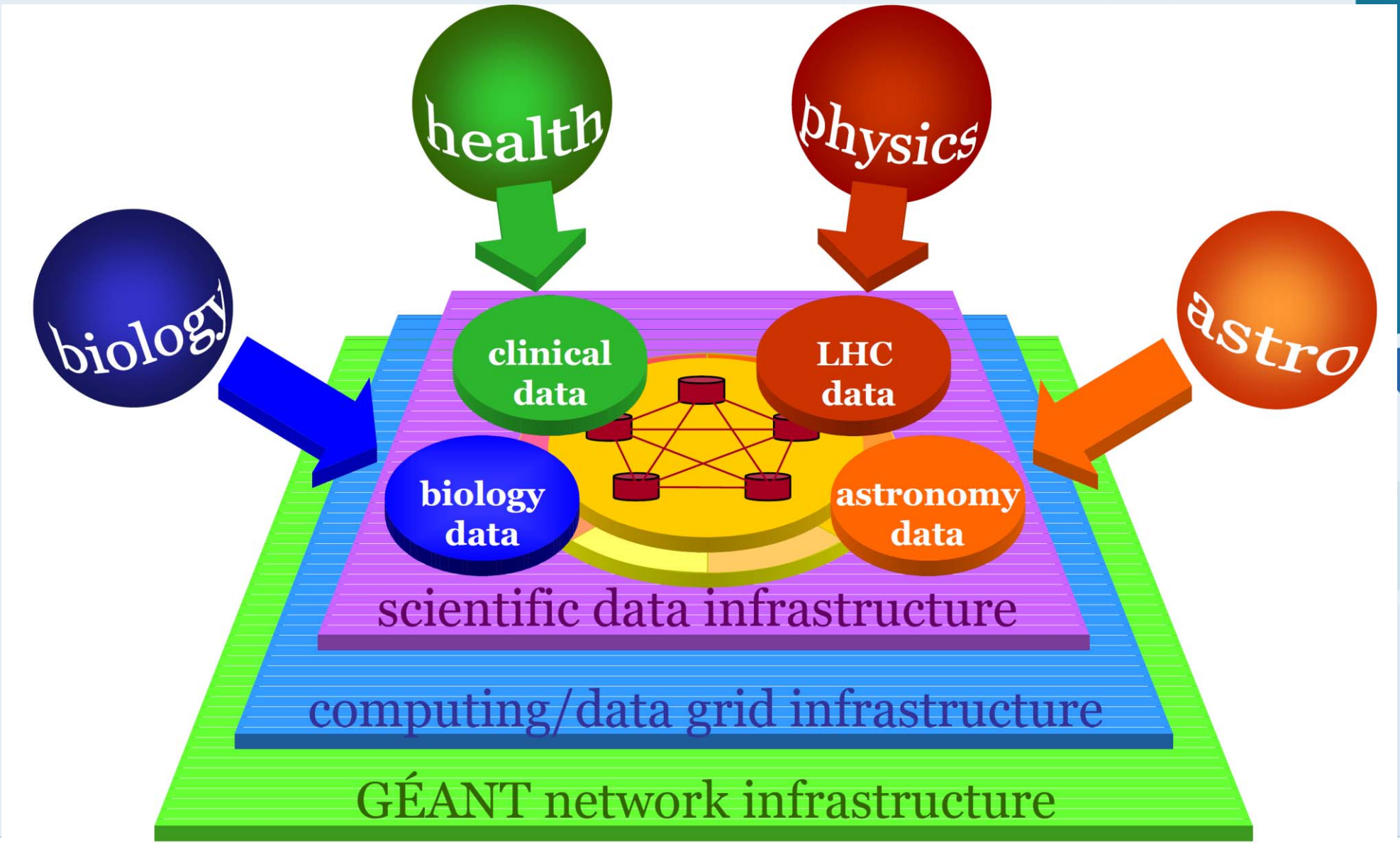
- Design and start-up of support for new domain-specific federated grids
- Development of new infrastructure services tools, environments and resources
- Extension of the resources available in the PL-Grid infrastructure by
  - 500 Tflops
  - 4.4 PB
- Keeping diversity
  - Clusters (thin and thick nodes)
  - Clusters with GPGPU
  - SMP
  - vSMP
- Deployment of Cloud infrastructure for users
- Deployment of Quality of Service system for usersby introducing SLA agreement
- Broad consultancy, training and dissemination offer




The scope is not limited to the selected domains.
Easy extension offered.

# Fits to European e-Infrastructure Plans

(thanks to Mario Campolargo)



# TOP500 Nov. 2013 Polish Sites

| Rank | Site | System | Cores | Rmax (TFlop/s) | Rpeak (TFlop/s) | Power (kW) |
|---|---|---|---|---|---|---|
| 106 | **Cyfronet Poland** | **Zeus** - Cluster Platform SL390/BL2x220, Xeon X5650 6C 2.660GHz, Infiniband QDR, NVIDIA 2090<br>Hewlett-Packard | 23932 | 234.3 | 357.5 | |
| 143 | ICM Warsaw Poland | BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect<br>IBM | 16384 | 172.7 | 209.7 | 82.2 |
| 344 | Grupa Allegro Poland | Cluster Platform 3000 BL 2x220, Xeon L5420 4C 2.50 GHz, Gigabit Ethernet<br>Hewlett-Packard | 16876 | 92.8 | 168.8 | |
| 375 | **PCSS Poland** | Rackable C1103-G15, Opteron 6234 12C 2.40 GHz, Infiniband QDR<br>SGI | 9498 | 89.8 | 211.1 | |

# Cyfronet at TOP500 lists

| List | Rank | System | Cores | Rmax (GFlop/s) | Rpeak (GFlop/s) |
|---|---|---|---|---|---|
| 11/2012 | 106 | **Zeus** - Cluster Platform SL390/BL2x220, Xeon X5650 6C 2.660GHz, Infiniband QDR, NVIDIA 2090, HP | 23932 | 234000 | 357500 |
| 06/2012 | 89 | **Zeus** - Cluster Platform SL390/BL2x220, Xeon X5650 6C 2.660GHz, Infiniband QDR, NVIDIA 2050/2090, HP | 13944 | 185316 | 271113 |
| 11/2011 | 88 | **Zeus** - Cluster Platform 3000 BL 2x220, Xeon X5650 6C 2.66 GHz, Infiniband, HP | 15264 | 128790 | 162409 |
| 06/2011 | 81 | **Zeus** - Cluster Platform 3000 BL2x220, L56xx 2.26 Ghz, Infiniband, HP | 11694 | 104765 | 124424 |
| 11/2010 | 85 | **Zeus** - Cluster Platform 3000 BL2x220, L56xx 2.26 Ghz, Infiniband, HP | 9840 | 88051 | 104698 |
| 06/2010 | 161 | Cluster Platform 3000 BL2x220, L56xx 2.26 Ghz, Infiniband, HP | 6144 | 39934 | 55542 |
| 11/2008 | 311 | **Zeus** - Cluster Platform 3000 BL2x220, L54xx 2.5 Ghz, Infiniband, HP | 2048 | 16179 | 20480 |
| 11/1996 | 408 | SPP1600/XA-32, HP (Convex) | 32 | 5.5 | 7.7 |
| 06/1996 | 408 | SPP1200/XA-32, HP (Convex) | 32 | 4.0 | 7.7 |

# Current PL-Grid Resources

## Computational Power

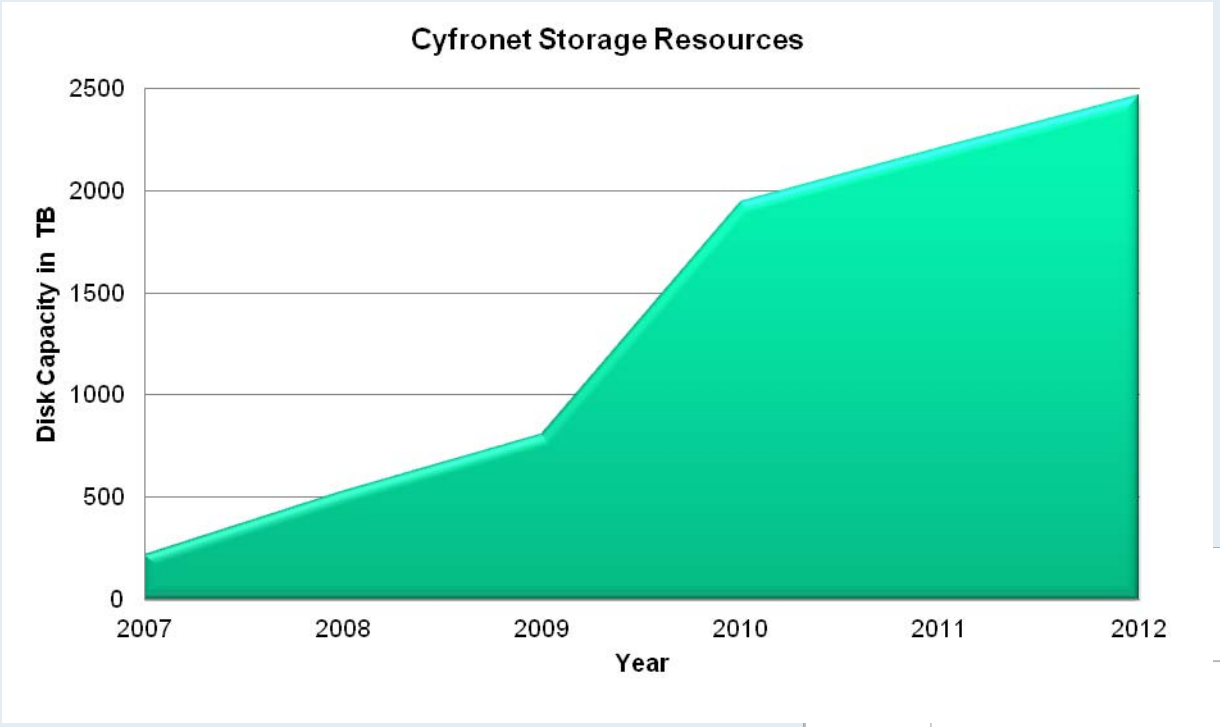
| Site | Total Rpeak , Tflops | Incl. GP GPU, Tflops |
|---|---|---|
| CYFRONET | 358 | 131 |
| ICM | 49 | -- |
| PCSS | 100 | 52 |
| TASK | 30 | -- |
| WCSS | 72 | 3 |

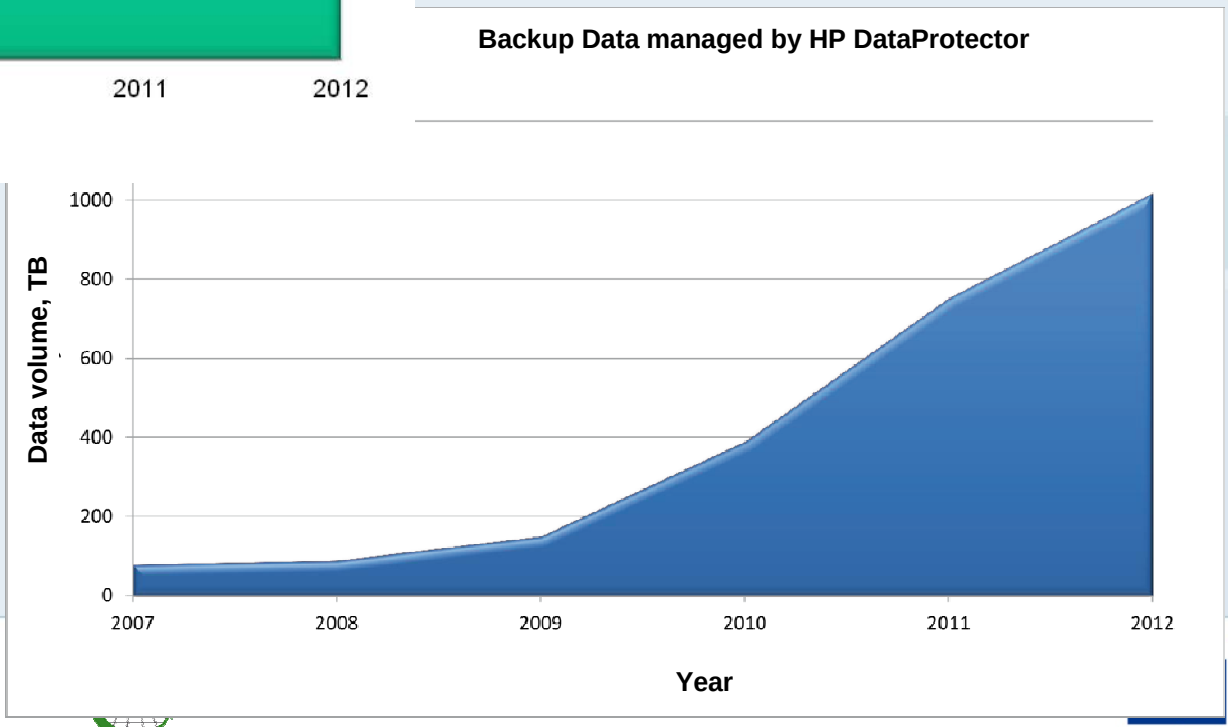
# Current PL-Grid Resources

## Operational Storage

| Site | TB (disks & tapes) |
|---|---|
| CYFRONET | ~3500 |
| ICM | 544 |
| PCSS | 847 |
| TASK | 3 |
| WCSS | 3491 |

# Cyfronet Storage Resources

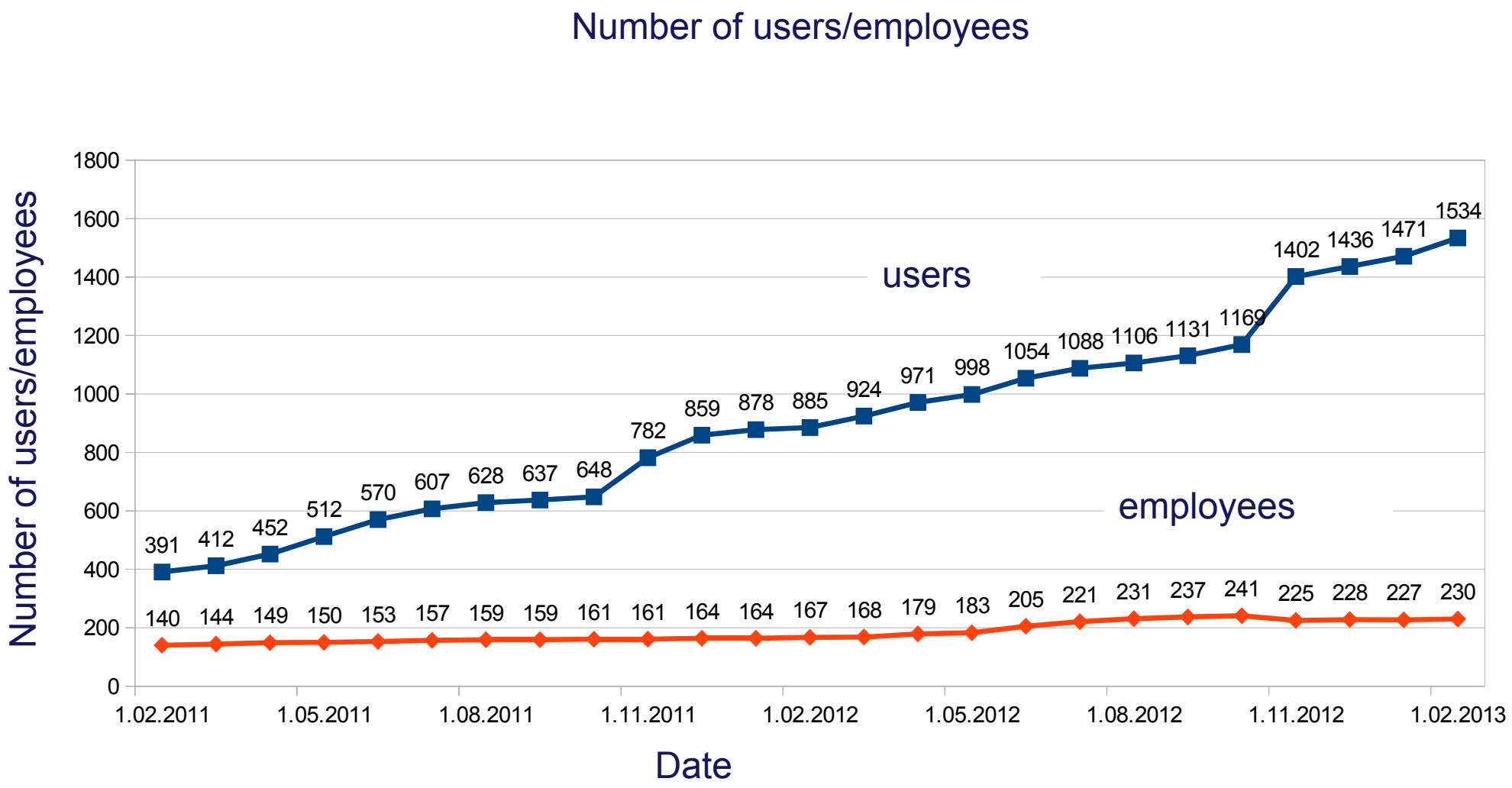


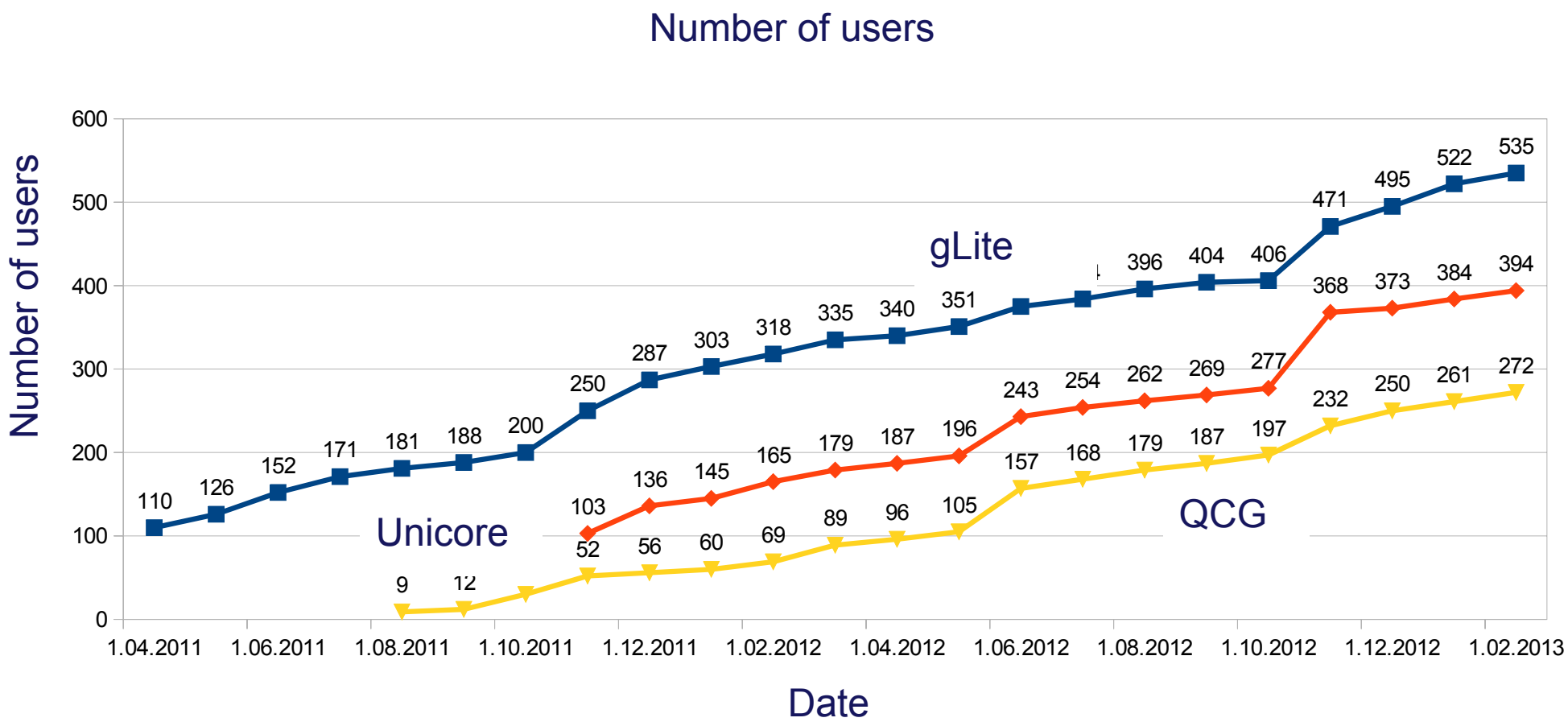
# Cyfronet Storage Resources

- Total disk systems capacity 2,468 PB, including:
  - 13,6 TB high performance FC disks,
  - 211 TB cost-effective FATA disks,
  - 1192 TB high performance SAS disks,
  - 1052 TB cost-effective SATA disks,
  - From:
  - HP StorageWorks: XP12000, EVA 8000, EVA 8100
  - SGI InifiniteStorage: 4600, 5000,5500
  - HDS AMS2500
  - Sun Fire: X4500, X4540
  - HP Blade  disk servers
  - HDS HNAS 3080 filers
- Total tape systems capacity 4 PB, including:
  - Tape library HP StorageWorks ESL712e
    - 6 drives Ultrium LTO-3,
    - 6 drives Ultrium LTO-4,
    - 636 slots for LTO.tapes
  - Tape library IBM System Storage TS3500
    - 16 drives Ultrium LTO-5,
    - 2003 slots for LTO tapes

# Current PL-Grid Users

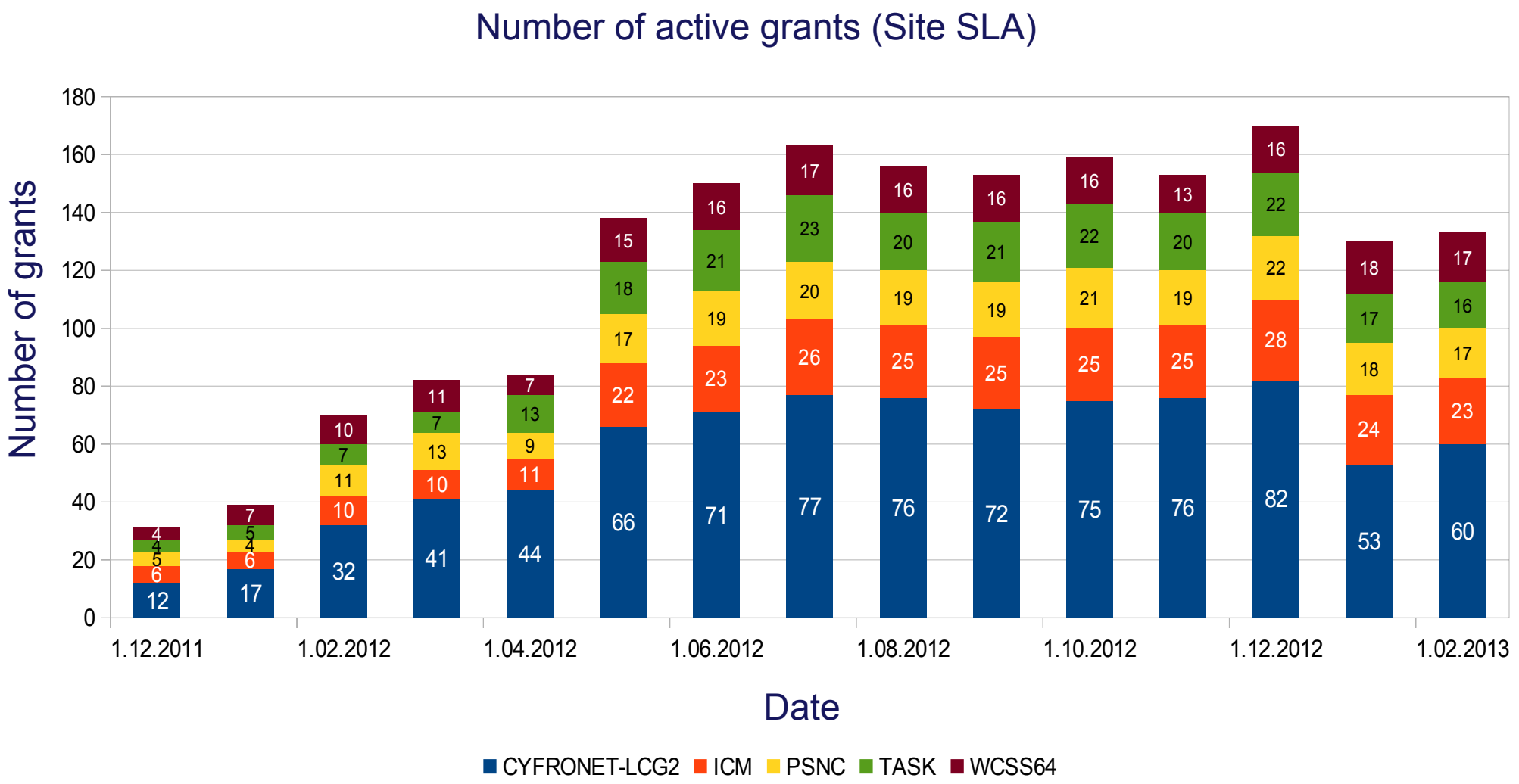


# Current PL-Grid Users of global services



# Computational Grants

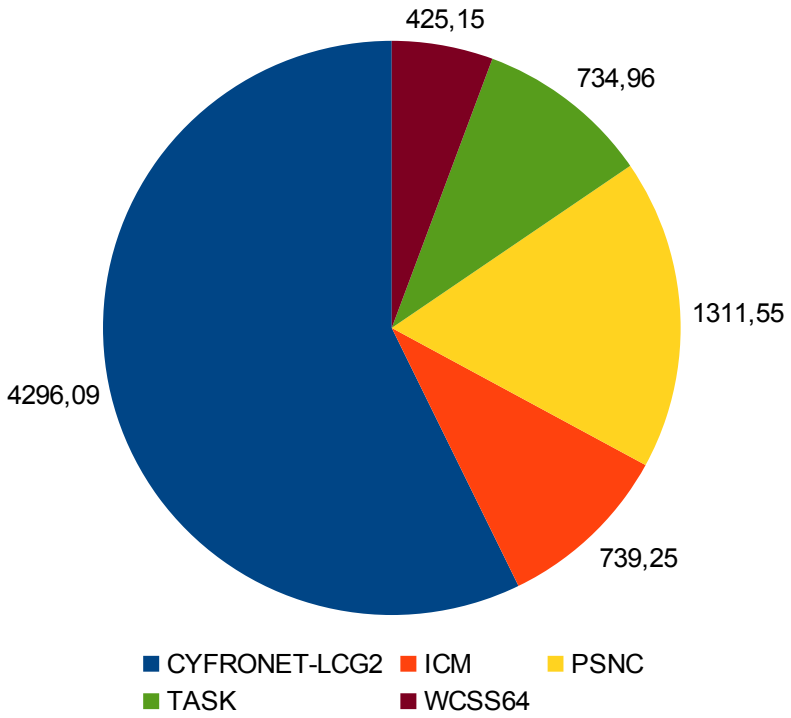
## Number of active grants



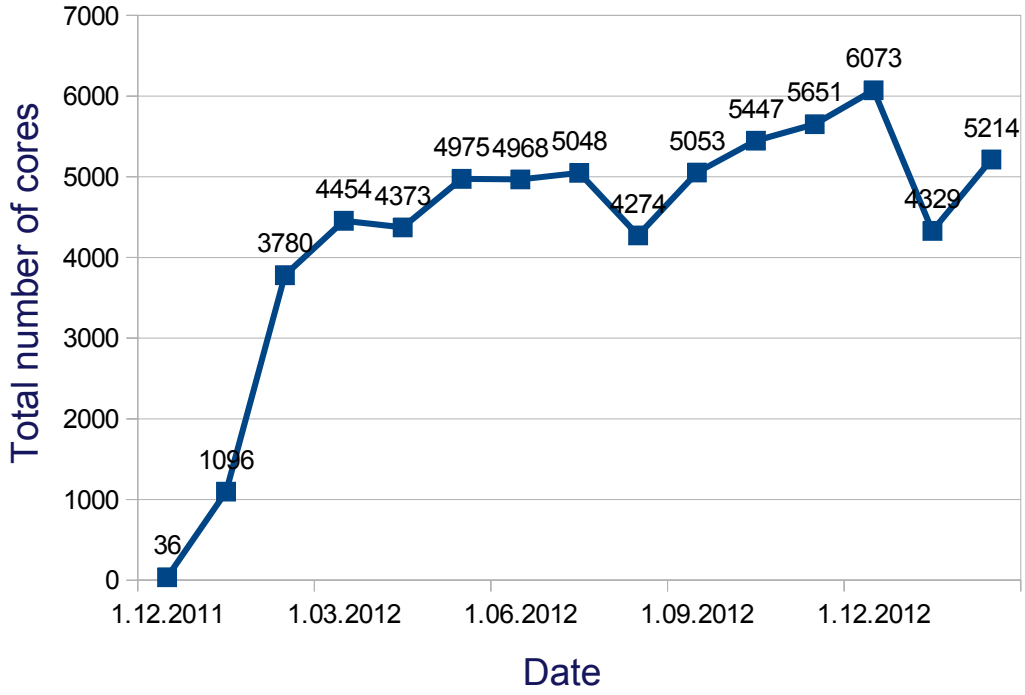
# Computational Grants

## Number of cores (x86)

### Number of cores for active grants (Site SLA)



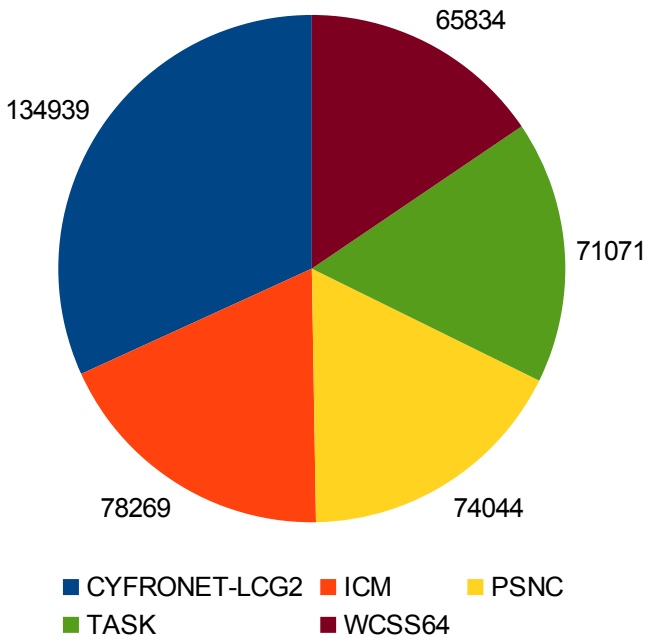

### Total number of cores for active grants (Grant SLA)



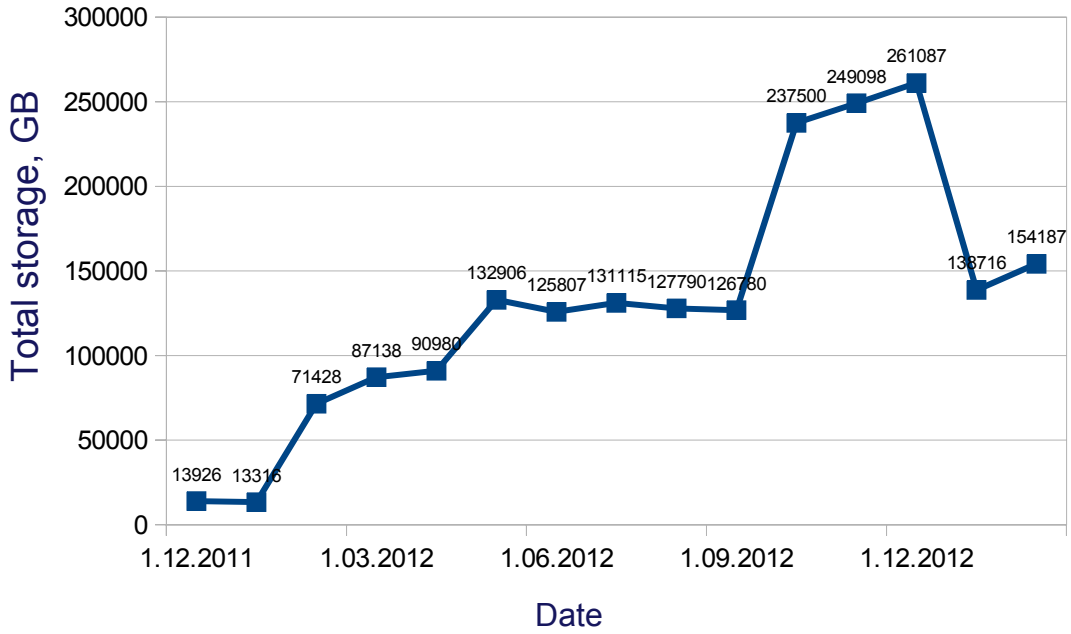
# Computational Grants

## Storage

### Storage for active grants (Site SLA)

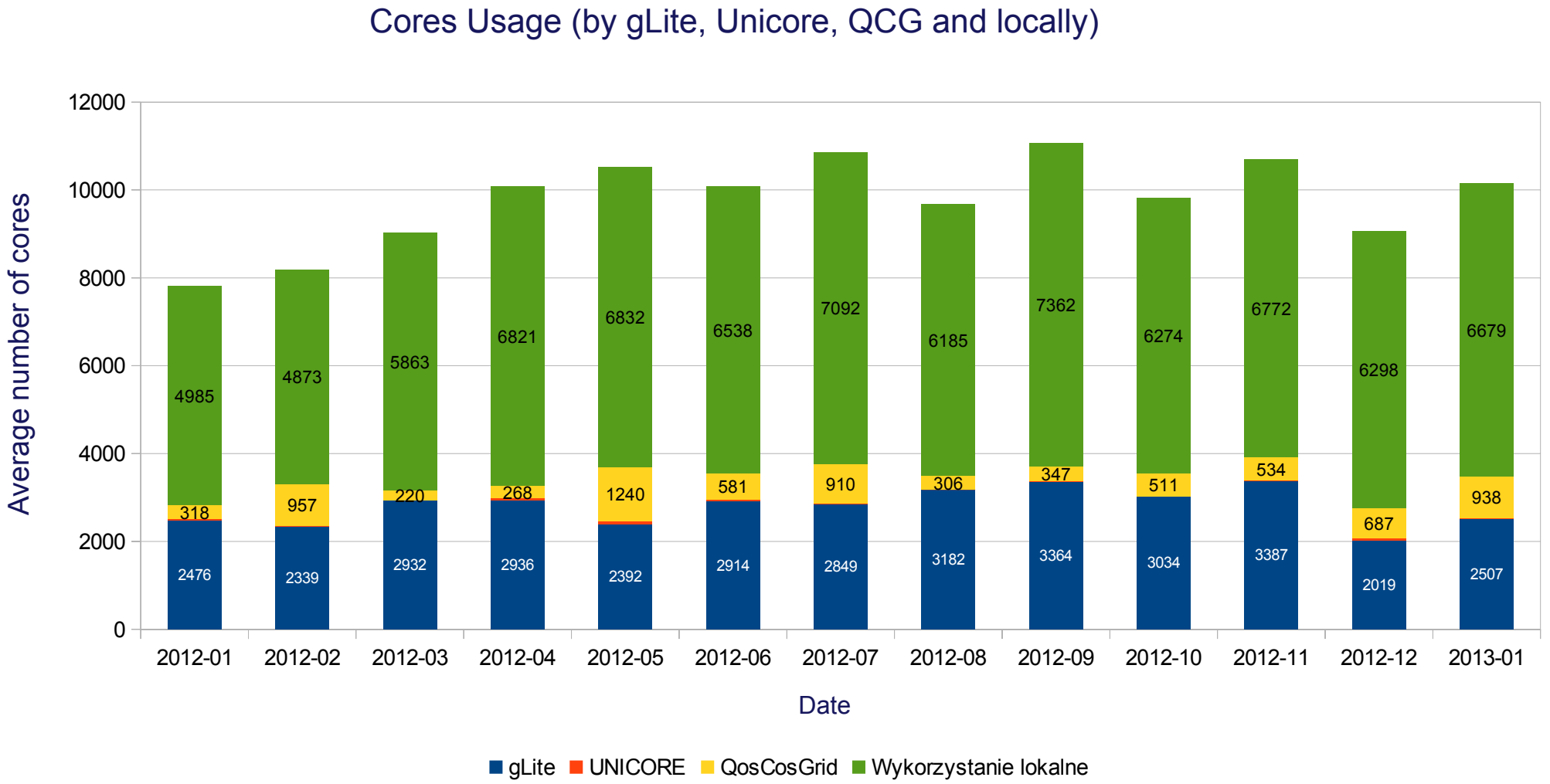



### Total storage for active grants (Grant SLA)

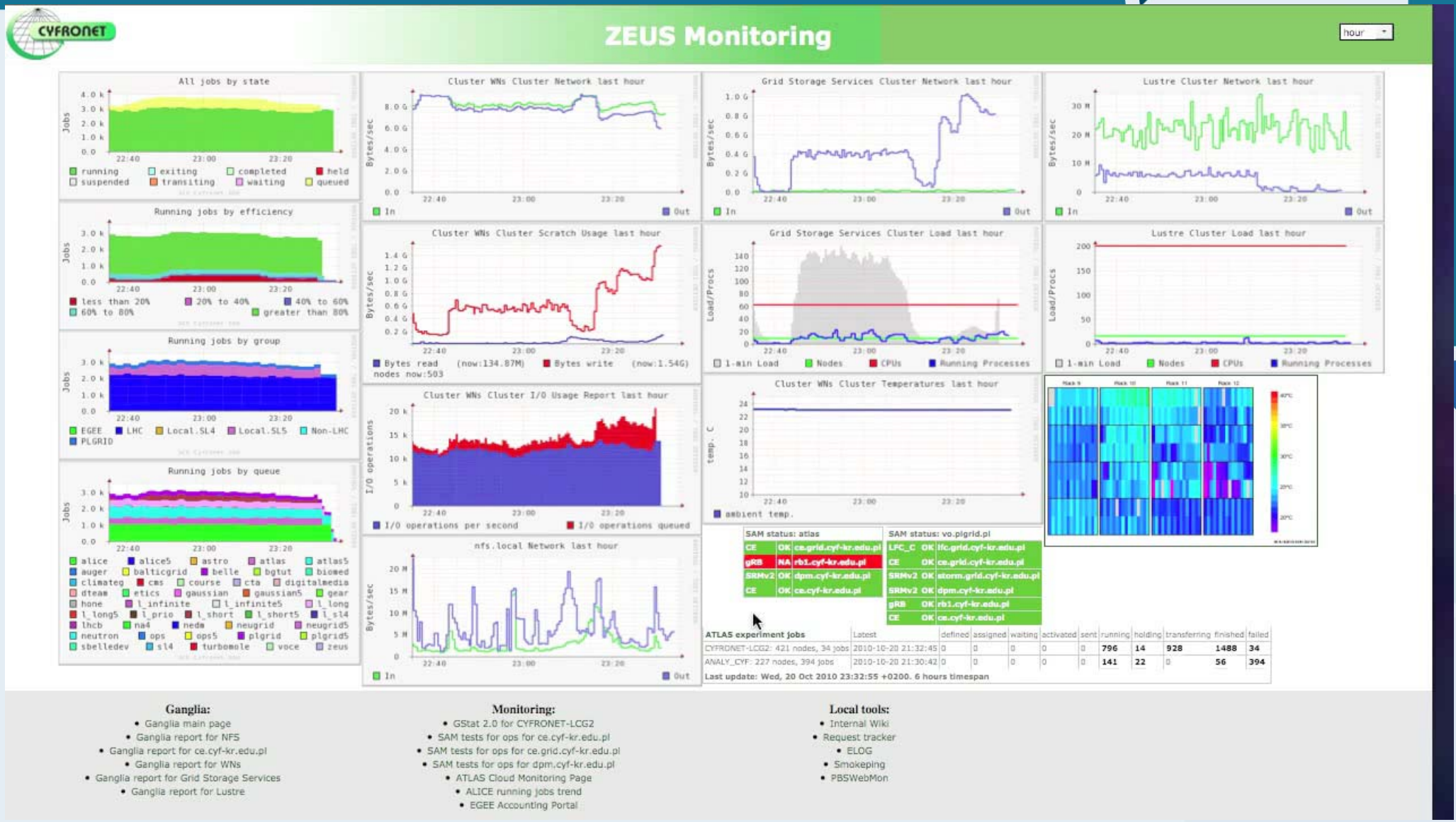


# Resource Usage

## Cores (x86)



# Zeus – Resource Monitoring



# New Software Packages

- Chemistry
  - Molpro – Coupled Cluster Methods
- Life Science
  - GeneSpring – Microarray management suite
  - NTI – gene sequence analysis software
- Energetics
  - GAMS – optimisation and modelling system
- Metallurgy
  - ProCast – metallurgy processes modelling suite
- Acoustics
  - NUMEICA – modelling and analysis suite

# Domain Grids

- Pilot program for strategic science domains and important topics of Polish/European Science
- Access to the software packages is provided by:
  - Glite
  - Unicore
  - QCG
- Already identified 13 communities/scientific topics:
  - Astrophysics
  - HEP
  - Life Sciences
  - Quantum Chemistry and Molecular Physics
  - Synchrotron Radiation
  - Power Systems
  - Metallurgy
  - Nanotechnology
  - Acoustics
  - Ecology
  - Bioinformatics
  - Health
  - Material Science

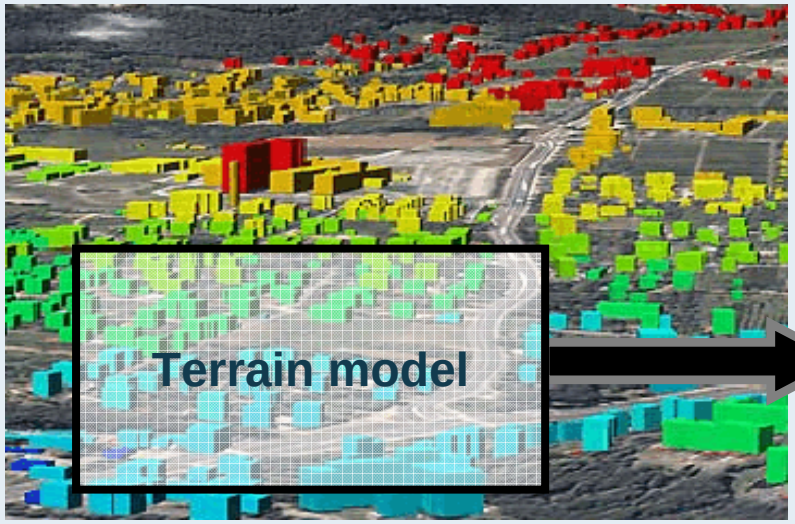
# (Near) Future Plans

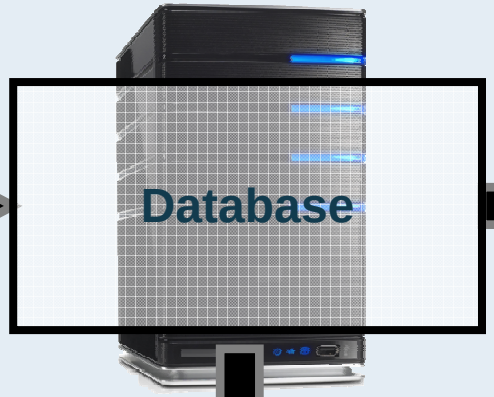
- First implementations (March 2013)
  - InsilicoLab (Chemistry)
  - Integromics ( Life Science)
  - Noise Maps (Acoustics)
- New community services (March 2013)
  - Virtual Synchrotron (SynchroGrid)
  - OptiMINE (Energetics)
  - Data processing prototype (Health)
  - Virtual Observatory (AstroGrid-PL)

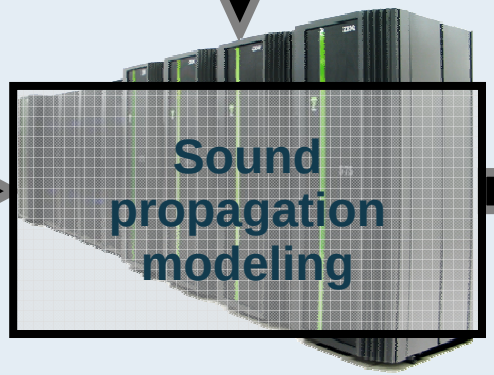
# Examples of domain specific solutions and services

# Acoustics

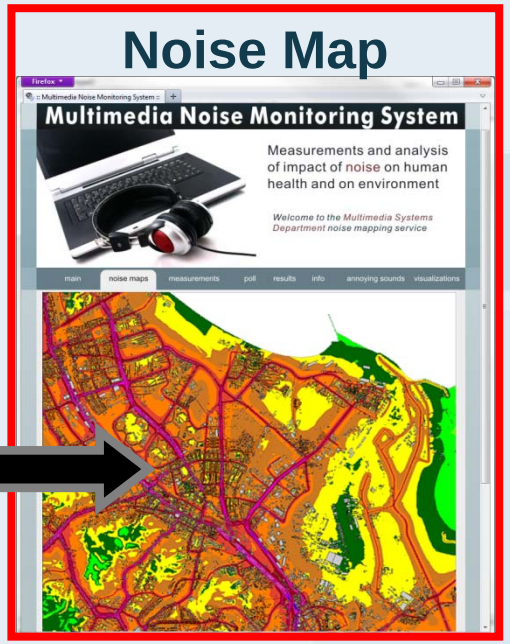
## Multimedia Noise Monitoring System and Simulation

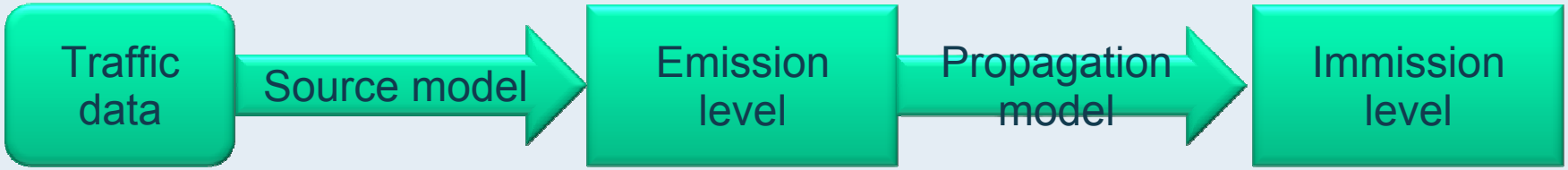







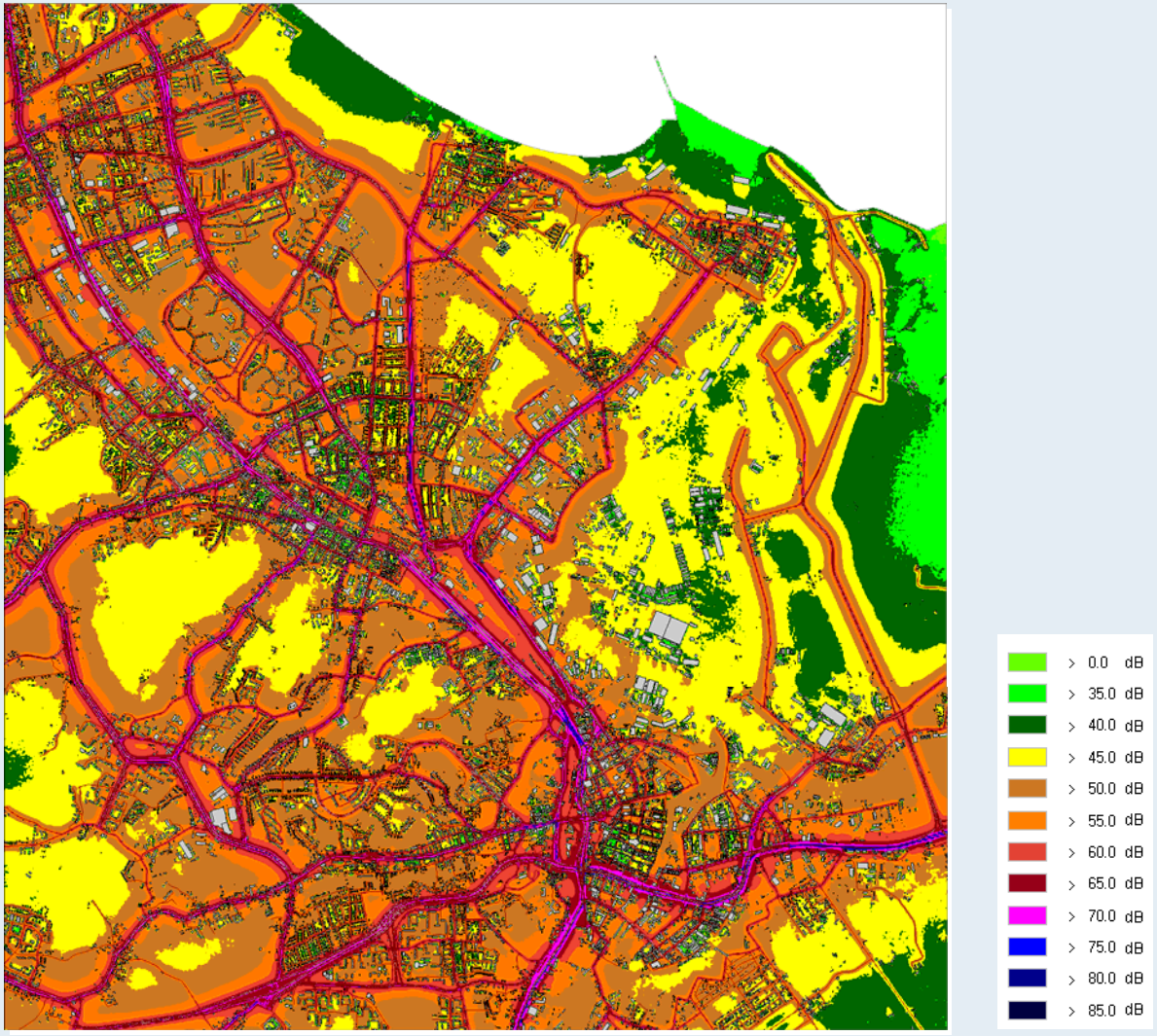
# Acoustics
## Methodology




- Source part, the Harmonoise model
  - Traffic volume
  - Vehicle speed
- Propagation part
  - The acoustic ray tracing method
  - Additional libraries: Harmonoise, CGAL, Tardem
  - Geometrical description of sources and buildings

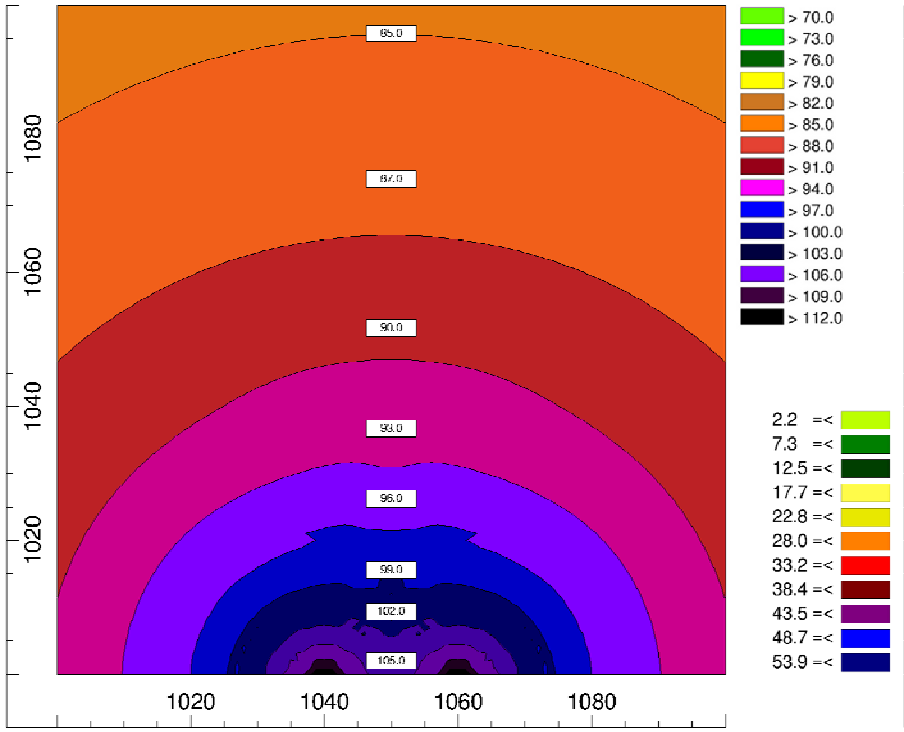
# Acoustics

## Computed noise map of large urban area (road noise)

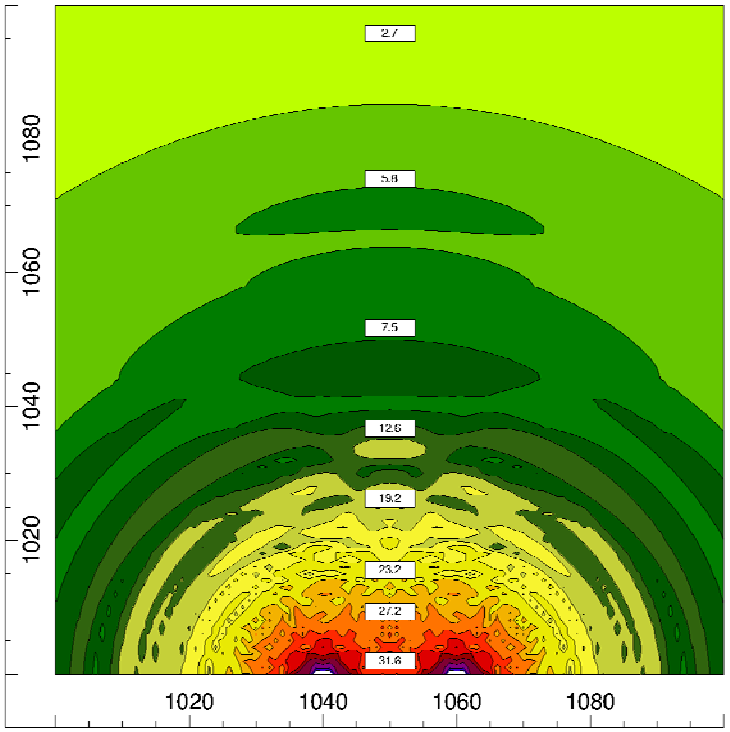


# Acoustics

## Simulation of noise exposure during outdoors concert




Noise map for the outdoor loud acoustic event (open field musical concert)




The map of maximum TTS values

# Nanotechnology

## The AuxEx Service: goals and features

### Goals:

- creation of central point of collection and distribution of experimental data
- reduction of the likelihood of duplication of work on getting the same results
- improvement of data security (access rules, backup)
- automated data processing
- providing a consistent interface to the advanced computing application

### Features:

- dedicated software (does not require the user to spend time to learn)
- requires no client installation Web computing (web interface)
- application tailored to the needs of a particular research project (for now NewLoks and Organometallics)
- the ability to install the server in the PLGrid Plus resource and locally on the user's machine

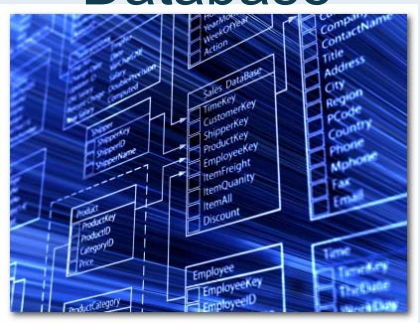
# Nanotechnology
## Application structure

Prototype

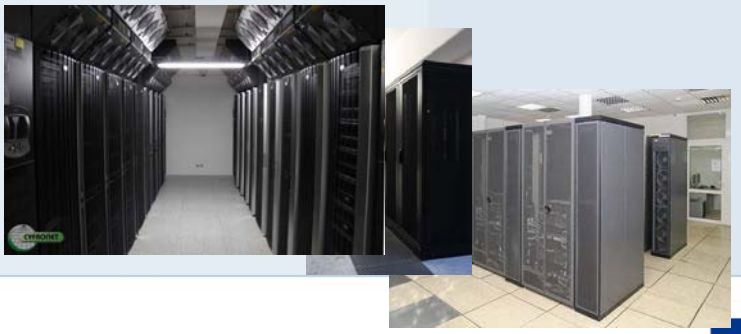
Client session

AuxEx server

Database



KDM



# Synchrogrid
## Overview

- Synchrogrid builds services for the synchrotron radiation scientific community
- It is expected that the establishment of the Research Centre of Polish Synchrotron (2014) will influence the rapid rise in the users of synchrotron radiation to 1,000 people
- Involved institutions:
  - Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences
  - AGH University of Science and Technology
  - Jagiellonian University
  - University of Silesia in Katowice
  - Adam Mickiewicz University
- Launching a synchrotron  makes its radiation easily accessible
- The world witnessed the rapid increase of the number of scientists using synchrotron radiation when the first synchrotron was opened in their country

# Synchrogrid
## Services in development

### Elegant Service

- Elegant („ELEctron Generation ANd Tracking”) is a fully 6D accelerator simulation program that now does much more than generation of particle distributions and tracking them
- Matlab configured to use the Self Describing Data Sets (SDDS) file protocol
- Additional scripts that ease submission of jobs locally on the cluster and with use of grid middleware
- **Status:** prototype delivered to specific users for evaluation

### Virtual Accelerator Service

- Requires Elegant service
- TANGO (The TAco Next Generation Objects) control system – open source object-oriented control system for controlling accelerators, experiments and any kind of hardware or software being actively developed by a consortium of (mainly) synchrotron radiation institutes
- Virtual Machine with User Interface for submitting grid jobs
- **Status:** prototype development (installation on cluster and preparation of modules)

# Synchrogrid

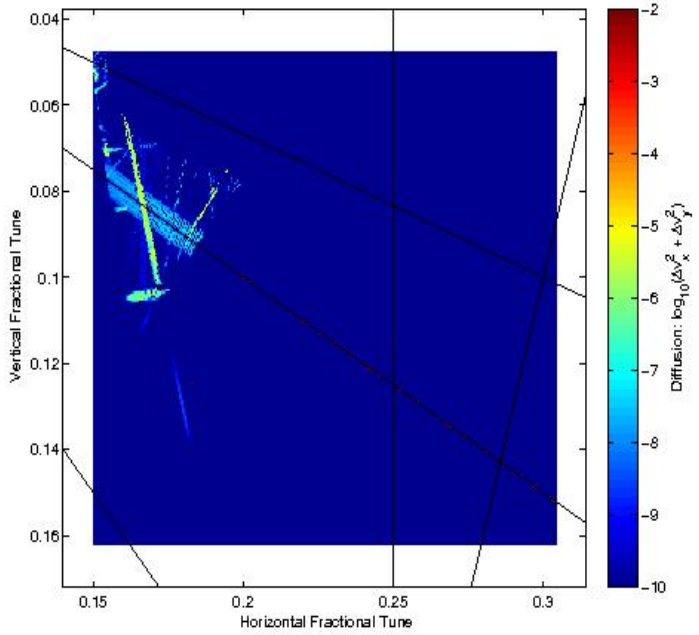
## Usage of Elegant service prototype

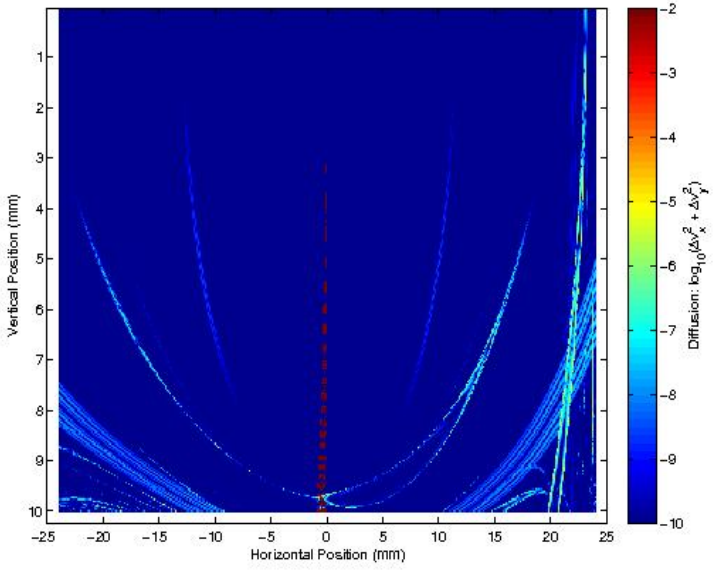
Preparation of input files

- Submission of jobs (local or grid) of parallel version of Elegant software
- Intermediate output file is automatically analysed by pre-prepaired Matlab scripts
- Final output (as figures on the right) is analysed by a user. Then, corrections to the input files are entered manually and the iteration is repeated.
- If the results are satisfactory for the user, the figures (prepared in eps and jpeg format) could be inserted into publication

Calculations in basic version (calculations in two dimensions only) required ca. 100h of walltime on iteration.

The introduction of scan in additional dimension is foreseen in the next release.

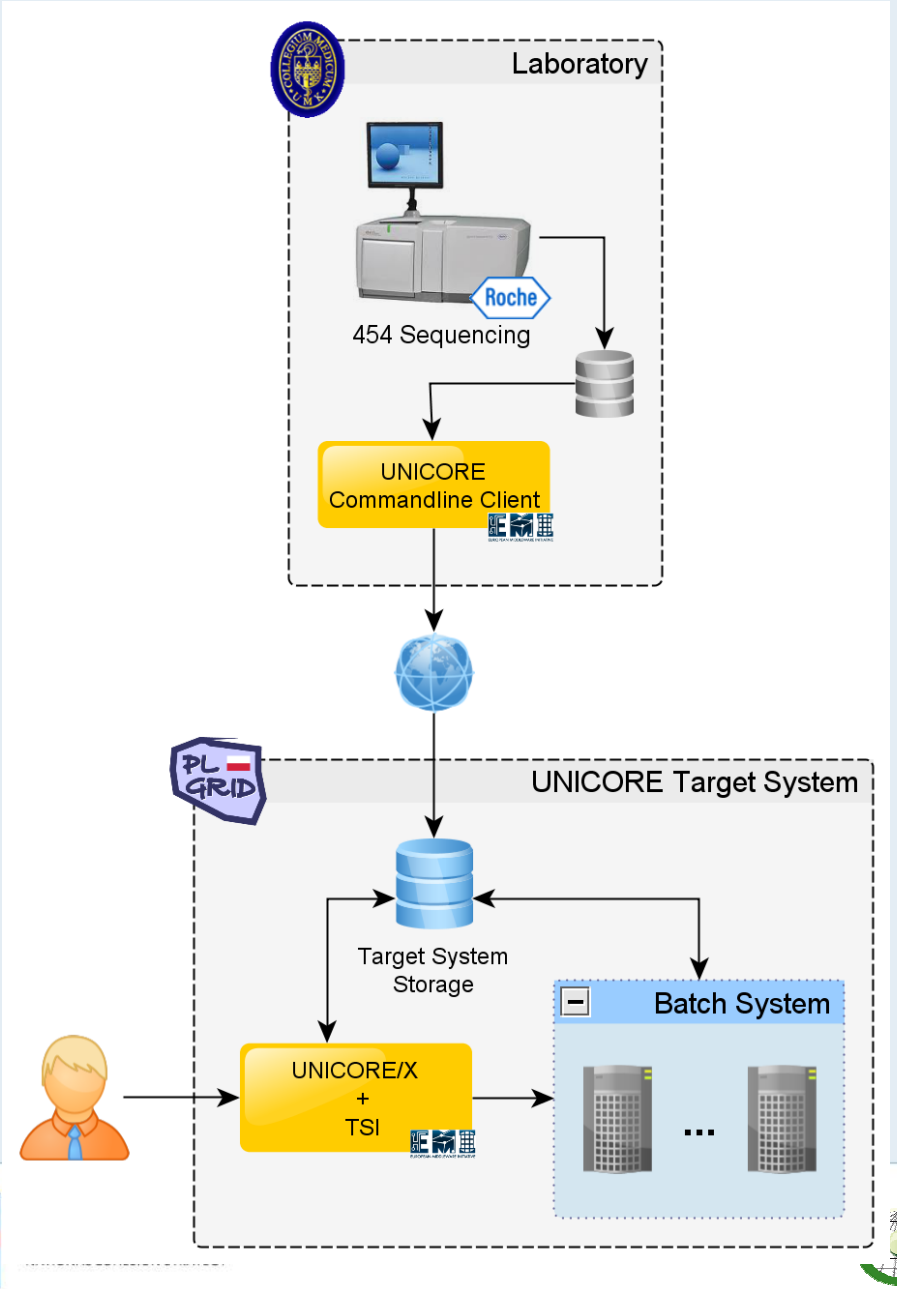



Storage ring requires a sufficiently large dynamic aperture in order to achieve high injection efficiency and long Touschek lifetime. In order to predict the performance of the storage ring, different simulations are done, e.g. to calculate the dynamic aperture in the 6D space, the frequency map analysis and diffusion maps analysis are made.**The Figure shows the diffusion map and frequency map for the electron bunch circulating in the storage ring. The diffusion is low for a blue color and for light blue where you see such circles it is a bit higher.**

# Bioinformatics

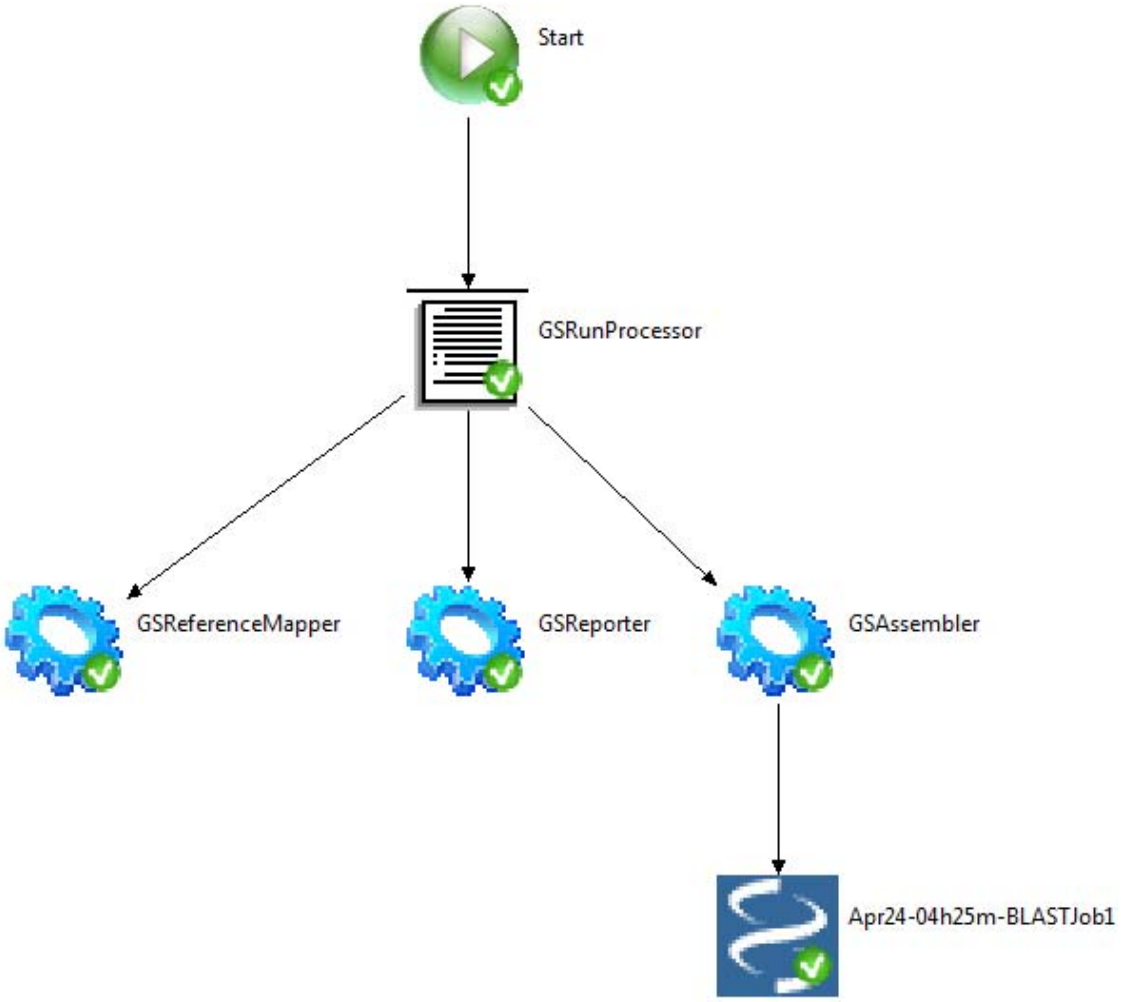
## Processing of DNA sequencing data




- High-throughput GS FLX Instrument (Roche Diagnostics)
- UNICORE Commandline Client (UFTP)
- Target System Storage (PL-Grid)
  - data storage
- Target System (PL-Grid)
  - workflow execution

# Bioinformatics

## Workflow for processing DNA sequencing data




PL-Grid allows to process data in 4h instead of 80h

- GS Run Processor
- GS Reporter
- GS Reference Mapper
- GS Assembler (run in parallel)
- BLAST

# Health
## Processing of medical images

An example result of the matching procedure visualized via volume rendering. Red image represents reference dataset that is transformed in the registration process, while the green image is the current object under examination. M Chlebiej *et al.*

- UNICORE Rich Client
- UNICORE Command line Client (UFTP)
- Web access

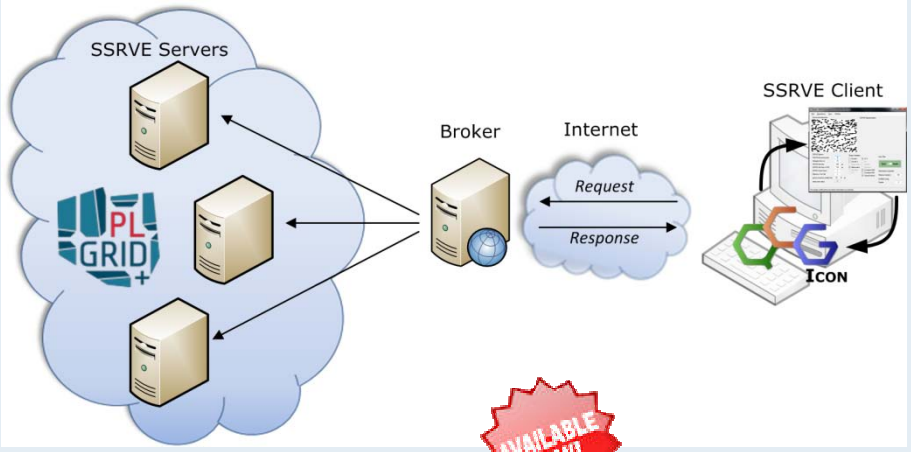
- UNICORE Storage (PL-Grid)
  - secure storage for medical images

- Target System (PL-Grid):
  - dedicated software to process medical images

# Metallurgy
## SSRVE – Existing Prototype

### SSRVE objective:

Creation of Grid Service, which supports creation of Statistically Similar Representative Volume Element by parallelization of optimization procedure allowing massive parallel calculations on grid infrastructure.




### SSRVE main workflow:

- SSRVE Client (MS Windows OS) – import of micrographs of dual phase steel, image processing, analysis of shapes coefficients, detection of histograms characteristics, export of *ssrve* input file, launch of QCG Icon,
- QCG Icon – automatic import of *ssrve* input file, configuration of a job (automatic configuration for basic and intermediate users is available, however all options can be set up by advanced users),
- SSRVE Server (Linux OS) – launch path includes *ssrve* file, which contains startup parameters for parallel optimization methods; the results are sent back to SSRVE Client.

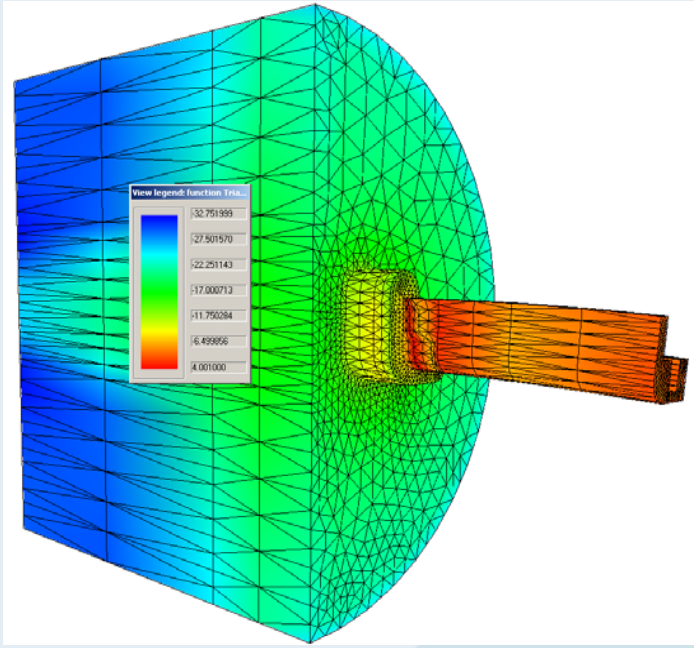
# Metallurgy

## Extrusion – Prototype for February 2013

### Main Objectives:

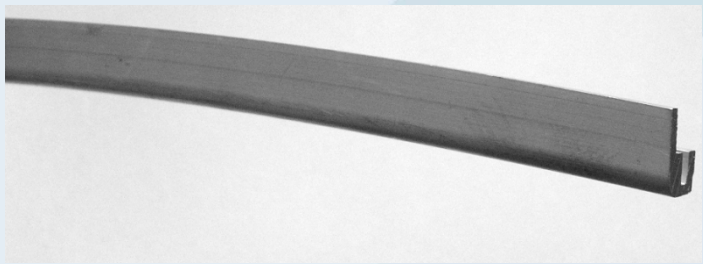
Support of engineers in demanding calculations for optimization of the metallurgical process of profiles extrusion. Optimization includes:

- shape of foramera,
- channel position on a die,
- calibration stripes,
- extrusion velocity, ingot temperatures, tools.



### Extrusion Service Realization:

- Implementation of parallel parts of Finite Element Method, used as the part on a Server side (implemented in Fortran),
- GUI will be created as Windows standalone application, integrated with QCG Icon (implemented in C++).



# Metallurgy

## MCMicro – Prototype planned in May 2013

### Main Objectives:

Material engineers support in numerical simulations of static recrystallization by using Monte Carlo approach.

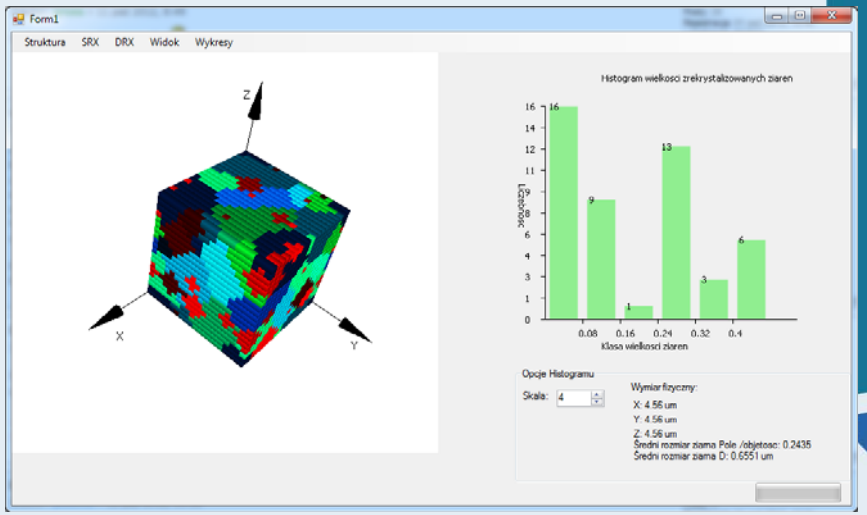
### Tasks:

- Implementation of graphical user interface for configuration of numerical calculations of the material model and visualization of obtained results,
- Implementation of module for generation of initial microstructure and export of input file for parallel calculations,
- Design and implementation of parallel Monte Carlo model for static recrystallization.

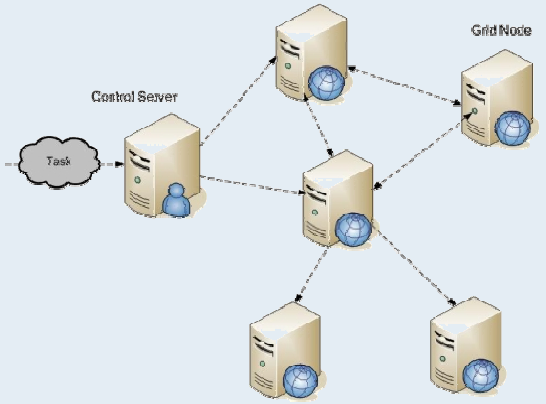
### Implementatoin issues:

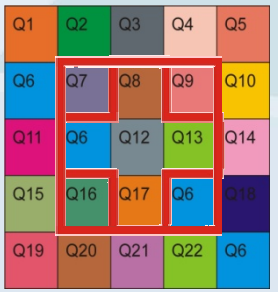
- Client's GUI – C++/CLI, ASP.NET,
- Server side – unmanaged C++, MPI.

Graphical User Interface on Client's Side




Parallel Model Calculation on Server's Side




$\Omega = \{Q_0, \ldots, Q_{n-1}\}$

# Ecology
## KIWI Eye (1.0) observation set

A set for automatic photo observations

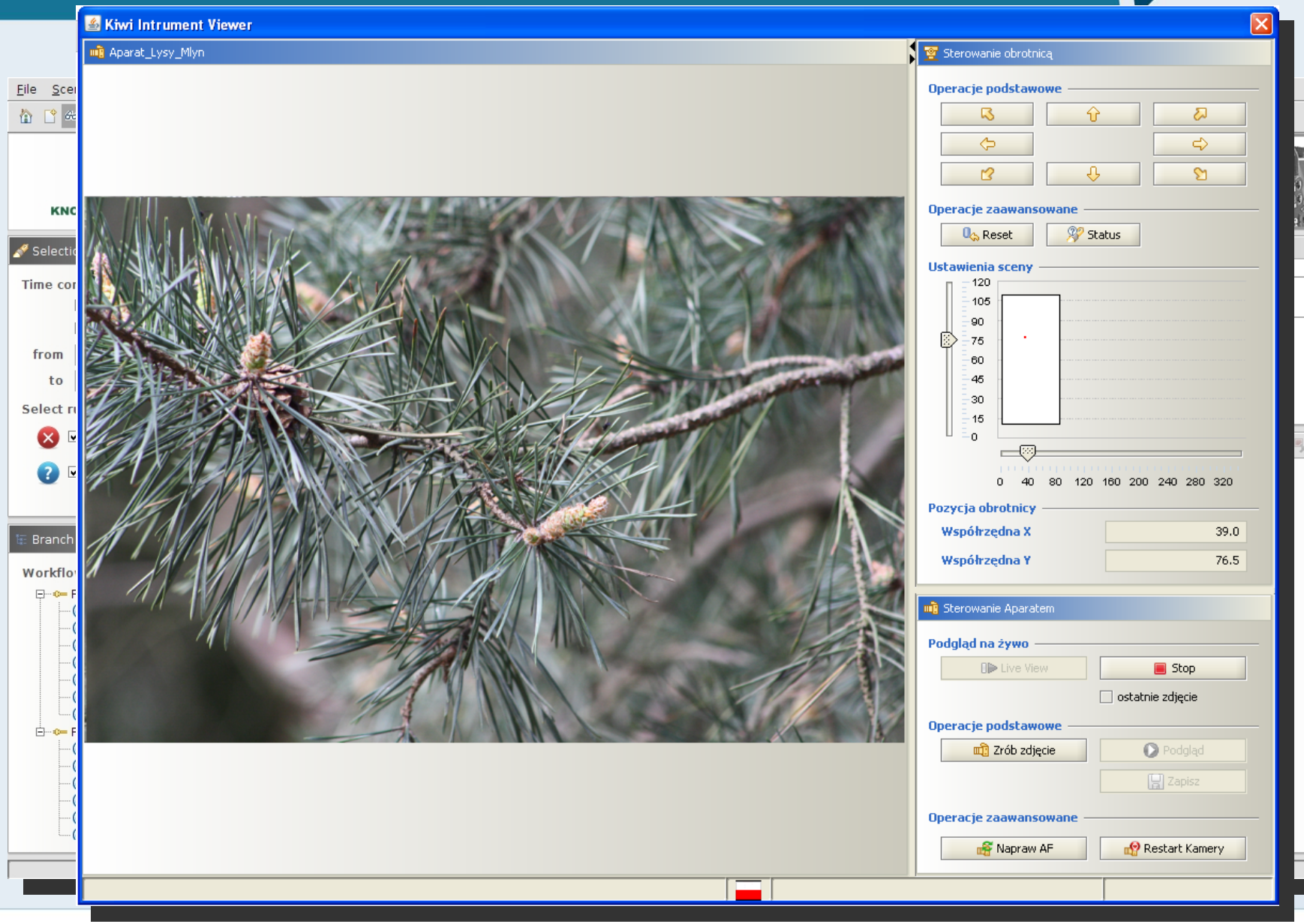
**Functionality:**

- Remote control of the camera
- Remote viewing of the video from the camera
- High resolution photos (DSLR type camera with interchangeable lenses)
- Scene and measuring points definition
- Workflow-type management software and remote access



# Ecology

## KIWI – workflows and remote access

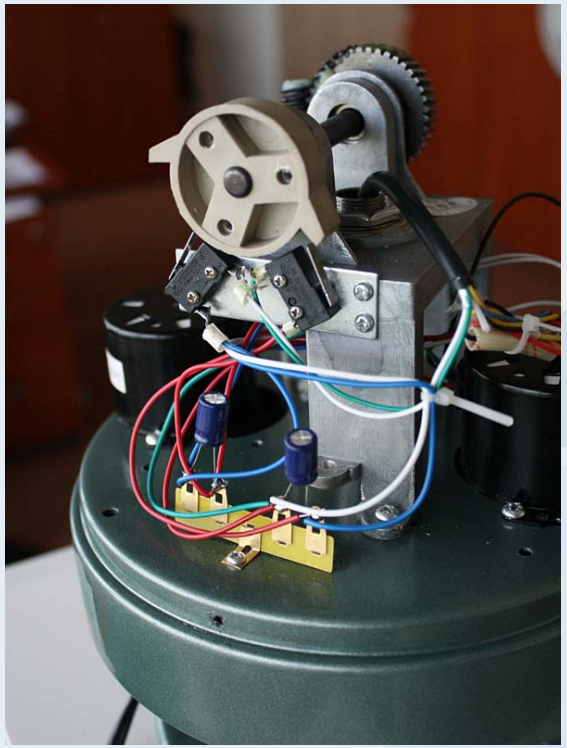


# Ecology

## KIWI – universal monitoring platform

Achievements:

- **KNOW-HOW** associated with the implementation of the observational sets for the **WLIN project**
- **Observation equipment**, hardware, software, materials, technologies, **problems and their solutions**

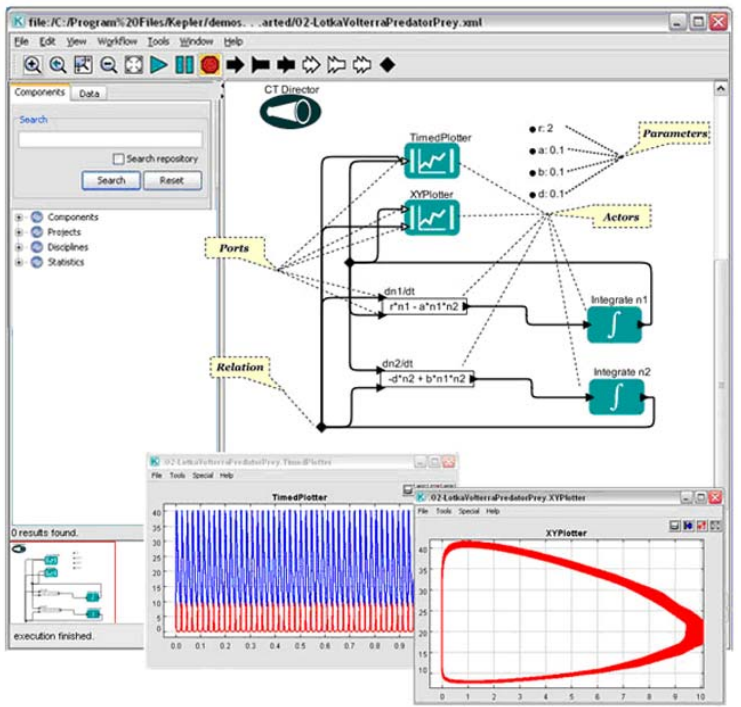
# AstroGrid-PL

- Whole-community astronomical grid
- Main Polish astronomical institutes involved CAMK PAN (coordinator), CA UMK, OA UJ and a few others
- Integrated platform for various areas of research
- Universal core services
- Data management very important in astronomy!
- Use of the Grid brings huge benefits (professional infrastructure, ease of data sharing, direct access from computational resources)
- Simple WWW & CLI interfaces for advanced data/metadata management (e.g. data receiving and archiving, cataloguing, sharing raw data or catalogues)
- Dedicated support for specific instrumental projects
- iRods solution is being considered & tested
- This service is basis for other services

# AstroGrid-PL core sevices

## Polish Virtual Observatory and Workflow Environment for Astronomy

- The Virtual Observatory (VObs) is an international astronomical community-based initiative aiming to provide transparent and distributed access to data available worldwide. The VObs consists of a collection of data centers each with unique collections of astronomical data, software systems and processing capabilities.
- Service goals:
  - Setup National VObs Data Center, integration of Polish data and join international efforst
- Workflow Environment
  - Provide astronomers with workflow environment
  - Enable easy resource switching: desktop – cluster – grid
  - Library of template scenarios for popular activities
  - Dedicated support for selected projects
  - Kepler environment is being tested...
- Universal Fluid Dynamics code Piernik



# Conclusions

- Further developement needed, as identified currently, mainly on Domain Specific Grids
- Request from the users' communities
- Capacity for organization of future development according to
  - Expertise and experience
  - Strong scientific potential of the users' communities being represented by PL-Grid Consortium
  - Wide international cooperation concerning the Consortium and individual Partners, good recognition worldwide
  - Good managerial capacity

- **Please visit our Web page: http://www.plgrid.pl/en**
- Credits

# Credits

- ACC Cyfronet AGH
  - Kazimierz Wiatr
  - Michał Turała
  - Marian Bubak
  - Krzysztof Zieliński
  - Karol Krawentek
  - Agnieszka Szymańska
  - Maciej Twardy
  - Teresa Ozga
  - Angelika Zaleska-Walterbach
  - Andrzej Oziębło
  - Zofia Mosurska
  - Marcin Radecki
  - Renata Słota
  - Tomasz Gubała
  - Darin Nikolow
  - Aleksandra Pałuk
  - Patryk Lasoń
  - Marek Magryś
  - Łukasz Flis
- ICM
  - Marek Niezgódka
  - Piotr Bała
  - Maciej Filocha
- PCSS
  - Maciej Stroiński
  - Norbert Meyer
  - Krzysztof Kurowski
  - Bartek Palak
  - Tomasz Piontek
  - Dawid Szejnfeld
  - Paweł Wolniewicz
- WCSS
  - Jerzy Janyszek
  - Paweł Tykierko
  - Paweł Dziekoński
  - Bartłomiej Balcerek
- TASK
  - Rafał Tylman
  - Mścislaw Nakonieczny
  - Jarosław  Rybicki

… and many others….

# Old slides

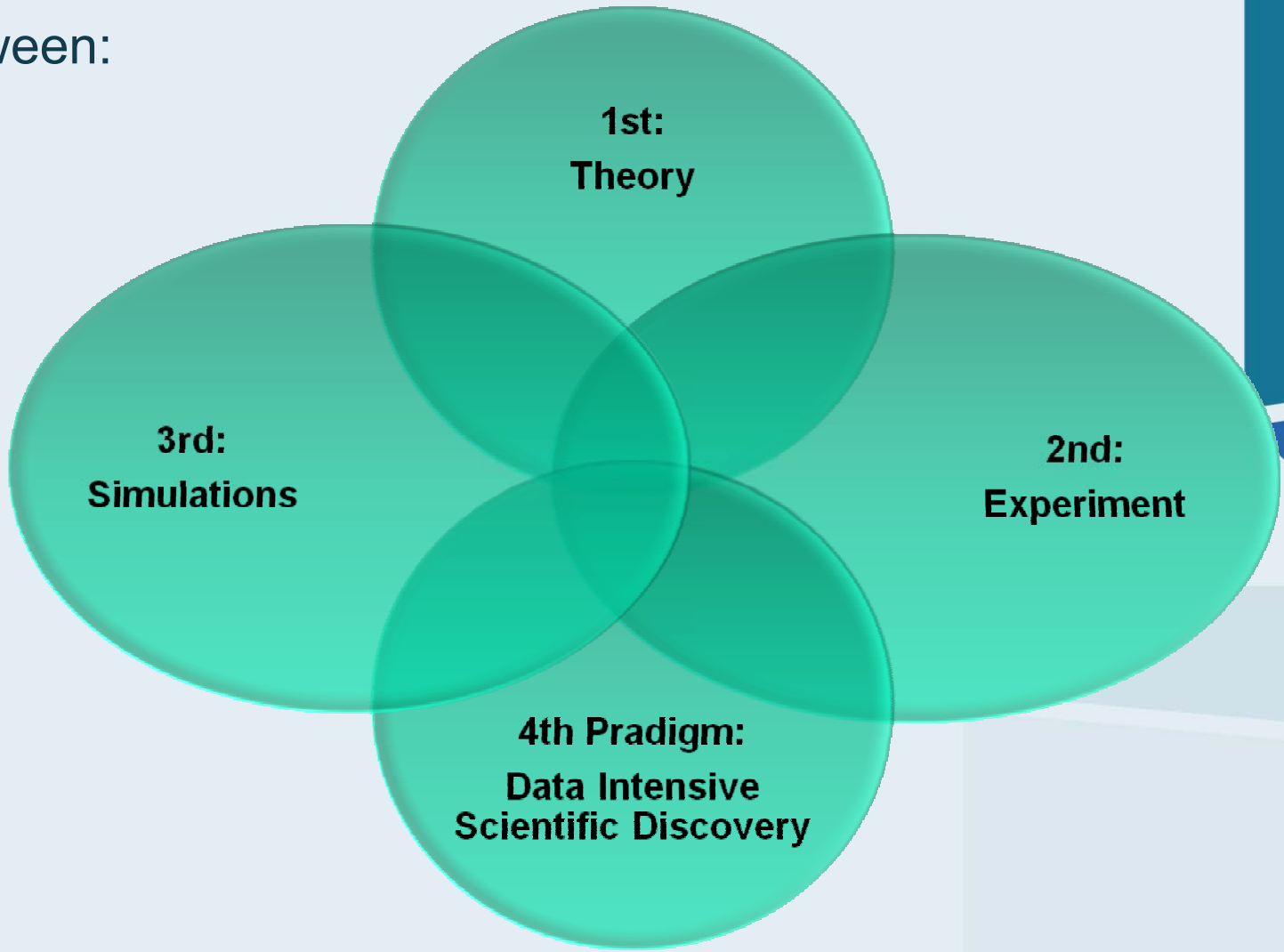
Old slides

# E-Science: Experiments in Silico

## Research Paradigms

Required Synergy between:

- Theory
- Simulation
- Experiment
- Data analysis



# Existing and Planned Resources

- Current PL-Grid resources:
  - 260 TFLOPs of CPU
  - 3.3 PB of storage

- Planned resource extension for PLGrid Plus
  - ca. 500 TFLOPs of CPU
  - ca. 4.4 PB of storage
- Accompanying equipment

# Extension of Computing Environment

- Keeping diversity
  - Clusters (thin and thick nodes)
  - Clusters with GPGPU
  - SMP machines
  - vSMP

# New Services in PLGrid Plus
(as defined in the Proposal)

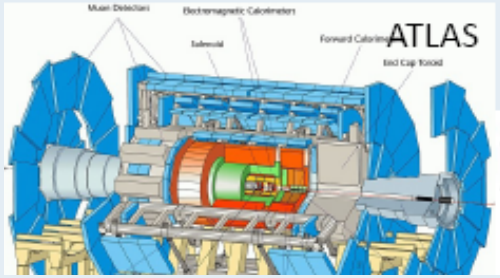
- **Cloud Computing** for Polish Science – new computing paradigm foreseen as a natural extension of the current Infrastructure offer
- **Platform for supporting e-Science**, resulting from the need for an international cooperation between various disciplines of scientific domains
- **Production infrastructure** oriented towards **domain specific services**, tools, environments and software packages
- **Professional support for specific disciplines** and topics important for Polish e-Science
- **Visualisation** of the scientific results via shared infrastructure servers equipped with possibility of binding domain specific visualisation tools

# Innovative Infrastructure Environment

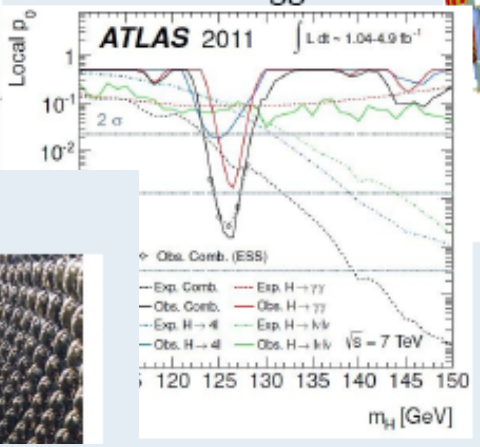
## PL-Grid extensions

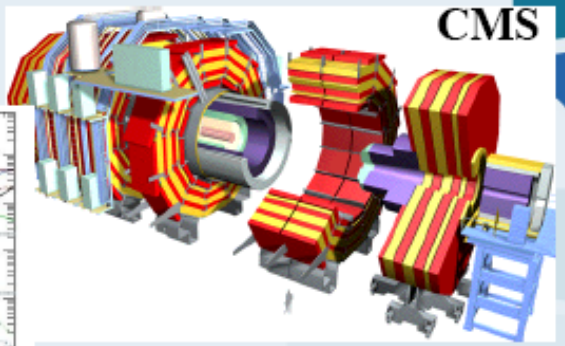
- Efficient Resource Allocation
  - **Grid Resource Bazaar**, mobile access to the infrastructure, new security modules and other tools for users and systems administrators, management of users request
- Experimental Workbenchs
  - **GridSpace2** platform extension for supporting for new domains and integration with new grid/cloud services
  - **InSilicoLab** – integrated environment for chemists and biologists
- Tools and Middleware
  - **Migrating Desktop**, **VineToolkit** and **gEclipse** tools integration with various PL-Grid domain services
  - **QStorMan Toolkit** – extension for domain requirements on optimization of data access
  - **QosCosGrid** continuation of development
  - Liferay **Portal** framework(s) – adoption to specific needs
  - **HelpDesk** Portal for the users (specialized versions)

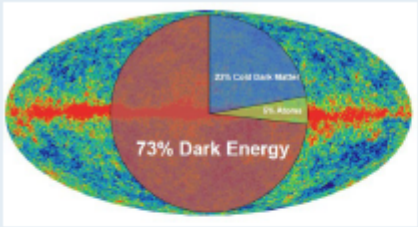
# HEP



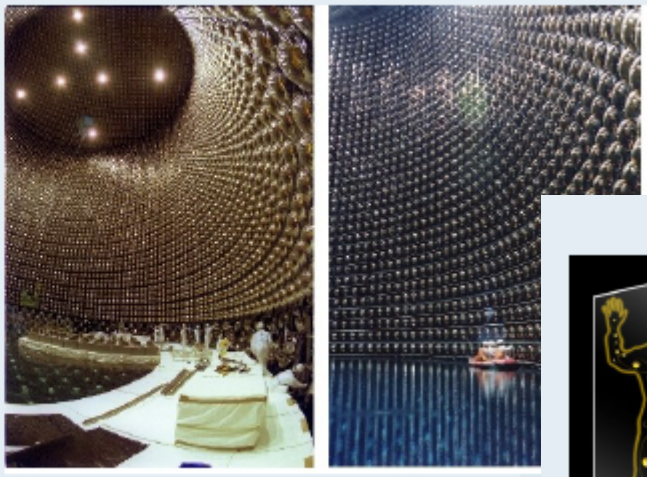

Bozon Higgsa?

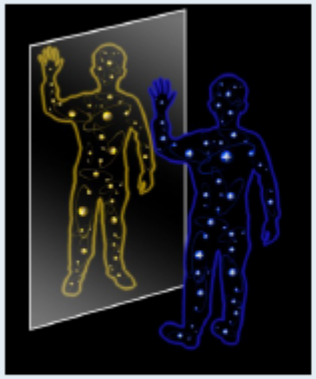


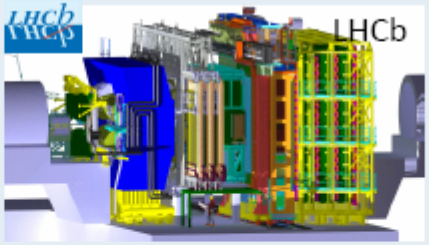



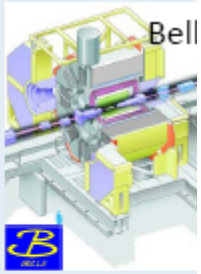



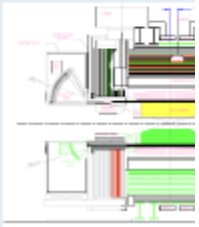

Eksperyment T2K



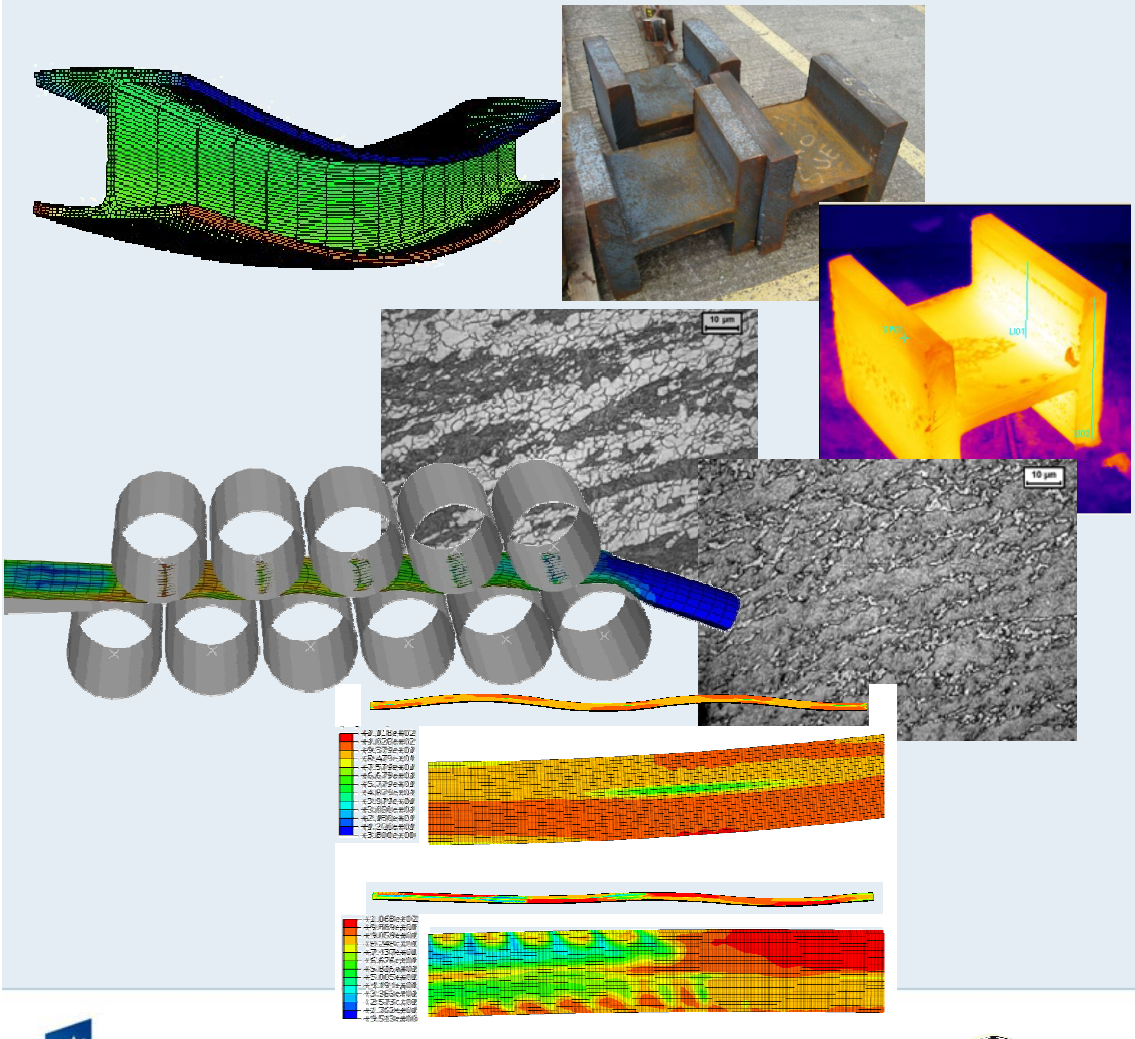


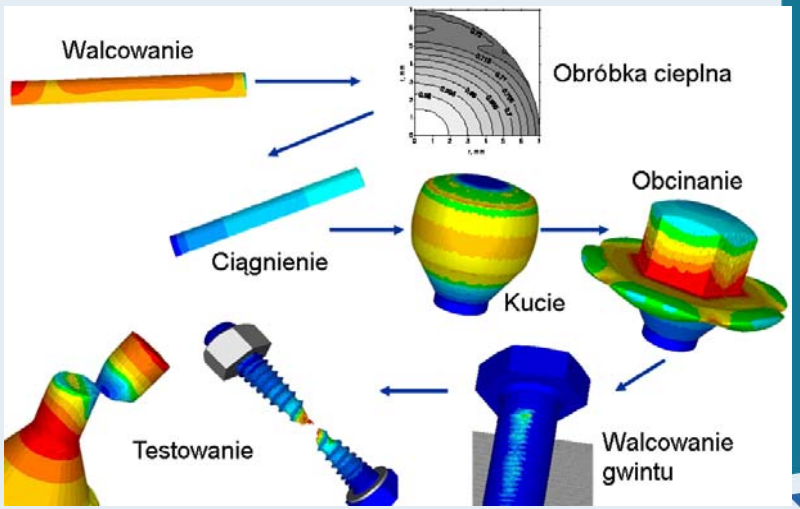



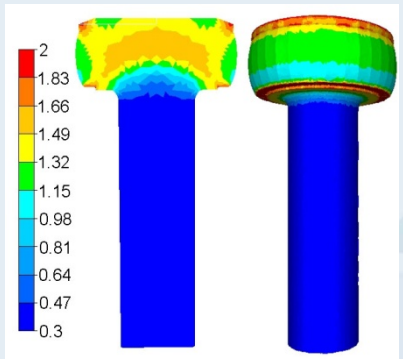



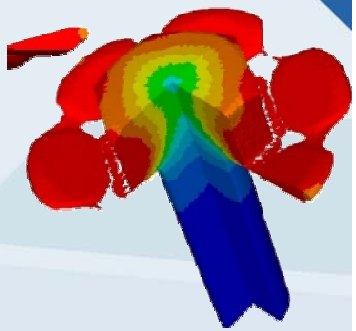
# Metallurgy

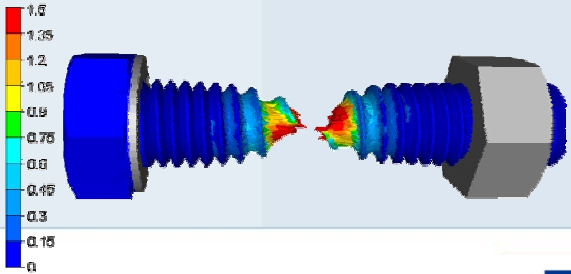
## Modelling of different kind of processes



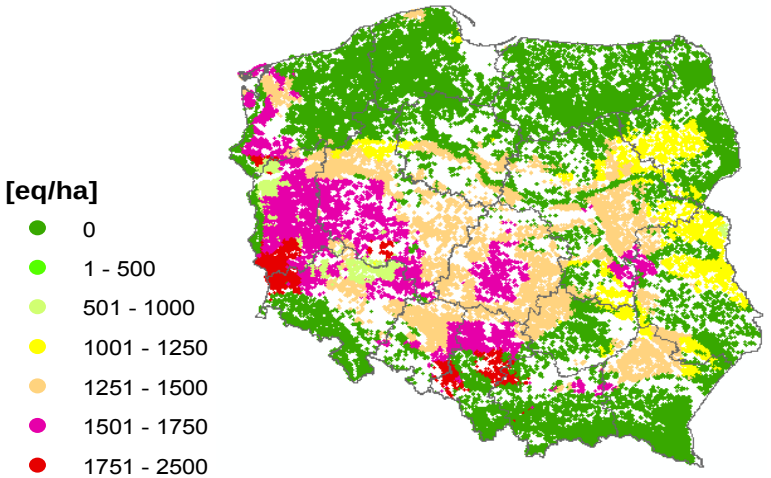


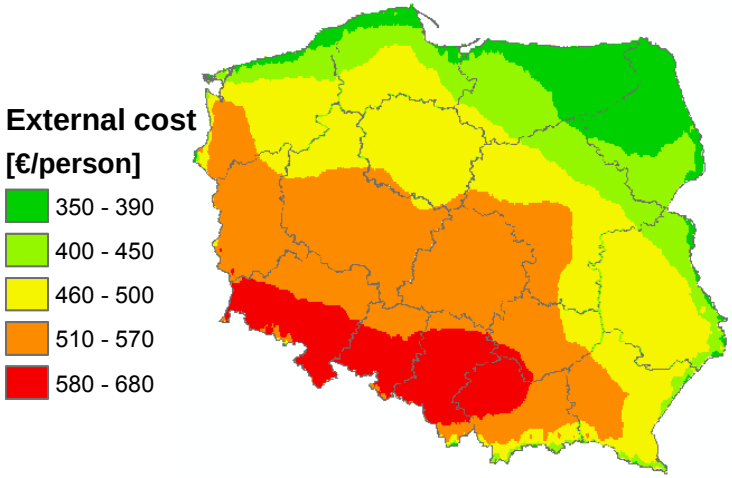





# Model for Assessment of Environmental & Health Impacts



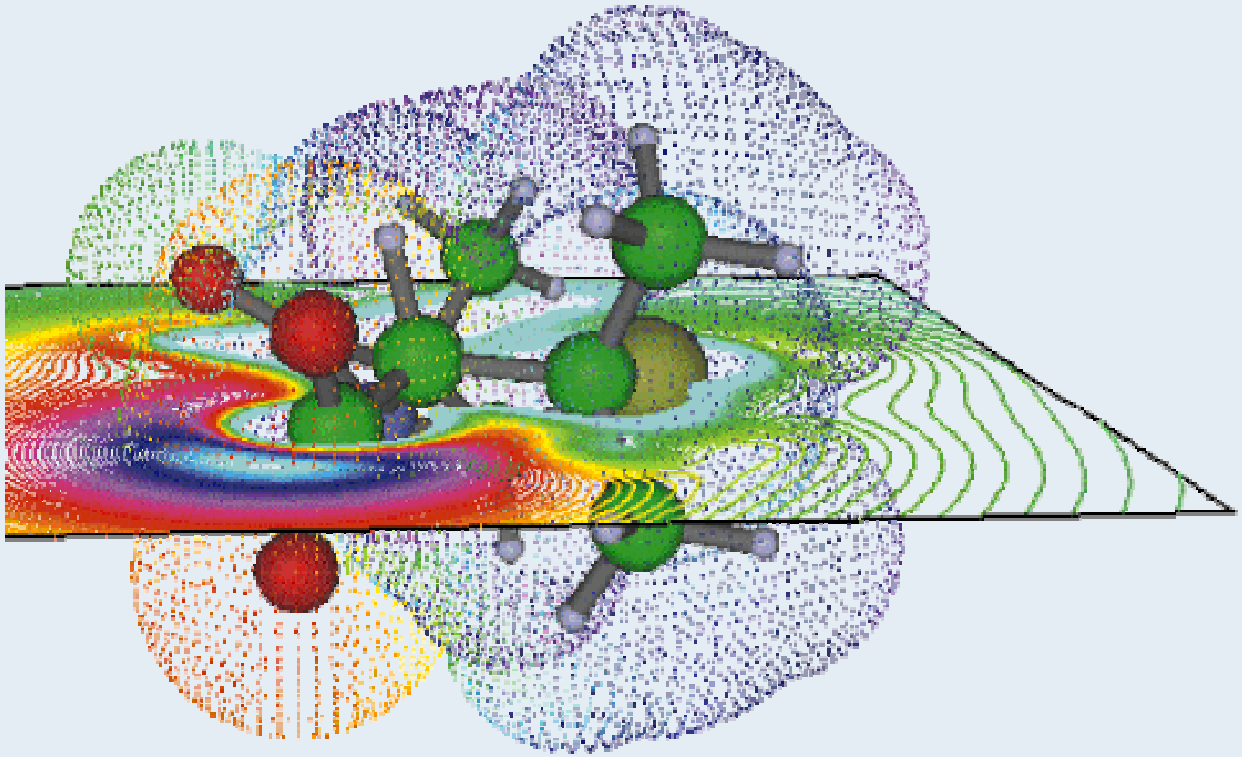

Exceedances of critical loads of acidity- 2005




External costs estimated for 2005

# Quantum Chemistry

## New original algorithms



$$H \Psi = E \Psi$$

# Nanotechnology


## Introduction to AuxEx

# Nanotechnology
## The AuxEx name

Auxiliar Experimentorum – Latin experimental assistant

In the Middle Ages it was believed that the Roman roads and aqueducts were built by giants. In fact, they were created by legions, the great builders of Rome.

The name of the service recalls the Roman auxiliary troops.

The basic goal is to build an application assisting in the daily work of experimentalists.


Downloaded from http://broeder10.wordpress.com 15.10.2012