

## WS-PGRADE: the second generation P-GRADE portal

*Gergely Sipos* [sipos@sztaki.hu](mailto:sipos@sztaki.hu)  
*Krisztián Karóczkai*  
*Péter Kacsuk*

*MTA SZTAKI* [www.lpds.sztaki.hu](http://www.lpds.sztaki.hu)

[www.wspgrade.hu](http://www.wspgrade.hu)

[www.guse.hu](http://www.guse.hu)



- **History, family of products**
  - P-GRADE Portal, WS-PGRADE, gUSE
- **WS-PGRADE features**
  - Scalable architecture
  - Seamless access to various types of resources
- **Advanced data-flows**
- **Comfort features**
  - Separated views, repository
- **Users and applications**
- **Next steps and conclusions**

- **P-GRADE portal**
  - Creating (basic) workflows and parameter sweeps for service grids
  - [www.portal.p-grade.hu](http://www.portal.p-grade.hu)
- **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 and desktop grids
  - Creating complex applications using embedded workflows, legacy codes and community components from workflow repository
  - [www.wspgrade.hu](http://www.wspgrade.hu)
    - Apply for an account!
    - Browse the User manual!

- **Pros.**

- Easy-to-use workflow system with graphical editor
- Easy-to-use parameter sweep concept at workflow level
- Multi-grid / multi-VO access mechanism: job submission to LCG, gLite and GT2
- Intelligent handling of grid errors
- Open source community on Sourceforge
- Reliable, production installations for several Grid, EGEE VOs
- Part of EGEE RESPECT programme

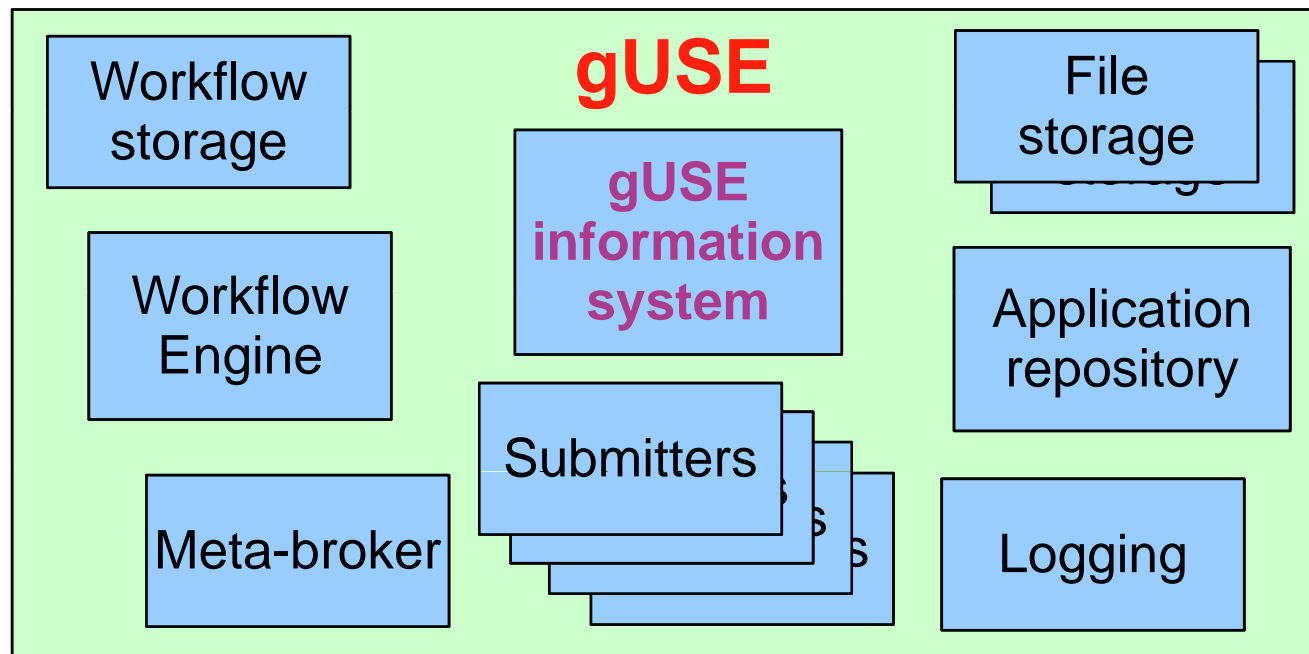
- **Cons.**

- Considered too simple by some IT people, while too complicated by some end users
- Workflow features found to be limited for some applications
- Internal structure is monolithic

- **To overcome (most of) the limitations of P-GRADE portal:**
  - To provide better modularity
  - To improve scalability
  - To enable advanced dataflow patterns
  - To interface with wider range of resources
  - To separate Application Developer view from Application User view
- **New products:**  
**WS-PGRADE (Web Services Parallel Grid Runtime and Developer Environment)**  
**and**  
**gUSE (Grid User Support Environment) architecture**
  - Web Services based Portal solution
    - Install it on a single machine
    - Install it on several machines

Graphical User Interface: **WS-PGRADE**

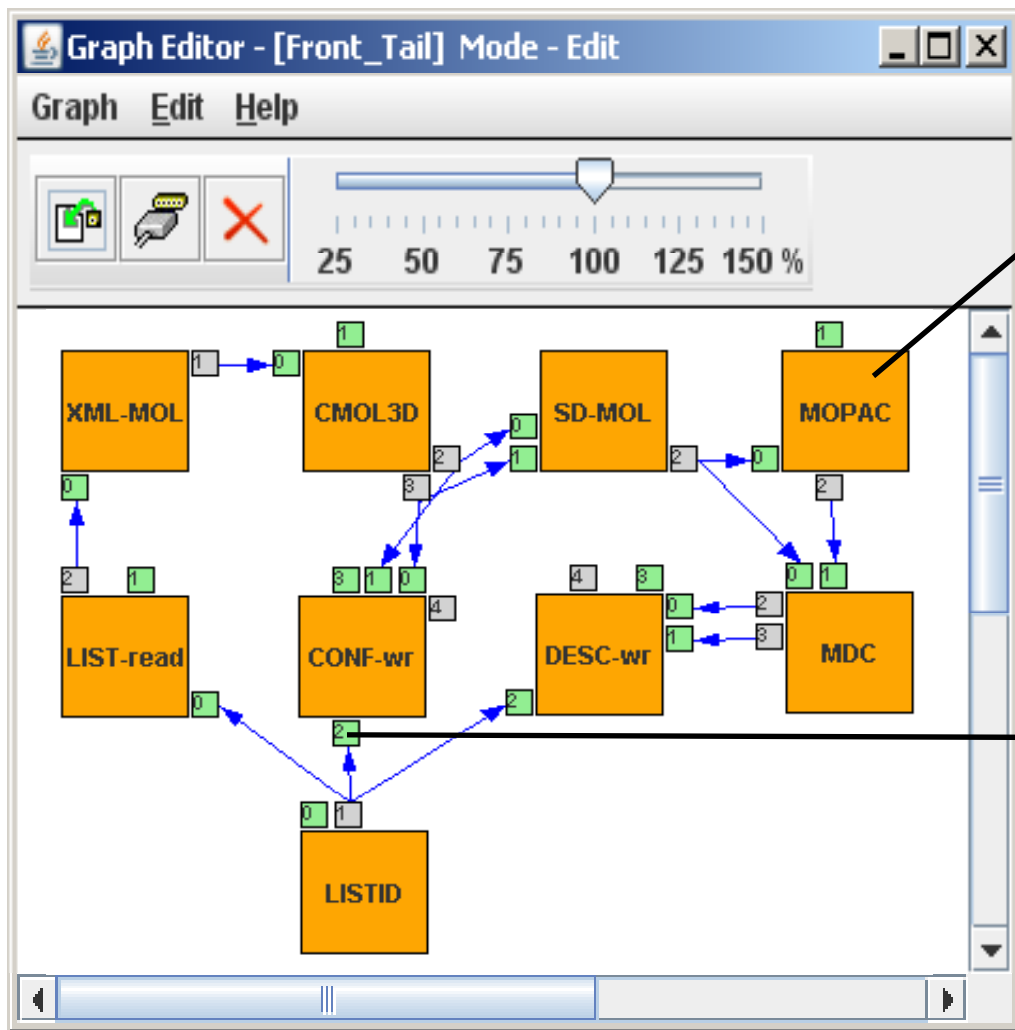
*Gridsphere  
portlets*



*Autonomous  
Services:  
high level  
middleware  
service layer*

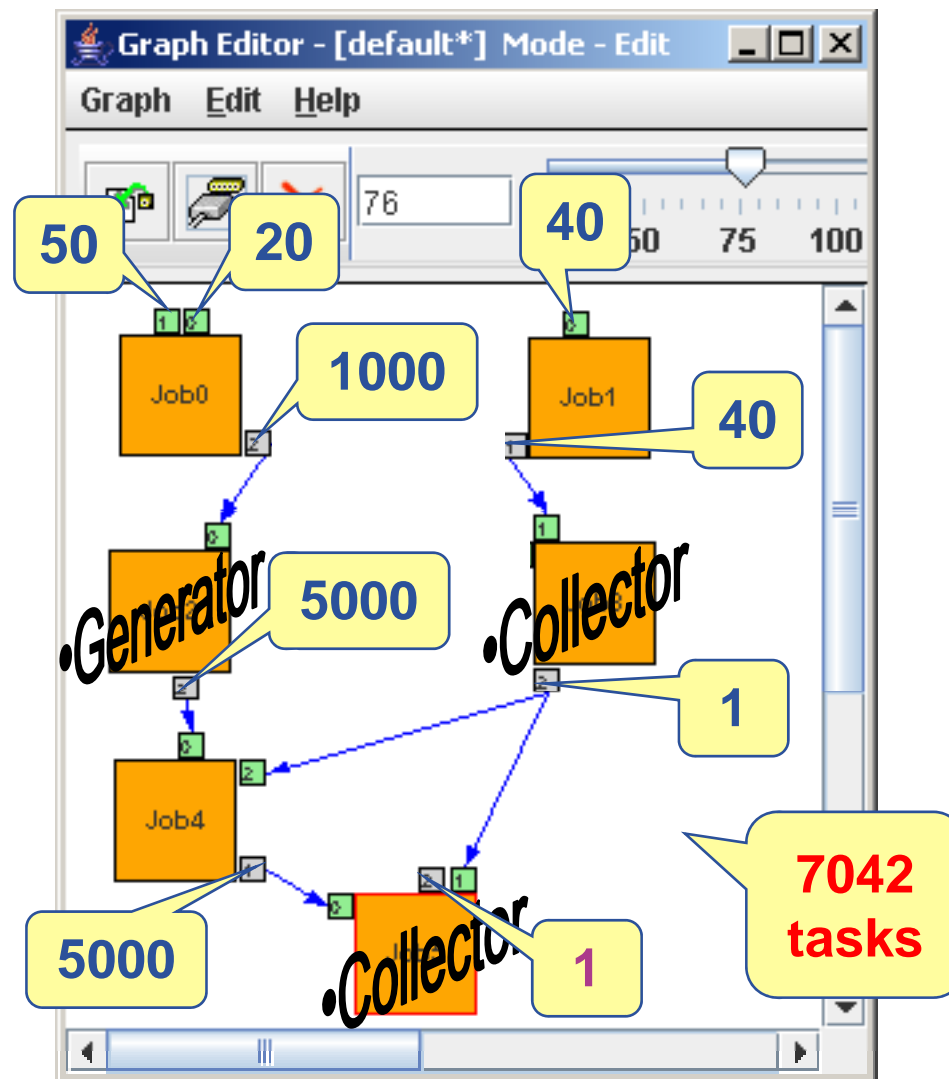
Local resources, Service grid resources,  
Desktop Grid resources, Web services, Databases

*Resources:  
middleware  
service layer*



- 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

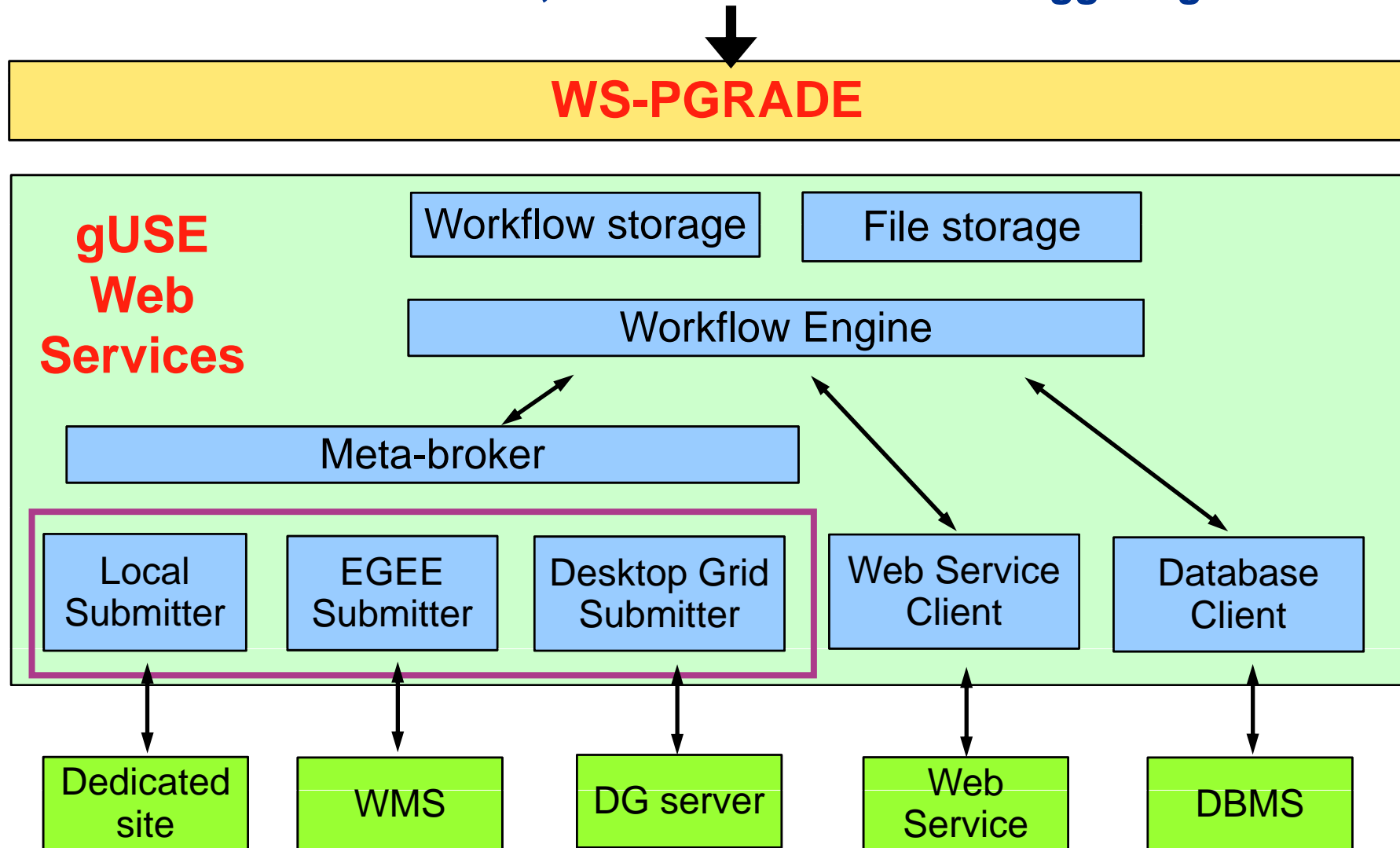
- **Separate application logic from data**
- **Cross & dot product data-pairing**
  - Concept from Taverna
  - All-to-all vs. one-to-one pairing of data items
- **Generator components:** to produce *many output files from 1 input file*
- **Collector components:** to produce *1 output file from many input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

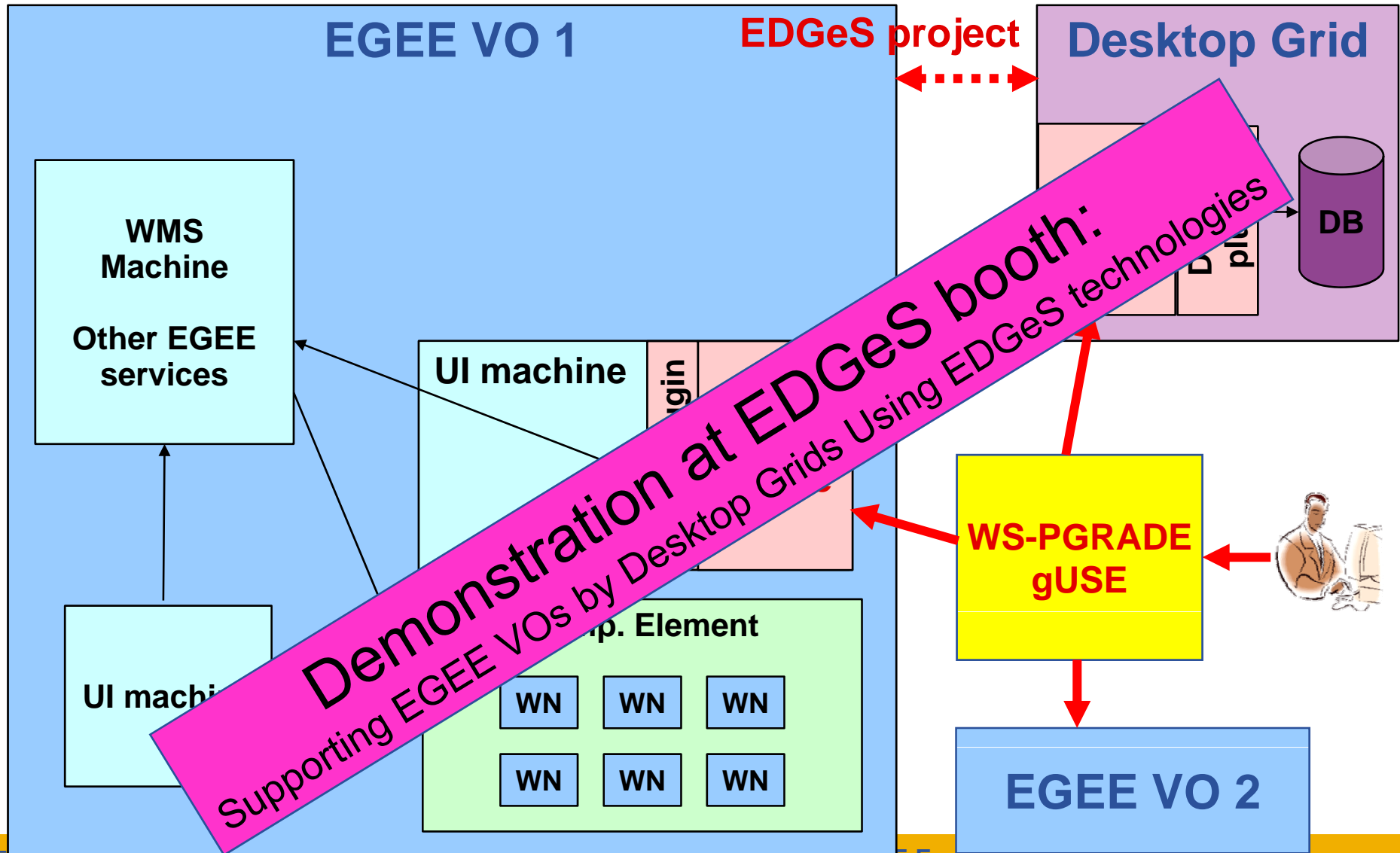




# Task execution process

User action, external event or time triggering





- **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

PGrade Grid portal - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://n47.hpcc.sztaki.hu:9080/gridsphere/gridsphere?cid=117&gs\_mode=view&gs\_...

Most Visited Getting Started Latest Headlines

Back

Workflow name: MathOpCascade  
 Note: 2008-6-25 command line parameter control  
 Workflow Graph: Front\_Tail --|-- Optional selection of a  
 Workflow Template:

Job's name: Front  
 optional note: Front has two free inputs  
**Job Executable** Job Inputs and Outputs  
 Job execution model:  
 Interpretation of job as Workflow  
 Interpretation of job as Service  
 Interpretation of job as Binary

Type

- gemlica
- YY1
- LCG-2
- Local
- YYY
- Hungrid\_BDII
- GLITE
- gUSE
- GT-4
- CancerGrid\_DB
- GT-2
- s

Grid: hungrid

Resource/Broker: [dropdown]

JobManager: [dropdown]

Replicate settings in all Jobs: [checkbox]

Kind of binary:  Sequential  Java

MPI Node Number: [input]

Executable code of binary: Recently stored: null [Browse...]

Parameter: [input]

Save... Quit


PGrade Grid portal - Mozilla Firefox

File Edit View History Bookmarks Tools Help


http://n47.hpcc.sztaki.hu:9080/gridsphere/gridsphere?cid=cwork2

Most Visited Getting Started Latest Headlines

gUSE RELEASE 3.7



**WS-PGRADE** portal



Logout  
Welcome, hermann

Welcome New Features Settings AMRI database Workflow Help Certificates Settings File Management Information System

Graph Create Concrete Concrete Applications Template Timing Remoting Storage Upload Import

Real Workflows

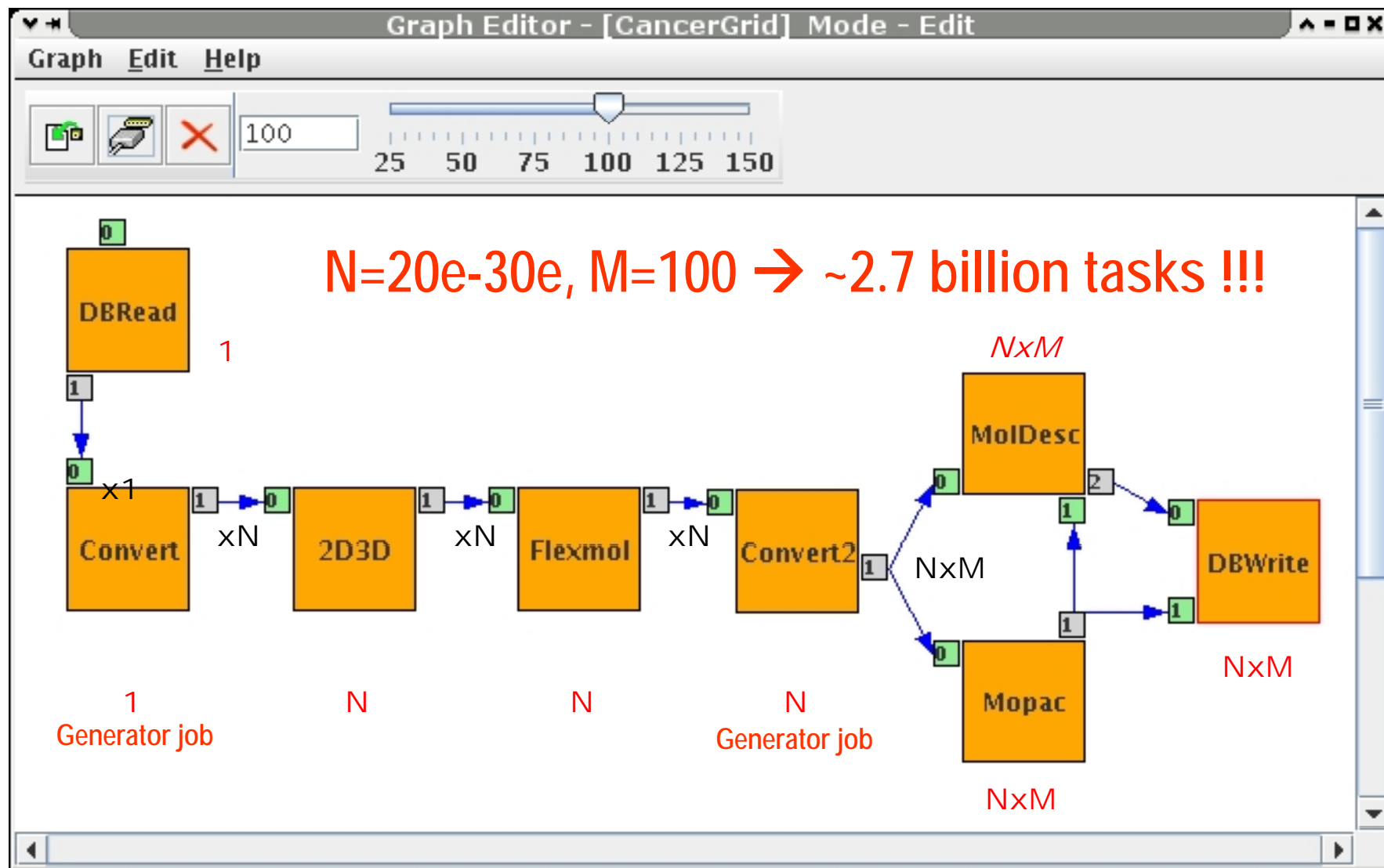
Submit All Refresh

Names of Workflows	Submitted	Running	Finished	Error	Actions
<b>MathOpCascade</b> 2008-6-25 command line parameter control	0	0	0	0	Configure Info Details Submit Delete Export

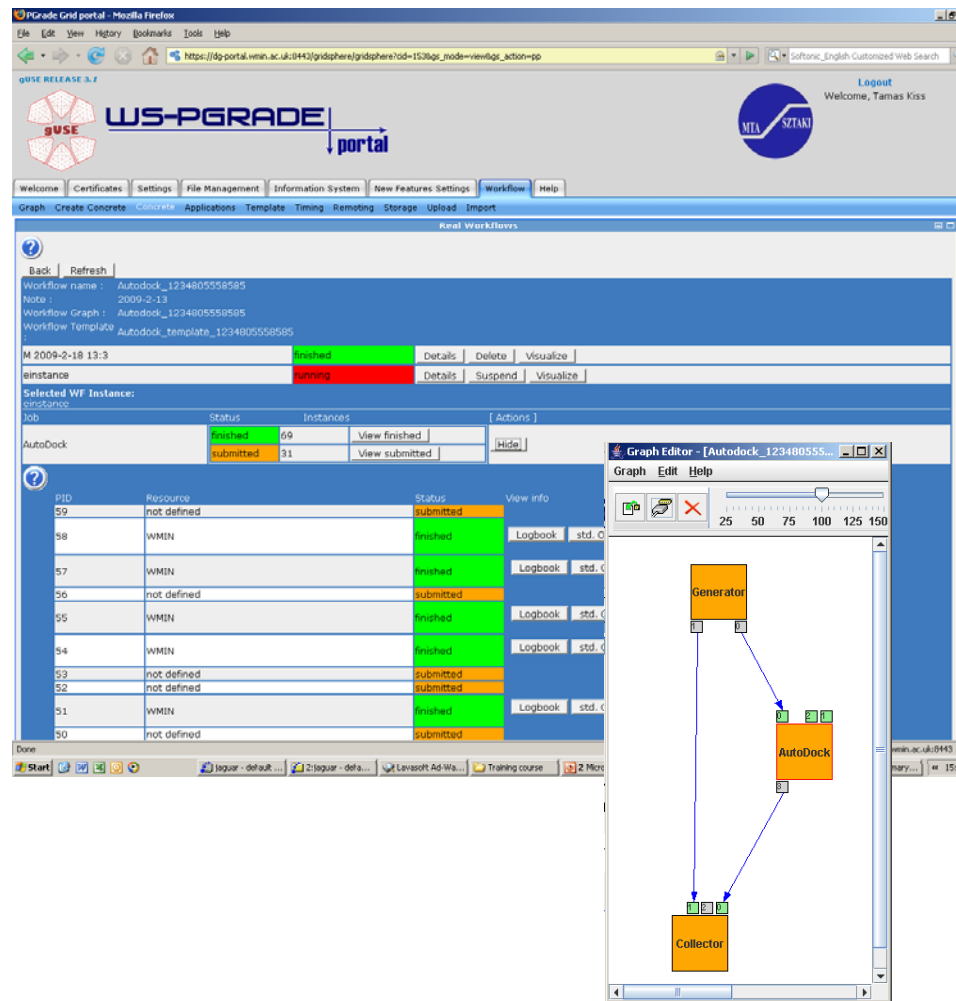
Message:

June 25, 2008

Done



- **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
- **University of Westminster Desktop Grid**
  - Using AutoDock on institutional PCs



The screenshot displays the gUSE portal interface. The top section shows the portal logo and navigation tabs. The main content area is titled 'Real Workflows' and displays a table of workflow instances. Below the table, there is a 'Selected WF Instance:' section with a table of job instances. On the right side, a 'Graph Editor' window is open, showing a workflow graph with three nodes: 'Generator', 'AutoDock', and 'Collector', connected by arrows.

Workflow name	Note	Workflow Graph	Workflow Template
Autodock_1234805558585	2009-2-13	Autodock_1234805558585	Autodock_template_1234805558585

instance	Status	Actions
M 2009-2-18 13:3	finished	Details   Delete   Visualize
	running	Details   Suspend   Visualize

job	Status	Instances	Actions
AutoDock	finished	69	View finished
	submitted	31	View submitted

PID	Resource	Status	View info
59	not defined	submitted	
58	WMIN	finished	Logbook   std. C
57	WMIN	finished	Logbook   std. C
56	not defined	submitted	
55	WMIN	finished	Logbook   std. C
54	WMIN	finished	Logbook   std. C
53	not defined	submitted	
52	not defined	submitted	
51	WMIN	finished	Logbook   std. C
50	not defined	submitted	

- **P-GRADE Portal remains supported**
  - Features can serve most grid scenarios
  - Open source project on Sourceforge
- **WS-PGRADE**
  - 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

A screenshot of a Windows Internet Explorer browser window displaying the gUSE website. The browser's address bar shows 'http://www.guse.hu/'. The website header features a logo on the left consisting of a red star-like shape with 'gUSE' in the center, and the text 'grid User Support Environment' on the right. A left-hand navigation menu lists various links: Home, Architecture, Features and Releases, Portal installations, Documents, For grid users (Client requirements, How to get access), For grid administrators (Install the portal), and Problem reporting (Report Problems). The main content area has a 'Home' heading followed by a sub-heading 'gUSE 3.1 released' and a paragraph: 'SZTAKI is glad to announce the release of gUSE, version 3.1.' The footer contains copyright information for 2008, MTA-SZTAKI LPDS, Hungary, and an email address: [webmaster@lpds.sztaki.hu](mailto:webmaster@lpds.sztaki.hu). The browser's status bar at the bottom shows 'Internet' and '100%' zoom.

User manual

Request a user account



# Thank you

**Gergely Sipos**

**[sipos@sztaki.hu](mailto:sipos@sztaki.hu)**

**[www.wspgrade.hu](http://www.wspgrade.hu)**

**[www.guse.hu](http://www.guse.hu)**

**[www.lpds.sztaki.hu](http://www.lpds.sztaki.hu)**

