

Polish Infrastructure for Supporting Computational Science in the European Research Space

UNICORE deployment in Polish NGI Lesson learned

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PL-Grid

- National Grid Initiative
- Partners:
 - Polish supercomputer centers
 - CYFRONET, ICM, PCSS, WCSS, TASK
- Project goals was:
 - Build and operate Polish National Grid
 - Provide training and user's support
 - Provide support for application deployment on the Grid
- ICM in PL-Grid
 - Training
 - Application support
 - UNICORE Operating Center

TOP500 List - November 2011

Cyfronet Poland Cluster Platform 3000 BL 2x220, Xeon X5650 6C 2.66 GHz, Infiniband / 2011

15264

128.79

162.41





PL-Grid resources

PL-Grid resources

Number of cores: 23 616

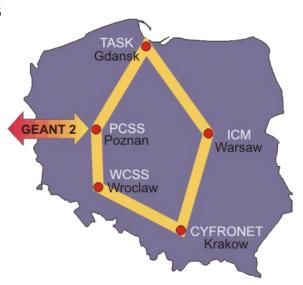
◆ CPU: 230,16 TFlops

◆ Disk: 3,6 PB

♦ Memory: 51,33 TB

Additional resources can be committed by partners

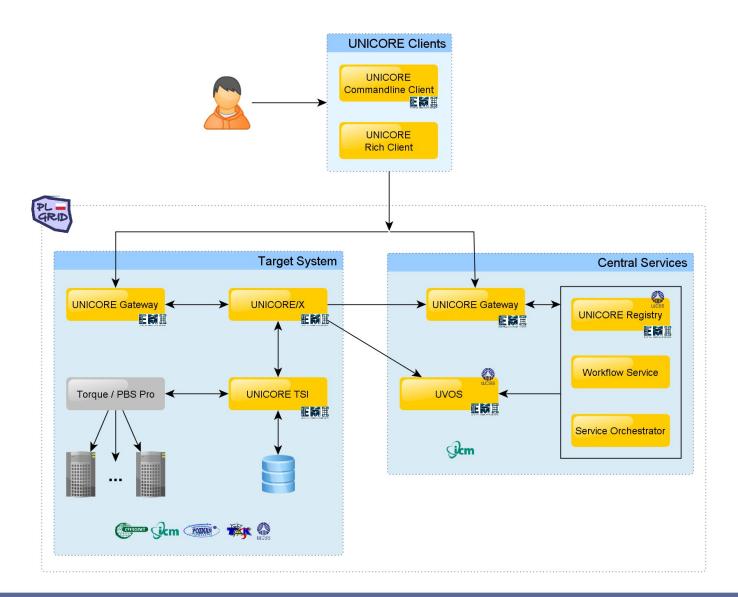
- UNICORE installed in all 5 centers
 - Services have to be maintained till 2017
- UNICORE central services run by ICM
 - Backup copy of Registry and UVOS run by WCSS





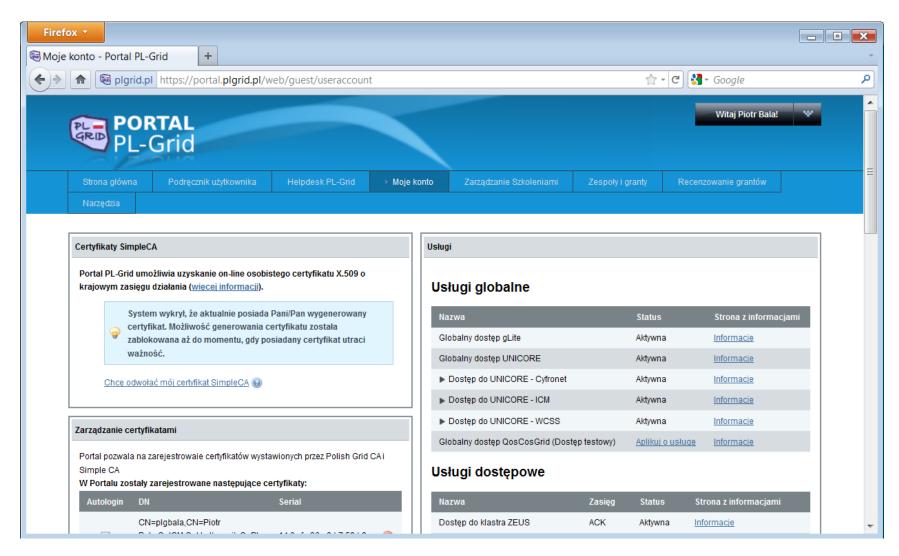


UNICORE Production Infrastructure





Integration with PL-Grid Portal

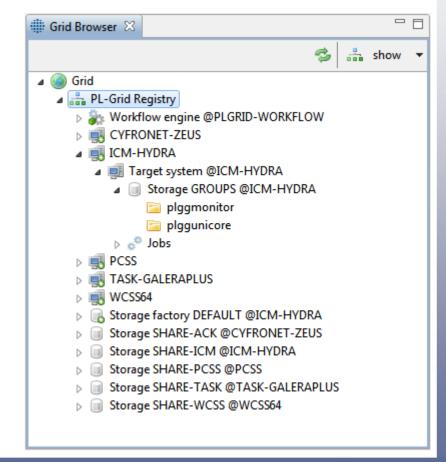






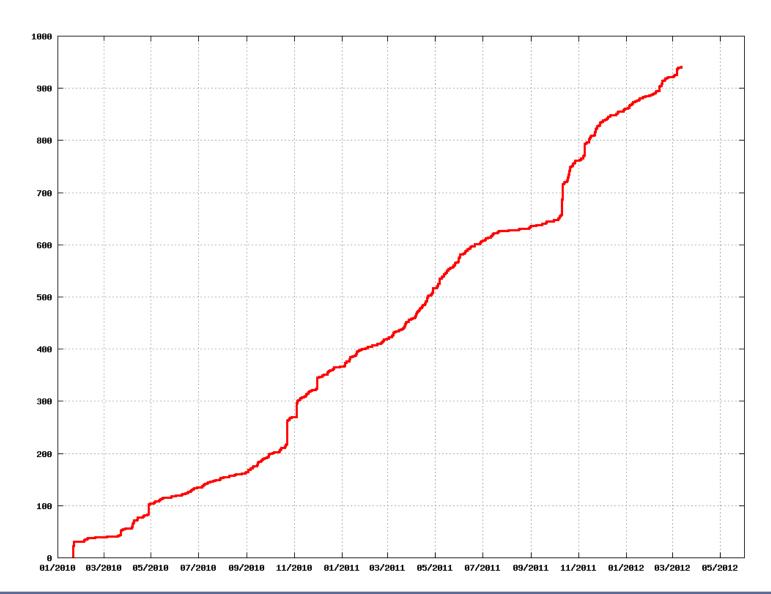
What User Needs to Know

- PL-Grid portal is central service responsible for users managements
 - Users registration
 - Integrated service of certificates issuing (PL-Grid Simple CA)
 - Certificate registration
 - Activation of UNICORE access
 - UNICORE e-learning materials
 - Scientific groups management
- http://helpdesk.plgrid.pl
 - When there are problems
- Grid Resource Bazaar
 - Groups' grants application
 - Only for groups' coordinators





Number of PL-Grid Users

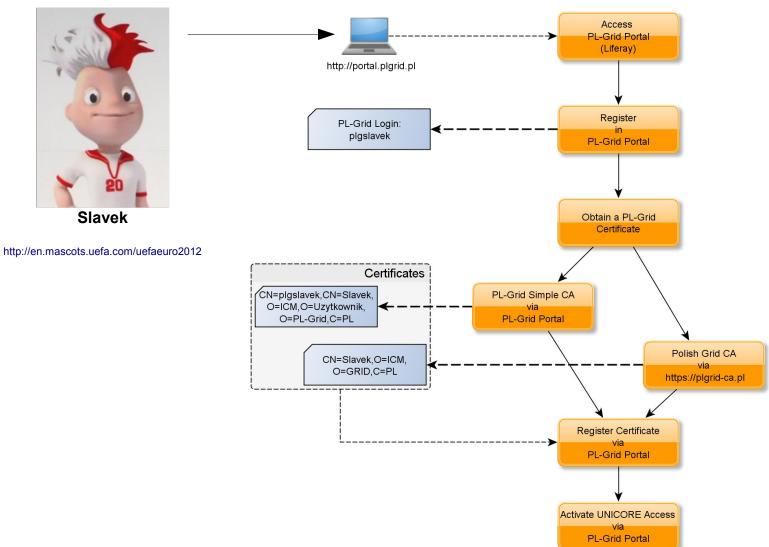








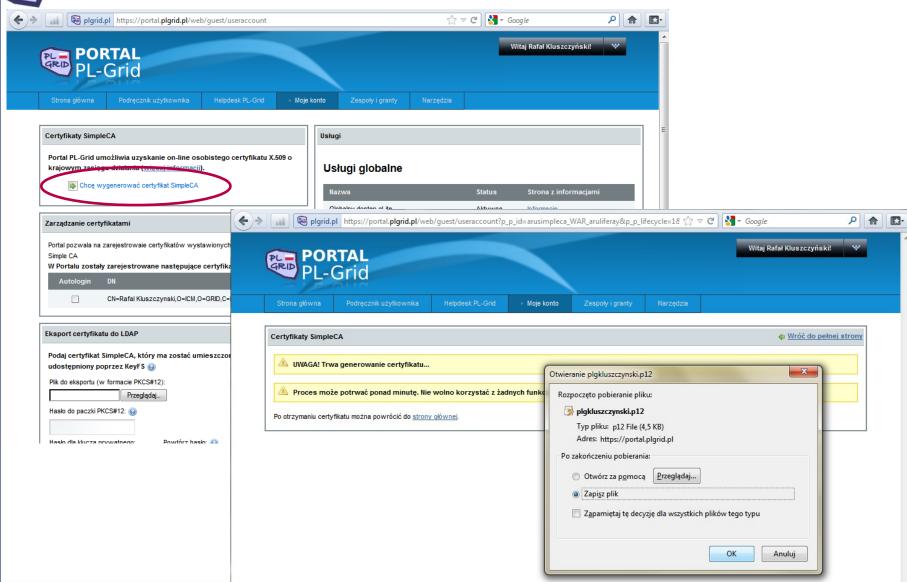
Getting Access to PL-Grid by Users







PL-Grid Simple CA Certificates



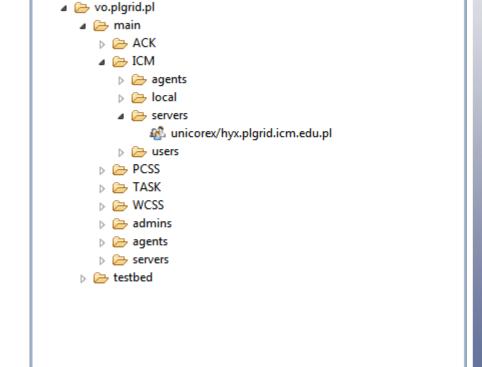






UVOS as UNICORE Attribute Source

- PL-Grid uses UVOS (UNICORE VO System) as users attribute source
 - Each site has its own branch
 - Site administrator may change roles and Xlogins of his branch
- UNICORE components in PL-Grid use "pull mode" of authorization
- For other tools UVOS server web authentication extensions is used
 - UNICORE accounting portal
- Second UVOS is run by WCSS for fail-over scenario



VOs Browser () Entities Browser

PLGridMainUVOS



INNOVATIVE ECONOMY

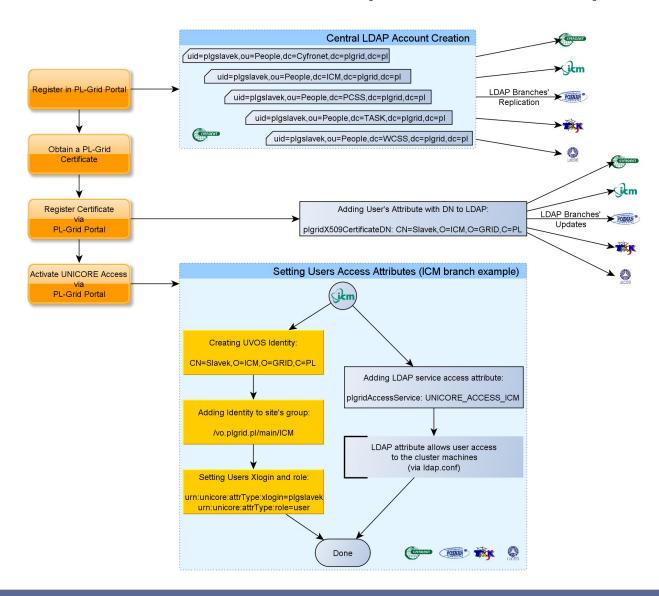


R.Kluszczyński

ॐ ₩ ← → □ □



Behind the Scenes (LDAP & UVOS)





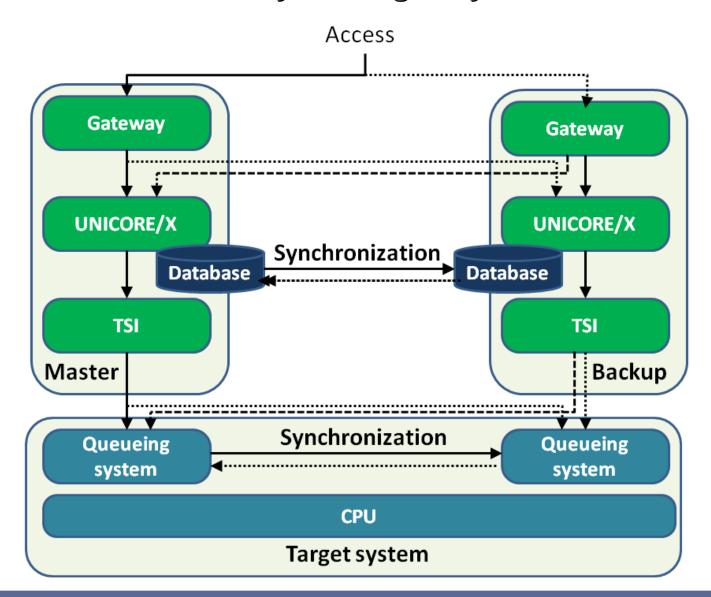
Reliability of Services

- ◆ In order to maintain reliability of services we need to:
 - Configure HA of services
 - Perform tests of release candidates
- Main central services redundancy run by another site WCSS (fail-over scenario)
- Target system services redundancy run by ICM (fail-over scenario of UNICORE/X and TSI services)
- Testing Infrastructure
 - Very important (!)
 - Allows to develop new tools and test new configurations and updates
 - Two dedicated virtual target systems:
 - ICM, University of Warsaw
 - NCU, Department of Mathematics and Computer Science in Toruń
 - Integrated with the production UVOS but with dedicated branch





Reliability of Target Systems





UNICORE Monitoring Infrastructure

- Based on Nagios probes
- Integrated with EGI
 - UNICORE GOCDB Types
 - Alarms escalation to Dashboard EGI
 - Included working probes in SAM 17 (announced as internal release):
 - emi.unicore.Gateway
 - emi.unicore.Registry
 - emi.unicore.TargetSystemFactory
 - emi.unicore.GlobalStorage
 - emi.unicore.UVOS
 - emi.unicore.ServiceOrchestartor
 - emi.unicore.WorkflowService
 - PL-Grid participate in Stage Rollout procedure of SAM

GOCDB Types:

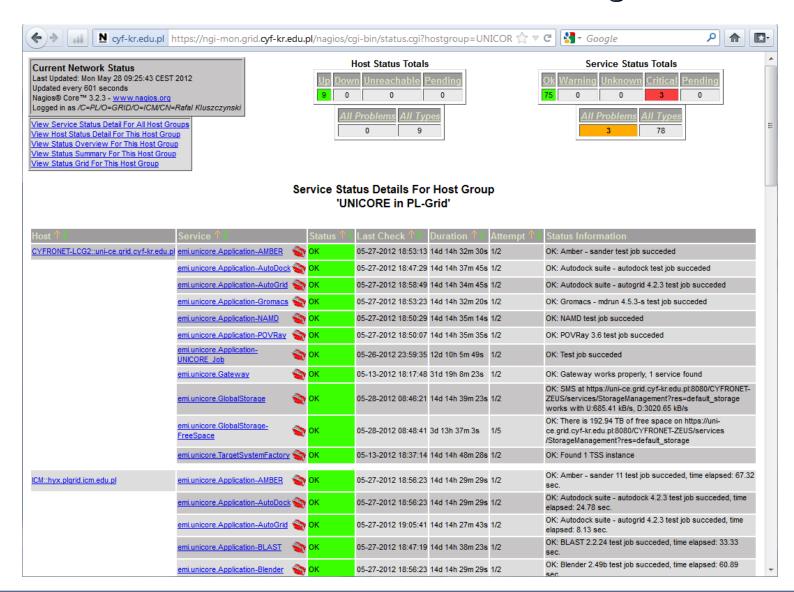
unicore6.Gateway
unicore6.Registry
unicore6.ServiceOrchestrator
unicore6.StorageFactory
unicore6.StorageManagement
unicore6.TargetSystemFactory
unicore6.UVOSAssertionQueryService
unicore6.WorkflowFactory

- Additional probes used in PL-Grid:
 - emi.unicore.UNICORE_Job, emi.unicore.GridWorkflow, emi.unicore.StorageFactory
 - emi.unicore.Application: Amber, AutoGrid, BLAST, Blender, Cfour, Clustal, Fluent, Gaussian, Gromacs, Lammps, Matlab, Mopac, Meep, NAMD, NWChem, NetLogo, Nmag, POVRay, R
 - LogWatcher for UNICORE





UNICORE Services Status in Nagios

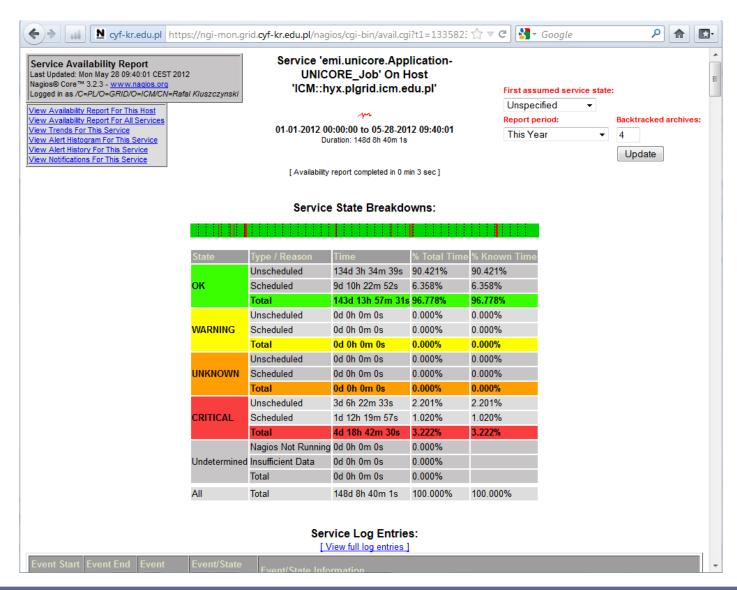








Nagios Availability Report







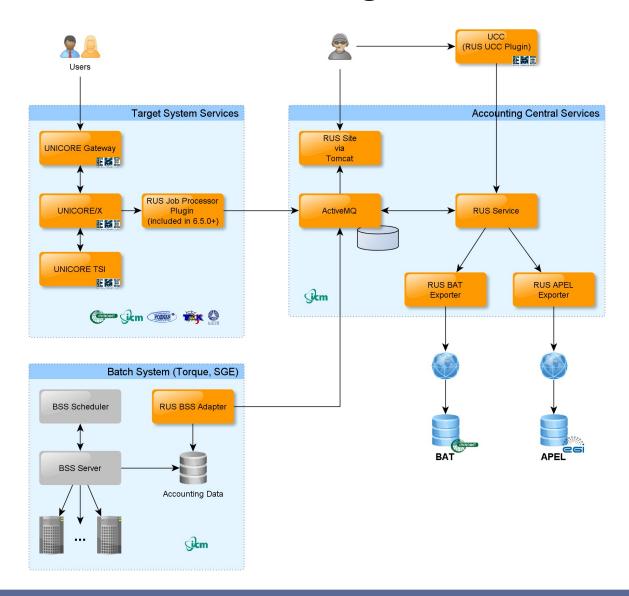
UNICORE Accounting

- Integrated with the PL-Grid Infrastructure
- Central Accounting Services:
 - RUS Service processes accounting data
 - RUS BAT Exporter publishing accounting data to national PL-Grid database
 - RUS Site accounting portal allowing to access data and statistics
 - ActiveMQ broker for storing messages
- Target System Services:
 - ♦ RUS Job Processor sends grid level accounting information about jobs
 - Included in UNICORE/X 6.5.0+
 - RUS BSSAdapter processing BSS accounting data based on log files
- RUS UCC Plugin allows to access data from command line and also to reprocess defined accounting data for exporters
- RUS APEL Exporter almost ready to publish accounting data to EGI database



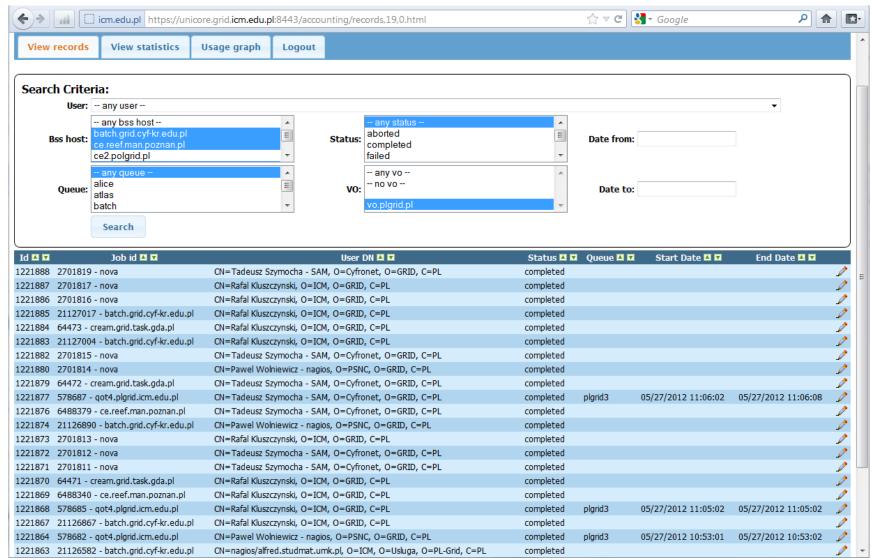


UNICORE Accounting Infrastructure





UNICORE Accounting Portal

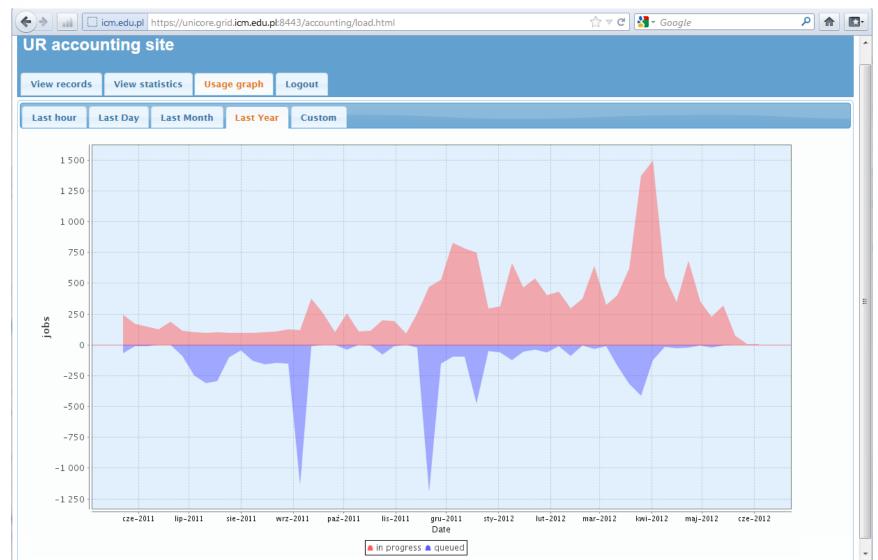








Usage Graph In Accounting Portal





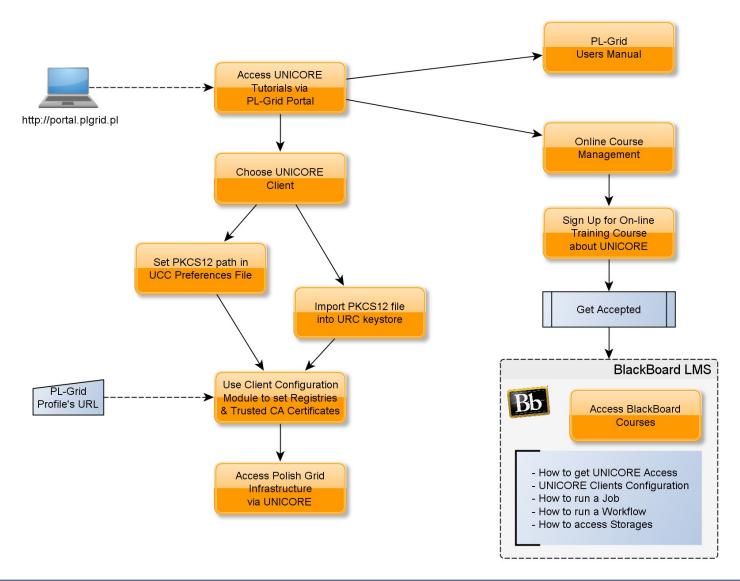
UNICORE Trainings

- PL-Grid portal support also organization of user trainings
 - Users register accounts available only for training
 - Organizer determines which services should users have (like "UNICORE Access")
- On-line course management
 - PL-Grid portal allows to apply for a course
 - Courses are integrated with BlackBoard
 - Many UNICORE tutorials like:
 - Getting UNICORE access in PL-Grid
 - UNICORE clients configuration
 - Running jobs and workflows with UNICORE
 - Accessing storage in UNICORE
- PL-Grid Users Manual available in PL-Grid Portal





Users' First UNICORE Access







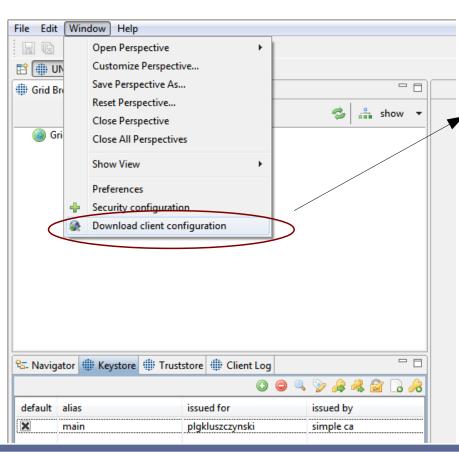
Client Configuration Manager (CCM)

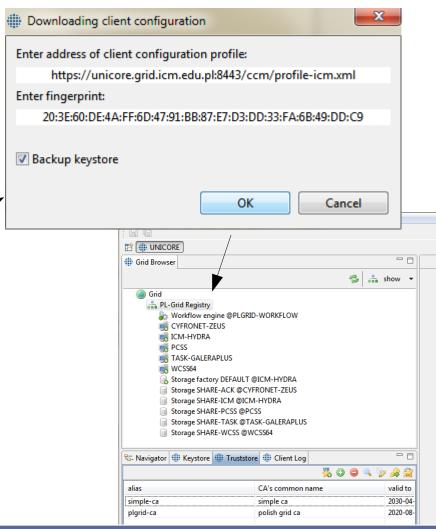
CCM allows to set quickly users' Grid environment by XML profile file:

Adds registries

Adds trusted CA certificates

Adds UNICORE clients extensions









Scientific Groups Support

- Scientific experiments often need collaboration
- PL-Grid offers support for scientific groups
 - Separate documents folder, forum and wiki portlets in PL-Grid portal
 - Storage accessible by all group members (via Target System Storage)
- Users can form a scientific groups:
 - Every group has a coordinator
 - Coordinator may apply for a grant
 - Grants are assigned to scientific groups (max. walltime, storage size)
- Every user has his personal grant at start to be able to use the Grid



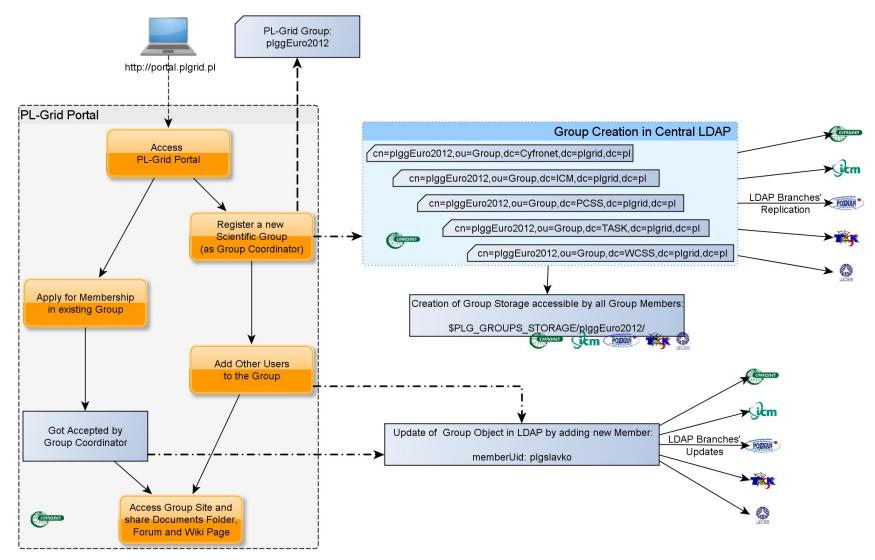








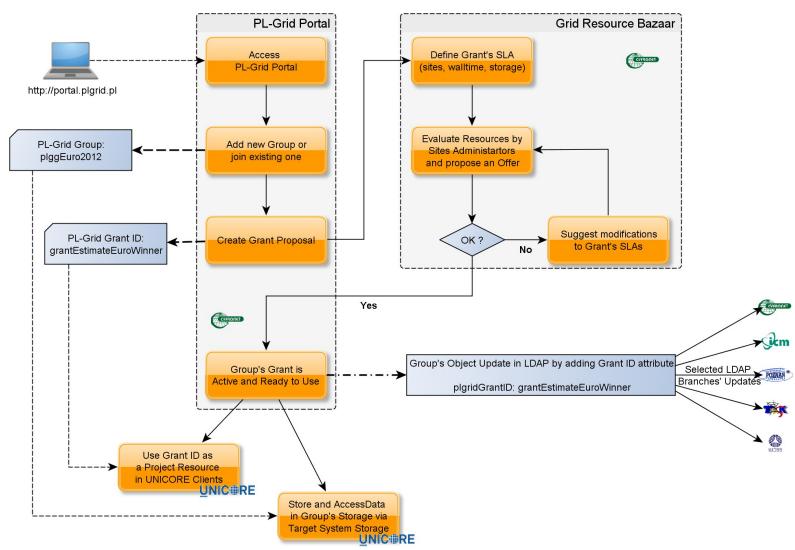
Scientific Group Registration





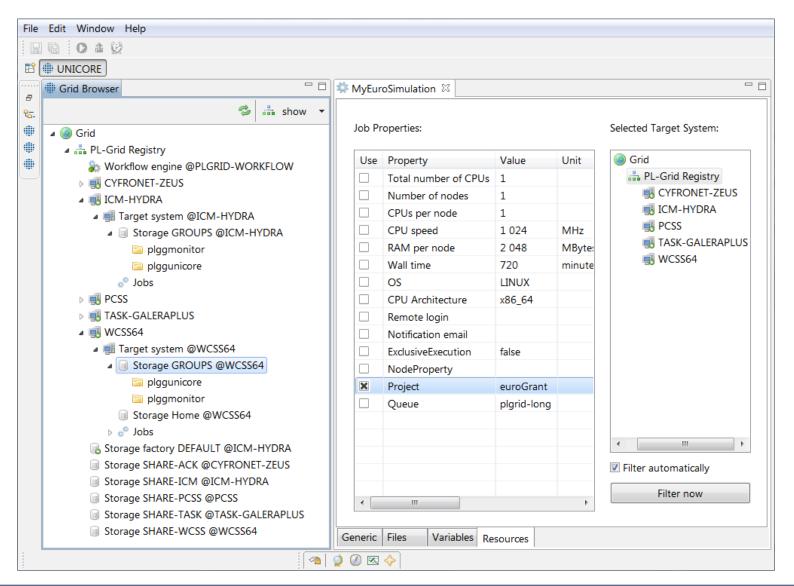


Group's Grant Application



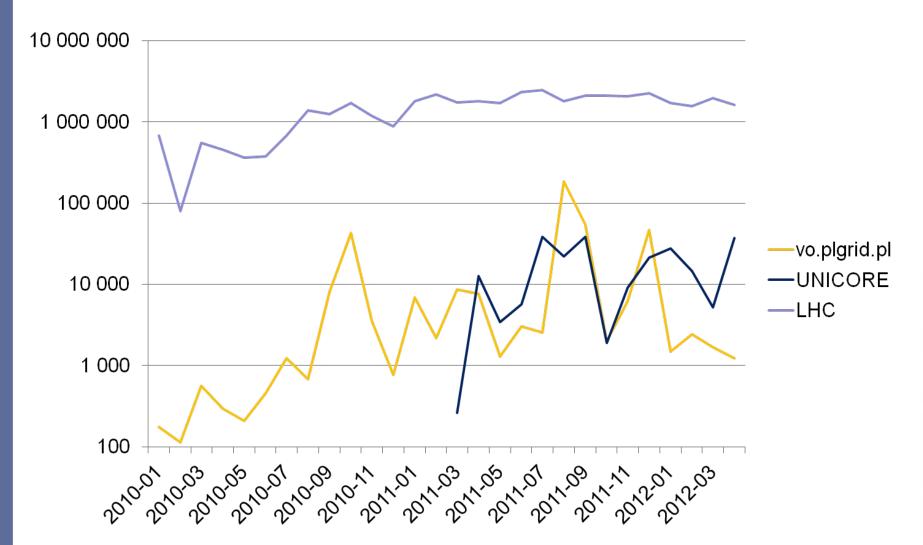


Groups and Grants in URC





PL-Grid Usage (walltime hours)



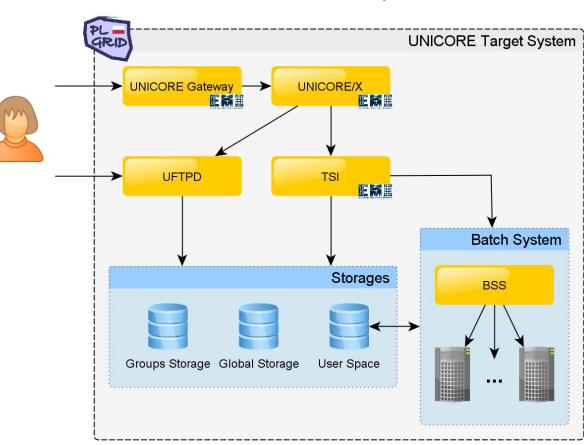






Example – Processing of Genetic Data

- Department of Molecular and Forensic Genetics, Institute of Forensic Medicine, Ludwik Rydygier Collegium Medicum, Nicolaus Copernicus University
- The Postgraduate School of Molecular Medicine, Medical University of Warsaw
- Analysis of patients' mtDNA having colorectal cancer (mutation identification)
- GS FLX Instrument (Roche Diagnostics) and its software
- Thanks for UNICORE
 File Transfer Daemon
 and UFTP clients
 support!

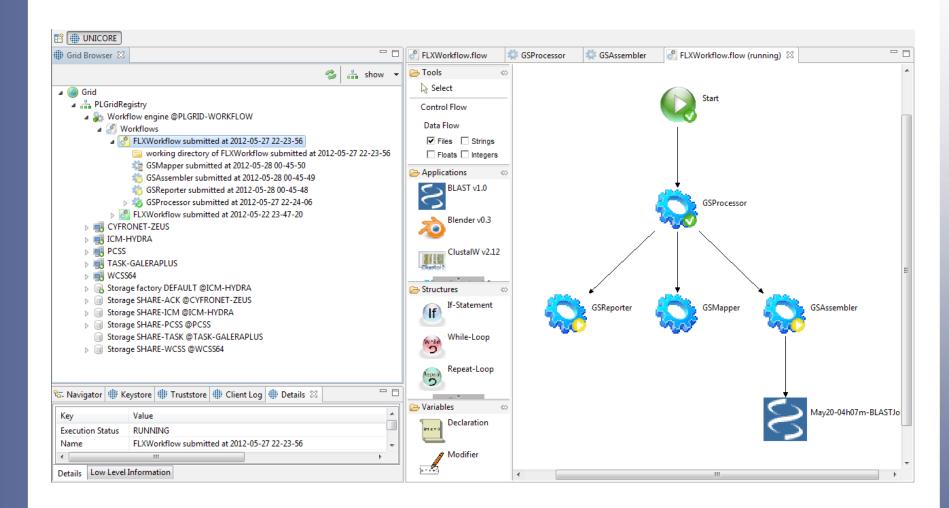








Experiment's Workflow





PL-Grid Plus

- 3 Year Project
- Focus on applications
- ICM coordinates 3 domain Grids:
 - Bioinformatics
 - Health and medicine
 - Material sciences
- Science gateways:
 - Still open issue
 - Hosted in Liferay portal

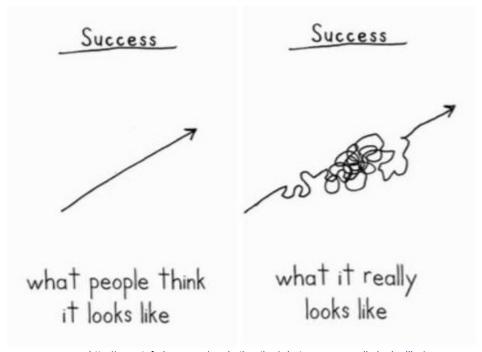






PL-Grid Plus

♦ Hopefully, it will also end with a success...



http://www.tofurious.com/marketing-tips/what-success-really-looks-like/





Many THANKS!

- What do we appreciate?
 - UNICORE itself;)
 - UNICORE Clients (URC, UCC)
 - UNICORE File Transfer Daemon !
 - RPM packages !
 (it really boosted deployment and is helping in maintaining services)



- Who do we thanks?
 - All UNICORE Team for a great support
 - B.Schuler and B.Demuth for suggestions and taking into account our requests
 - M.Strzelecki for great UNICORE monitoring support
 - M.Lewandowski for UNICORE Accounting framework
 - UNICORE administrators of other PL-Grid sites:
 - L.Flis (CYFRONET)
 - F.Klajn (WCSS)
 - M.Samson (TASK)
 - Z.Filutowska (PCSS)
 - ICM Hydra cluster administrators







Thank You for Your Attention



