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

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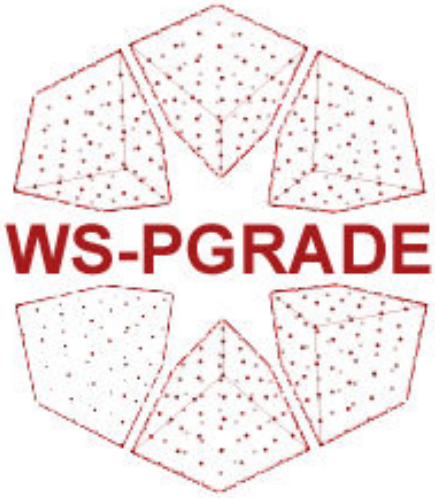



www.eu-egee.org

5th EGEE User Forum
Uppsala, 12-15 April 2010

e-infrastructure

# Outline

- **WSPGRADE in context**
  - P-GRADE Portal, GEMLCA P-GRADE Portal, WS-PGRADE
- **WS-PGRADE features**
  - Scalable architecture
  - Seamless access to various types of resources
- **Advanced data-flows**
- **Comfort features**
  - Separated views for different roles, repository
- **Users and applications**
- **Next steps and conclusions**

# Family of P-GRADE Portal products

- **P-GRADE portal**
  - Creating (basic) workflows and parameter sweeps for clusters, service grids, desktop grids
  - *www.portal.p-grade.hu*
  - *Over 1700 Sourceforge downloads*
- **P-GRADE/GEMLCA portal (University of Westminster)**
  - To wrap legacy applications into Grid Services
  - To add legacy code services to P-GRADE Portal workflows
  - *http://www.cpc.wmin.ac.uk/cpcsite/gemlca*
- **WS-PGRADE**
  - Creating complex workflow and parameter sweeps for clusters, service grids, desktop grids, databases
  - Creating complex applications using embedded workflows, legacy codes and community components from workflow repository
  - *www.wspgrade.hu*

# Motivations of creating gUSE

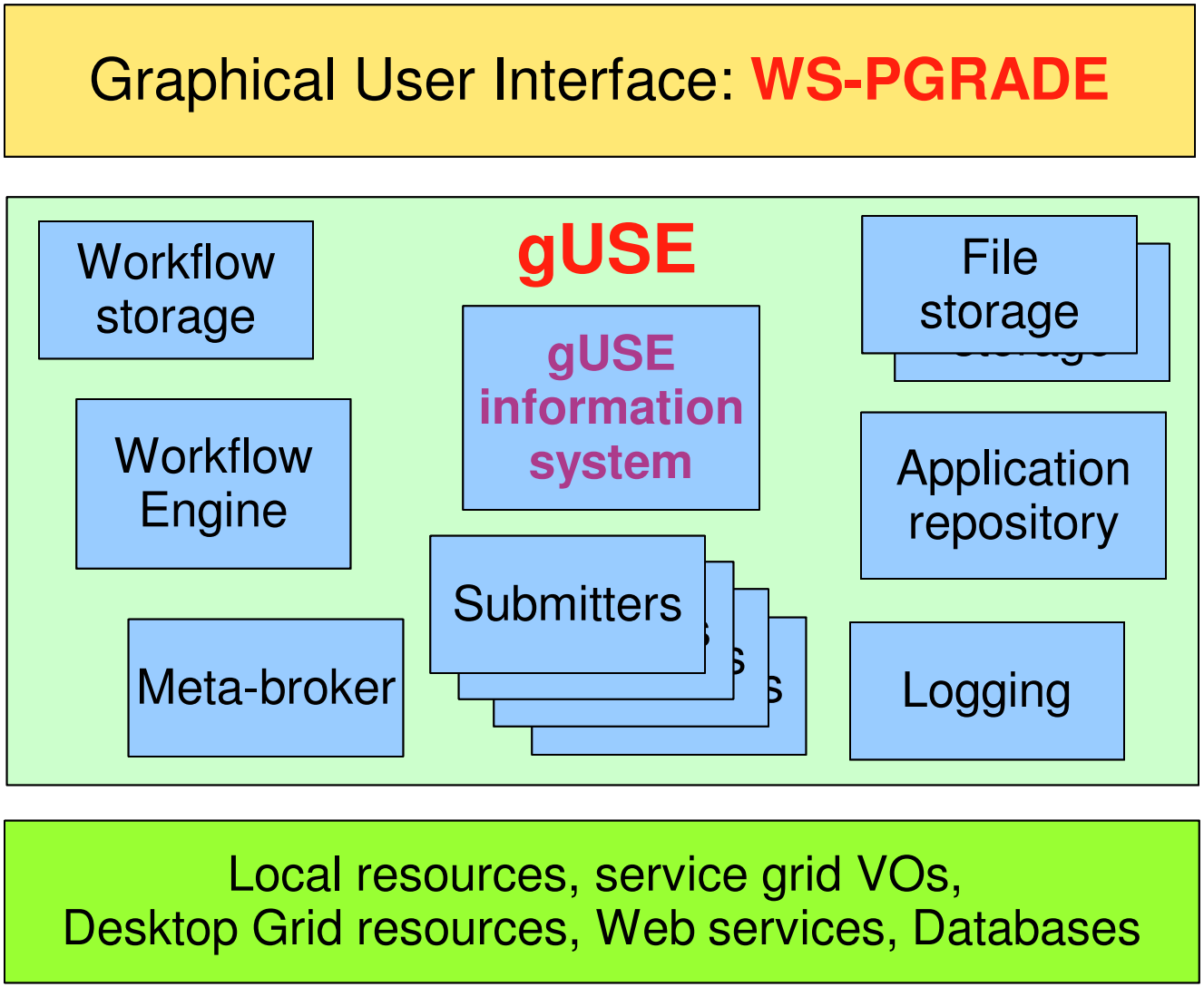
- **To overcome (most of) the limitations of P-GRADE portal:**
  - Provide better modularity → you can replace any service
  - Improve scalability → to millions of jobs
  - Enable advanced dataflow patterns
  - Interface with wider range of resources
  - Separate Application Developer view from Application User view

- **WS-PGRADE (Web Services Parallel Grid Runtime and Developer Environment)**

  **and**

  **gUSE (Grid User Support Environment) architecture**

# WS-PGRADE architecture




*Gridsphere portlets*

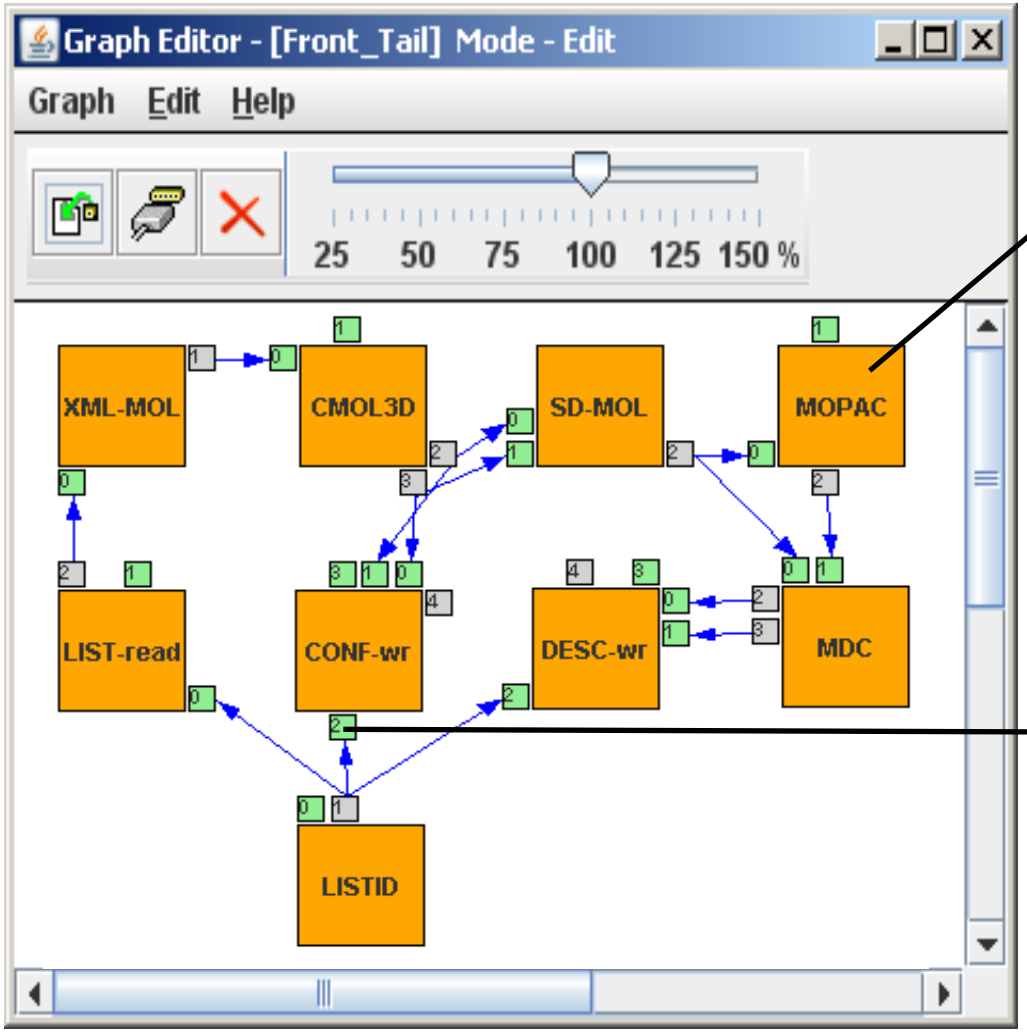
*Autonomous Services: high level middleware service layer*

*Resources: middleware service layer*

# Application lifecycle in WS-PGRADE

- **Define workflow structure**
- **Configure workflow**
  - Define the meaning of computational tasks
- **Run a test**
  - Use local resources, Web services, Databases
- **Scale workflow for large simulations**
  - Use batch systems, use cluster grids, use desktop grids
- **Fix some parameters, leave some open**
  - Application specific science gateway for end users

# WS-PGRADE application: Acyclic dataflow

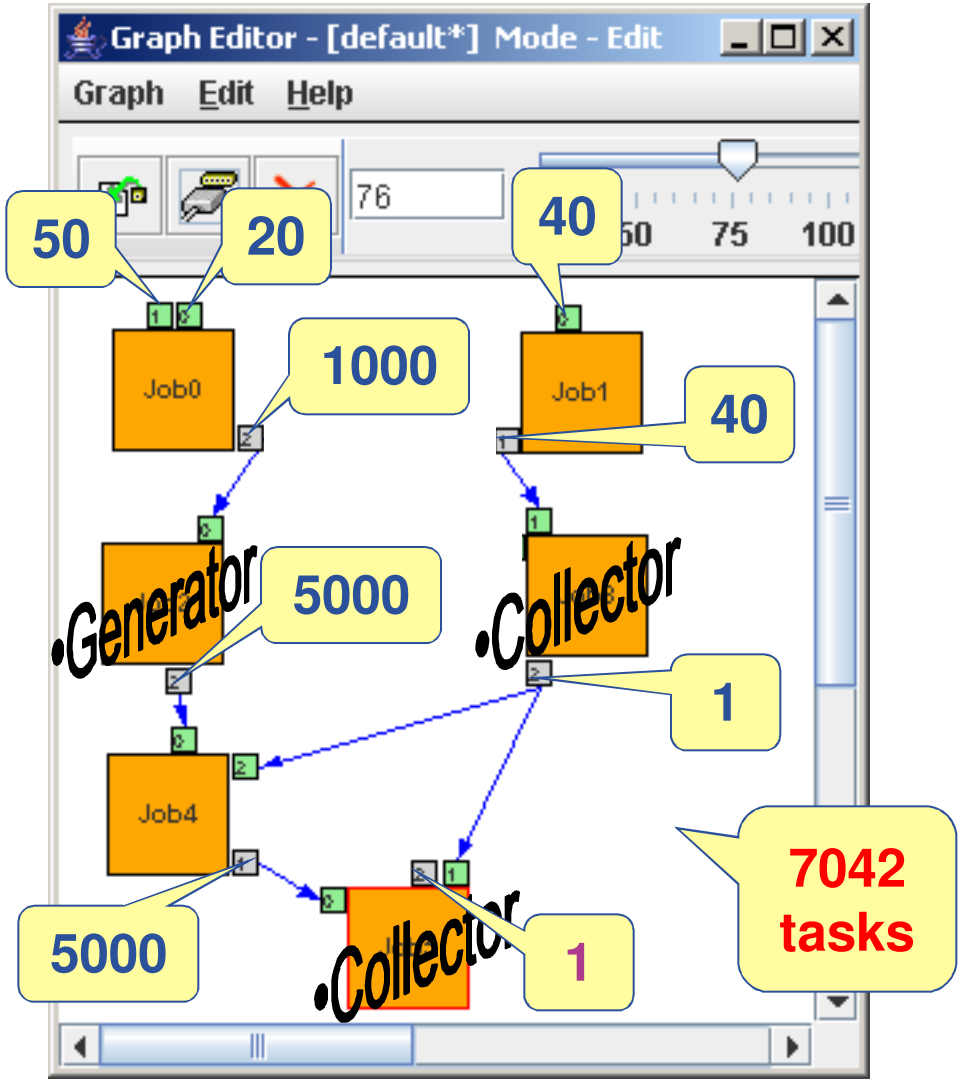



- Job to run on dedicated machine
- Job to run in a gLite VO
- Job to run in a Globus 2 VO
- Job to run in a Globus 4 VO
- Task to run in a BOINC Grid
- Web service invocation
- Database operation (R / W)

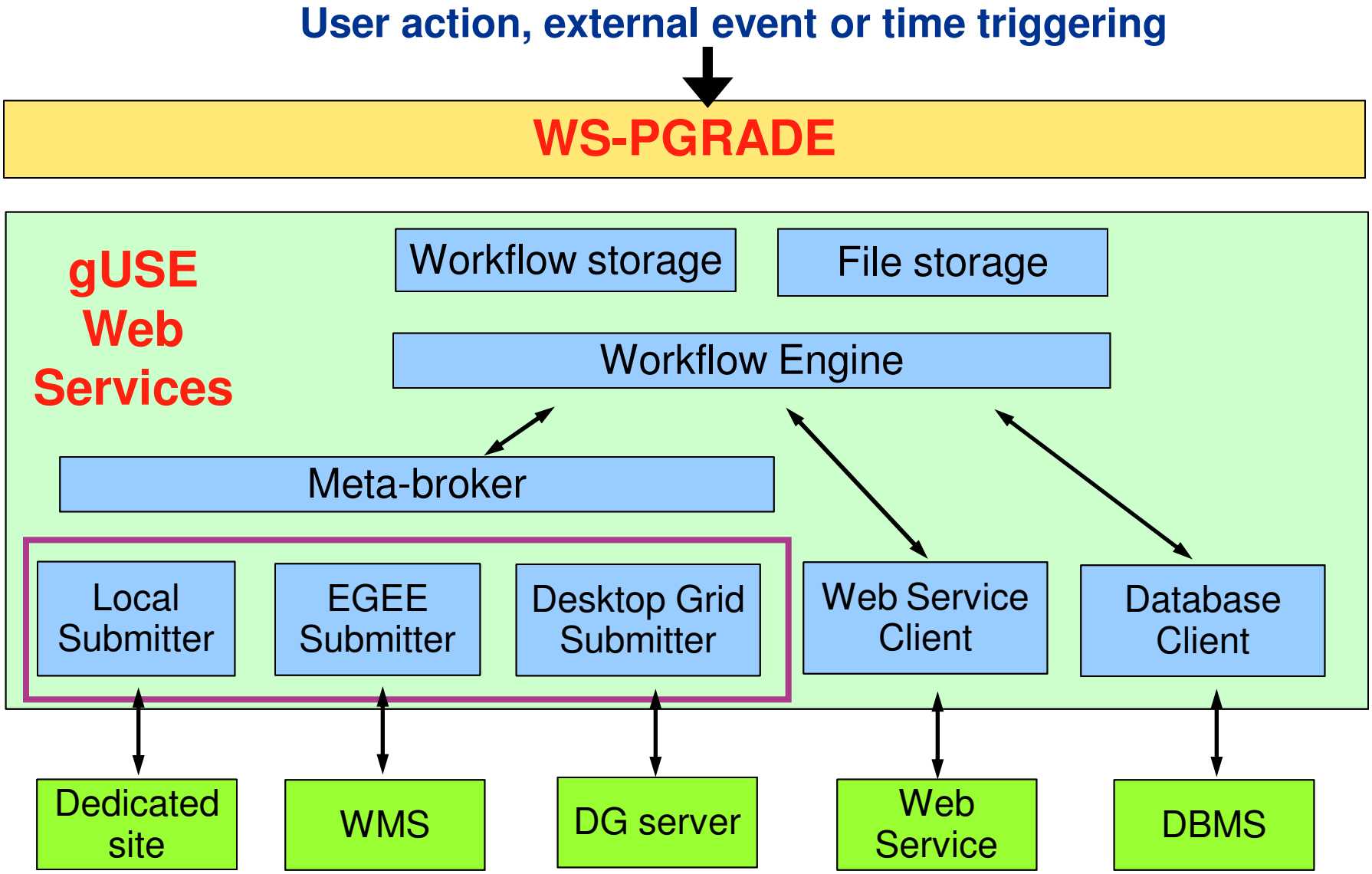
- File from the client host
- File from a GridFTP site
- File from an LFC catalog
- Input string for a task or service
- Result of a Database query

# Dataflow programming with gUSE

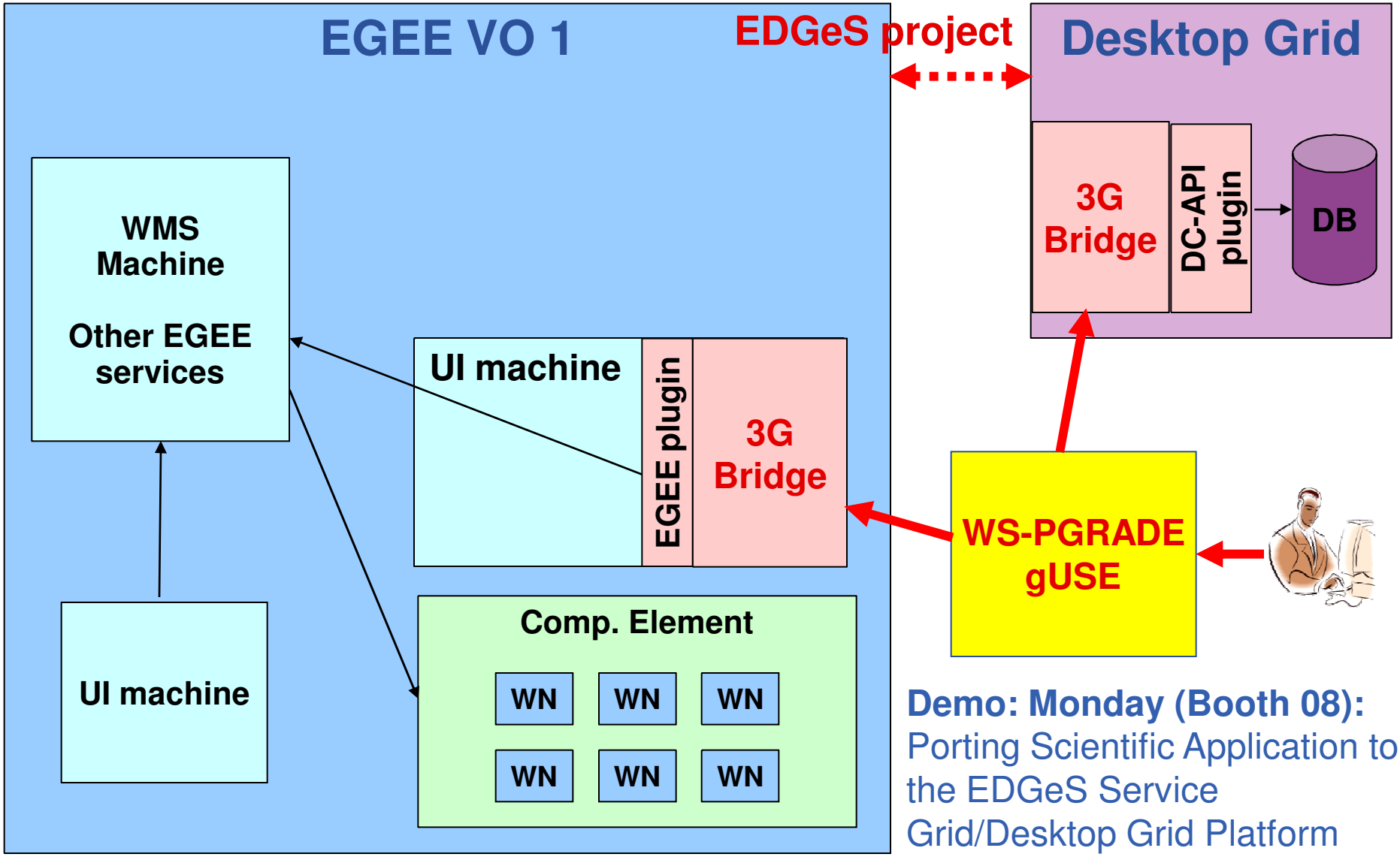
- **Separate application logic from data**
- **Cross & dot product data-pairing**
  - Concept from Taverna
  - All-to-all vs. one-to-one pairing of data items
- **Generator components:** to produce *many output files from 1 input file*
- **Collector components:** to produce *1 output file from many input files*
- **Any component** can be generator or collector
- Conditional execution **based on equality of data**
- Nesting, cycle, recursion



# Task execution process



# Generic Grid-Grid bridge – 3G bridge

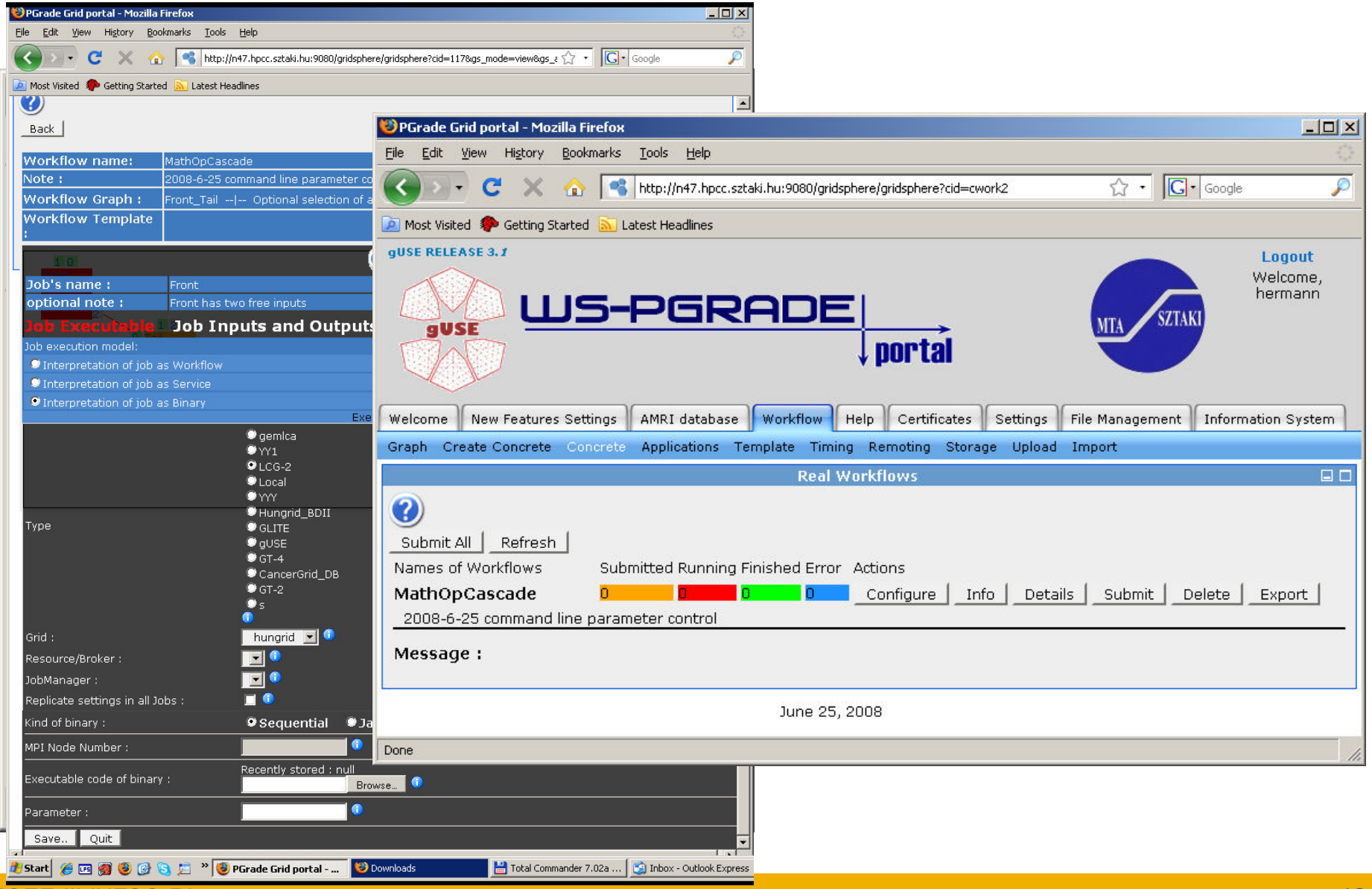



**Demo: Monday (Booth 08):**
Porting Scientific Application to the EDGeS Service Grid/Desktop Grid Platform

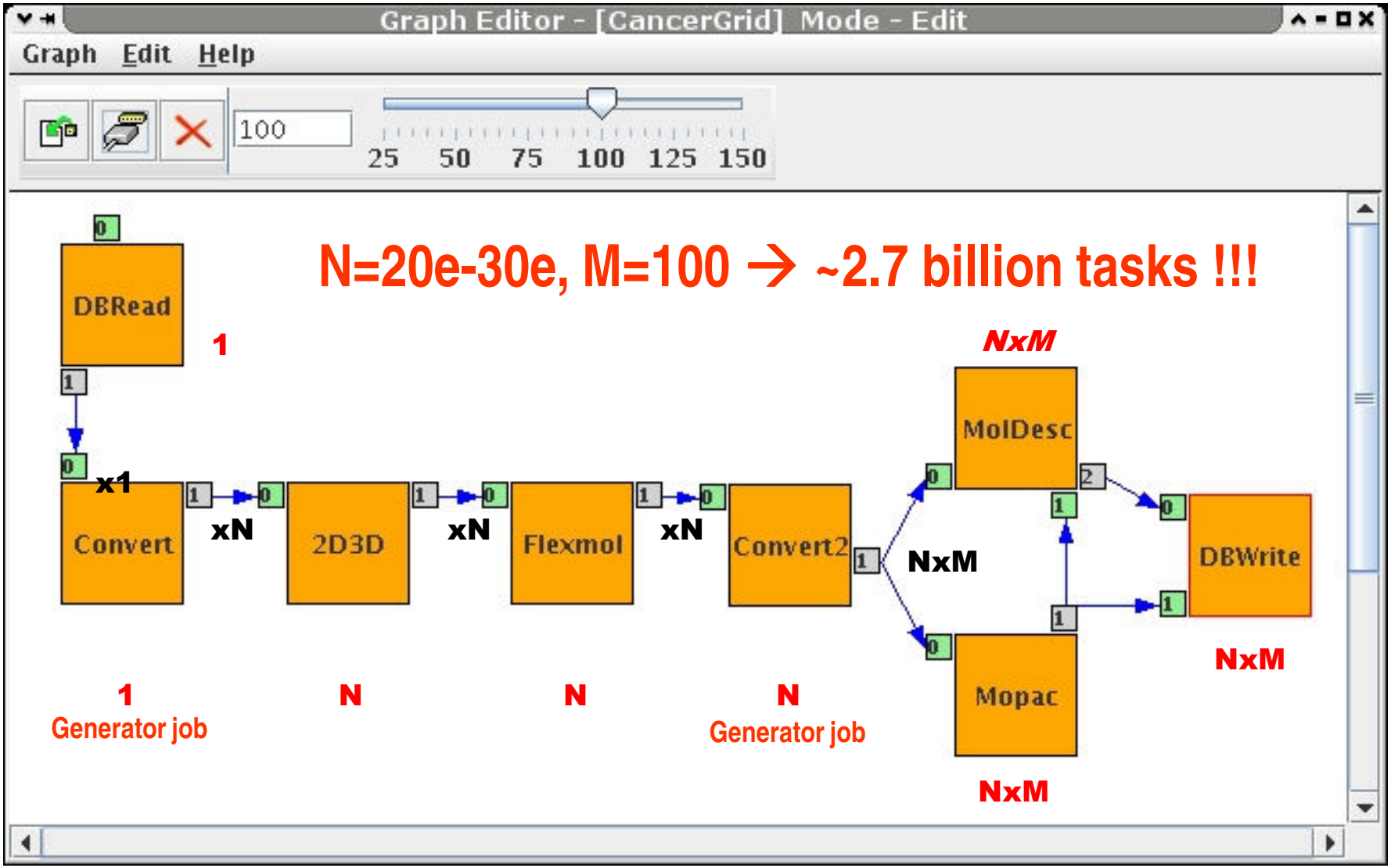
# Ergonomics

- **Users can be grid application developers or end-users.**
- **Application developers design sophisticated dataflow graphs**
  - embedding into any depth, recursive invocations, conditional structures, generators and collectors at any position
  - Publish applications in the repository at certain stages of work
    - Applications
    - Projects
    - Concrete
    - Templates
    - Graphs
- **End-users see gUSE as a science gateway**
  - List of ready to use applications in repository
  - Import and execute application without knowledge of programming, dataflow or grid

# Developer view vs. End-user view

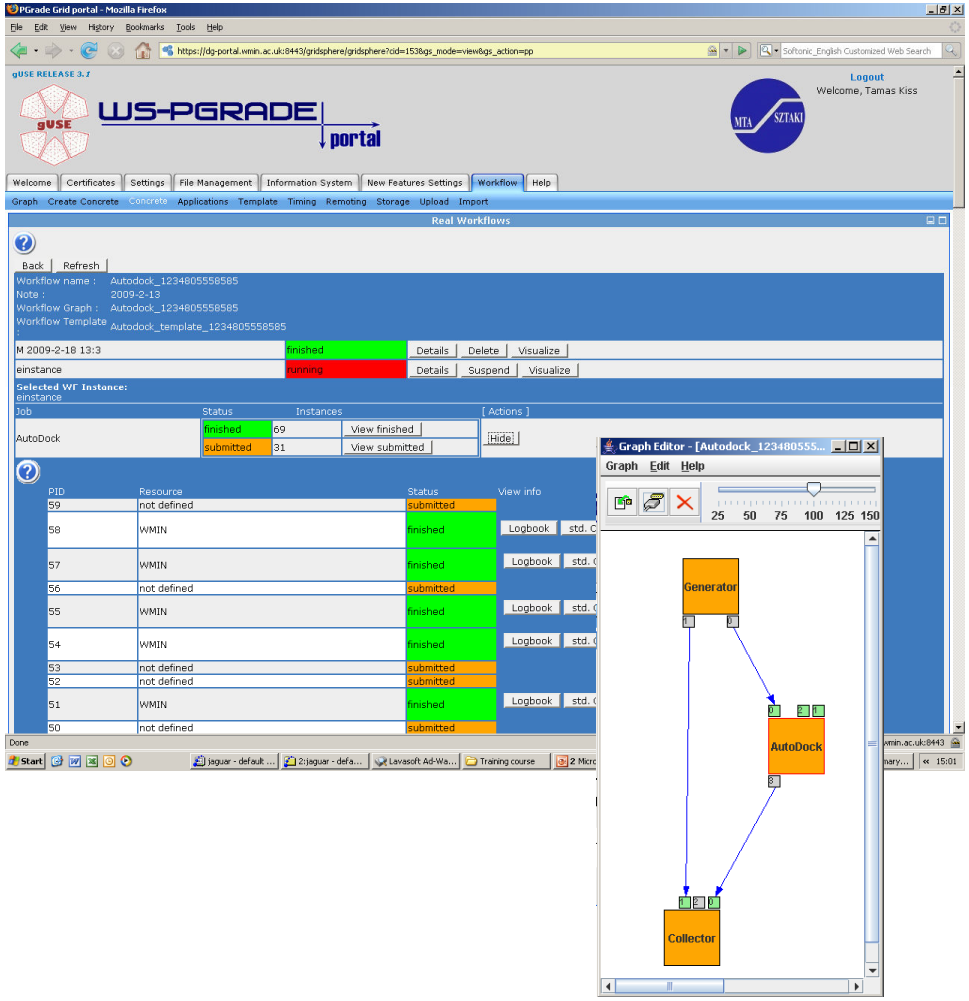


# Scalability example CancerGrid workflow



# Current users of gUSE

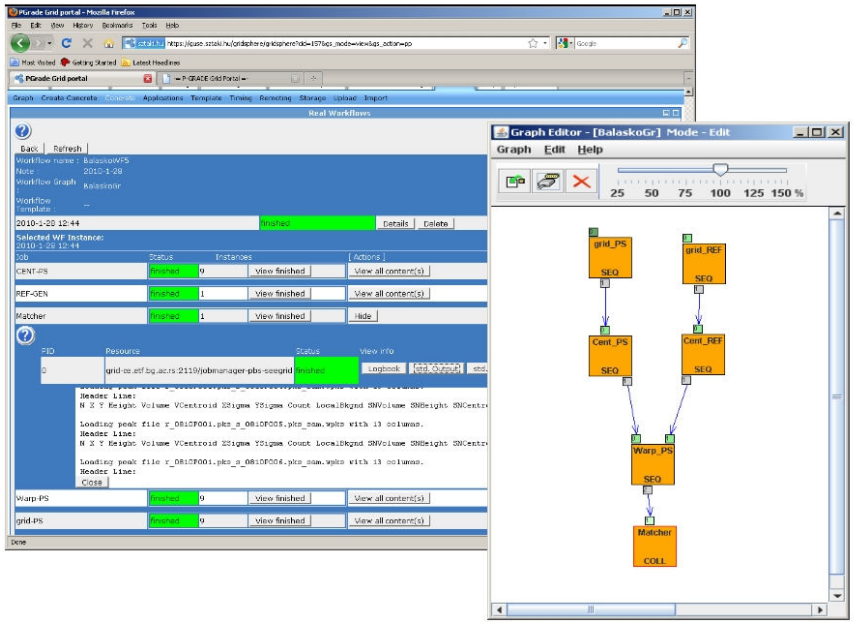
- **CancerGrid project**
  - Predicting various properties of molecules to find anti-cancer leads
  - Creating science gateway for chemists
- **EDGeS project (Enabling Desktop Grids for e-Science)**
  - Integrating EGEE with BOINC and XtremWeb technologies
  - User interfaces and tools
- **ProSim project**
  - In silico simulation of intermolecular recognition
  - JISC ENGAGE program
  - Demo on Wednesday
- **University of Westminster Desktop Grid**
  - Using AutoDock on institutional PCs

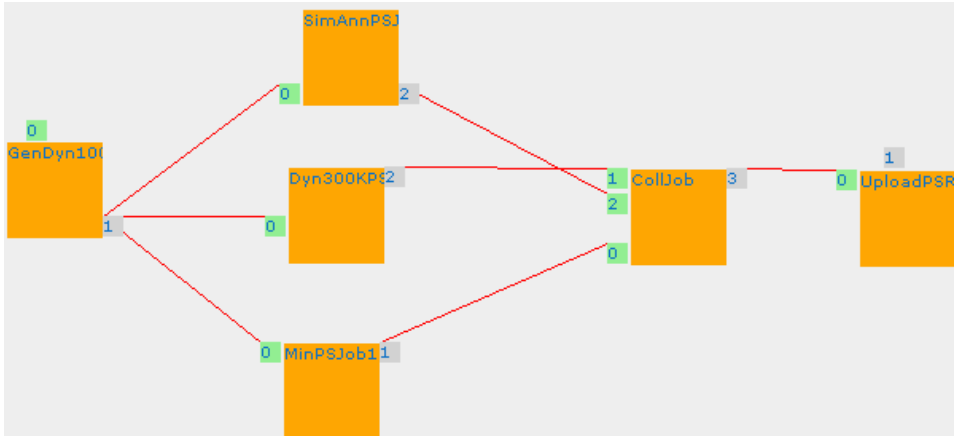


# Porting applications to grids with WS-PGRADE

- **EGEE Application Porting Support Group**
  - www.lpds.sztaki.hu/gasuc

- **Current applications with WS-PGRADE (Presentation on Monday)**
  - Proteomics analysis for biomarker discovery
    - http://www.lpds.sztaki.hu/gasuc/index.php?m=6&r=15
  - TINKER Conformer Generator
    - http://www.lpds.sztaki.hu/gasuc/index.php?m=6&r=12



# Conclusions

- **P-GRADE Portal is still supported and open source**
  - Features can serve most grid scenarios
  - Open source project on Sourceforge

- **WS-PGRADE provide more advanced services**
  - Implemented on top of scalable, WS based gUSE architecture
  - More expressive dataflow patterns
  - Transparent access to
    - Local resources
    - Service Grids
    - Desktop Grids
    - Databases
    - Web services
  - Application repository
    - Service for collaboration of developers and end-users
  - **Create science gateways with few clicks**

# Next steps at www.guse.hu


User manual

Request a user account

# PUCOWO

www.portal.p-grade.hu/pucowo

**1st P-GRADE Portal User COmmunity WOrkshop**

**Zurich, Switzerland**
**June 10-11, 2010**

•Free event!
•Register now!

- Home
- Program
- Tutorial
- Program committee
- Organizing committee
- Call for presentations
- Important dates
- Contact

•WS-PGRADE
•tutorial

## Home

In the last two years P-GRADE portal became popular and many Grids and VOs selected it as their science ga
their user communities (see **http://portal.p-grade.hu/?m=installations&s=0**). Due to the increased inte
number of user communities, the developers would like to provide stronger support and faster response
requirements of the user communities. In order to achieve this goal we organize the 1st P-GRADE Po
COmmunity WOrkshop. The major goal is to share experience of using P-GRADE Portal among the vari
communities and portal developers. The program is discussion-oriented. Every presentation will be followed by
minutes discussion time in order to give opportunity for the users to express their P-GRADE experience
developers to better understand the problems.

The presentations and discussions will be organized in the following sessions:

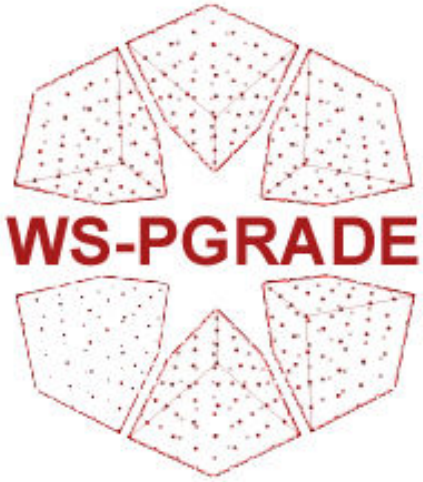
1. P-GRADE portal installation, administration and maintenance This session is for system admins who
   manage P-GRADE portal installations. Here we would like to discuss problems they encountered and
   improvements they recommend.
2. Applications developed by P-GRADE portal This session is for application developers who develop appli
   the portal. Here we would like to discuss what they like and what they do not like or miss in the portal.
3. End-user experience with P-GRADE portal Representatives of end-user communities are welcome to sh
   experience wit the portal.
4. Further development of P-GRADE portal Portal developers will present future plans on the further develo
   the portal. User communities are welcome to give presentation on their additional needs to improve the p

A half-day WS-PGRADE portal tutorial will be also part of the program. WS-PGRADE is the second generation
portal that will be presented and demonstrated during the tutorial. Two application-specific portals developed
the generic purpose WS-PGRADE portal will also be presented: ProSim portal for protein folding simula
CancerGrid portal for drug design.

The whole event is **free of charge**. We would like to share experience with the P-GRADE portal user community in
improve the portal for their sake and not to make profit from this event.

# Thank you

***www.wspgrade.hu***

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