



Enabling Grids for E-science

User friendly high level application support for EGEE/gLite

Jan Kmuníček
NA4 CE region coordinator

www.eu-egee.org



- **CE region specifics**
- **VOCE infrastructure**
- **Application support - CHARON**
- **Application support - P-GRADE**
- **Additional CE regional tools**
- **Plans & further progress**

- **Central European federation (CE)**

- regional descriptor **heterogeneity**
(in both partners & organizations)



Austria

GUP, UNIINNSBRUCK



Czech Republic

CESNET



Hungary

MTA SZTAKI, NIIF, KFKI RMKI, ELUB, BUTE



Poland

ICM, PSNC, CYFRONET



Slovakia

II-SAS



Slovenia

JSI

- EGEE II

regional newcomer



Croatia

- **VOCE - Virtual Organization for Central Europe**
 - provides **complete grid infrastructure** under EGEE wings
 - officially registered as currently the one and only “Regional VO” for Central European (CE) region
 - based on **regional principle**
 - VOCE spans the whole CE Federation
 - core services operated by CESNET
 - resources are provided by several institutions across the CE (these resources are available to all / experienced users registered in VOCE)

- **VOCE - Description**
 - **fully production environment**
 - VOCE environment allows Grid newcomers to get quickly first experience with Grid computing
 - simultaneously allows users to smoothly move to production use of the Grid in the same environment
 - **self-contained infrastructure**
 - all the relevant services run by VOCE administration
 - currently on LCG middleware but simultaneously available gLite 1.4 installation (undergoing task)

- **VOCE - Aims**

- **incubator** for new applications / new application areas

- assistance in adapting a software for use on the Grid
- even for applications that do not have any Grid/cluster/remote computing experience
- outsourcing the burden of running an grid infrastructure to VOCE

- **generic VO**

- VOCE is an application neutral virtual organization
 - *not bound to any particular application*
 - *interested in broad scale of application areas*
- also suitable for training purposes (in cooperation with P-GRADE)

- **VOCE - Features**

- comparison VOCE to GILDA VO

- **VOCE security**

- *no anonymous users (importance for resource owners)*
- *based on accredited CA's approved by the EUGridPMA body*

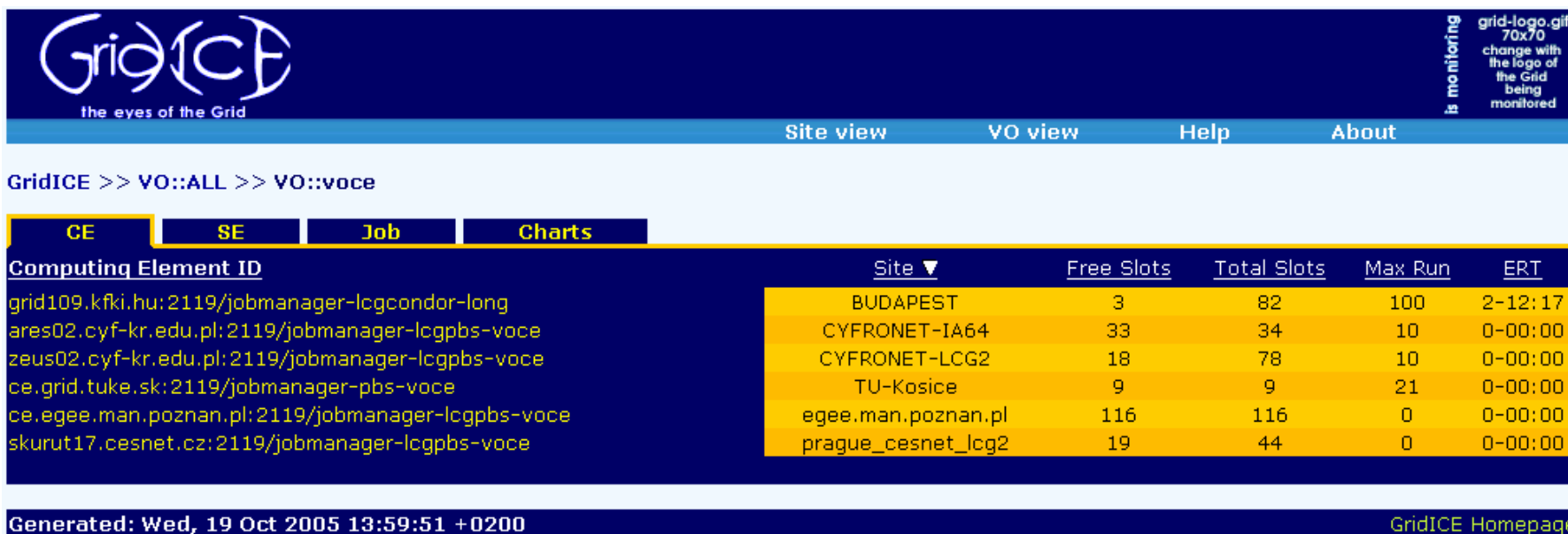
- **VOCE CA**

- *short-term certificates (days) dedicated for training purposes*
- *users can access only limited group of available resources (it is up to the resources owners if they will provide resource also for training purposes utilizing only “training” certificates)*

- **VOCE resources**

- *allocated guaranteed resources, not best effort approach*

- VOCE - Summary of resources



The screenshot shows the GridICE interface for the VOCE infrastructure. It includes a navigation menu with 'Site view', 'VO view', 'Help', and 'About'. The main content area displays a table of resources with columns for 'CE', 'SE', 'Job', and 'Charts'. Below the table, it shows the 'Generated' timestamp and the 'GridICE Homepage' link.

CE	SE	Job	Charts	Site ▼	Free Slots	Total Slots	Max Run	ERT
Computing Element ID								
grid109.kfki.hu:2119/jobmanager-lcgcondor-long				BUDAPEST	3	82	100	2-12:17
ares02.cyf-kr.edu.pl:2119/jobmanager-lcgpbs-voce				CYFRONET-IA64	33	34	10	0-00:00
zeus02.cyf-kr.edu.pl:2119/jobmanager-lcgpbs-voce				CYFRONET-LCG2	18	78	10	0-00:00
ce.grid.tuke.sk:2119/jobmanager-pbs-voce				TU-Kosice	9	9	21	0-00:00
ce.egee.man.poznan.pl:2119/jobmanager-lcgpbs-voce				egee.man.poznan.pl	116	116	0	0-00:00
skurut17.cesnet.cz:2119/jobmanager-lcgpbs-voce				prague_cesnet_lcg2	19	44	0	0-00:00

Generated: Wed, 19 Oct 2005 13:59:51 +0200 GridICE Homepage

- resources from
 - CESNET (Czech Republic)
 - PSNC, CYFRONET, ICM (Poland)
 - II-SAS (Slovakia)
 - KFKI (Hungary)
- more than 40 registered users from 10 institutes and 4 countries
- in total **539 CPUs, about 5.9 TB disk space**

- **VOCE - Advantages**

- **regional self-organization**

- users are not tightly bound around specific applications
 - the region itself is self-organized from the bottom level

resources	...	infrastructure
applications	...	high level middleware

- potential users are not required to invest special effort to easy use the environment in a production mode

- **application neutrality**

- **VOCE - Summary**

- user registration

- VOCE registration at <http://voce-register.farm.particle.cz/>

- documentation

- VOCE portal at <http://egee.cesnet.cz/en/voce/>

- request tracking

- send requests to voce@cesnet.cz

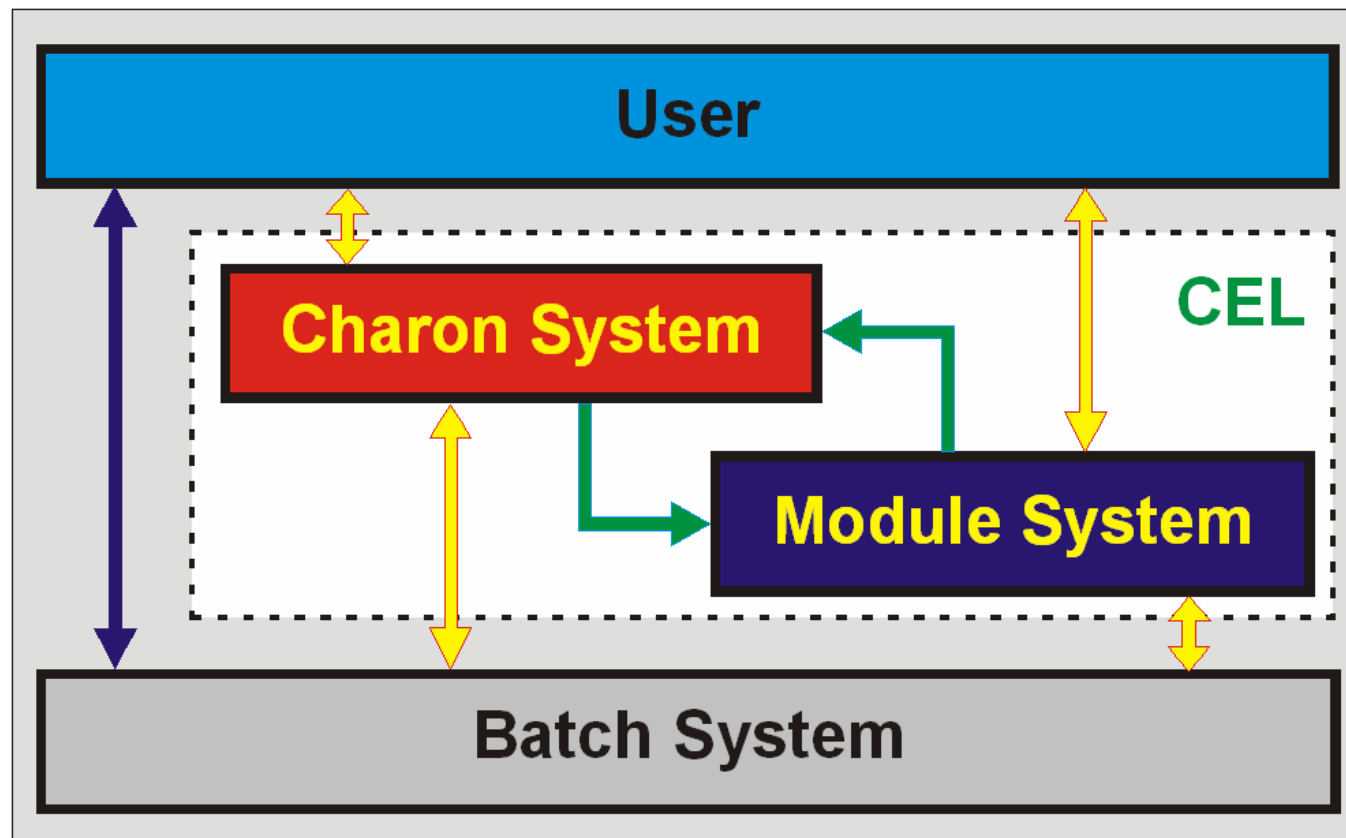
- **What is Charon?**

- uniform, and modular approach for (complex) computational jobs submission and management
- generic system for use of application programs in the Grid environment (LCG/gLite middleware, ...)

- **Why Charon?**

- many various batch systems & scheduling components used in grid environment
- each batch system has unique tools and different philosophy of its utilization
- LCG/gLite provided tools are quite raw and simple
- many additional tasks to use computer resources properly

- Charon Extension Layer (CEL)



- **Module system**

- manages application software

- each software package is described by a specific module
- configuration information is internally stored in XML format

name[:**version**[:**architecture**[:**parallelmode**]]]

- find the architecture and parallel mode that best fit available computational resources
- solve conflicts or dependencies between individual modules
- list available modules sorted into categories
- use pre-installed modules on WNs or install them on the fly if they are missing

- **Application portfolio**
 - **currently supported programs** from
 - computational chemistry and molecular modelling
 - *AMBER, AutoDock, Turbomole, CPMD*
 - numerical computations
 - *Octave*
 - vizualizations
 - *Grace, PovRay, Raster3D, Molscript*
 - **planned programs to be ported** (based on users feedback)
 - *Abinit, Dalton, Gromacs*
 - *Corsika (astrophysics), image processing tools*

- Application areas

```

skurut4.cesnet.cz - PuTTY
EXPORTED MODULES

[none]

AVAILABLE MODULES

--- Molecular Mechanics and Dynamics ---
amber:8.0m      amber-pmf:1.0    amber-rexp:8.0  autodock:3.0    autodock:3.0big

--- Quantum Mechanics and Dynamics ---
turbomole:5.6m  cpmd:3.9.1

--- Conversion and Analysis ---
babel:1.6      cats:dev         caver:0.99     qhull:2003.1    octave:2.1.71
wham:1.0

--- Vizualization ---
grace:5.1.18   povray:3.6       raster3d:2.7c  molscript:2.1.2

--- System ---
mpichrun:1.2.6

[kmunicek@skurut4 kmunicek]$
  
```

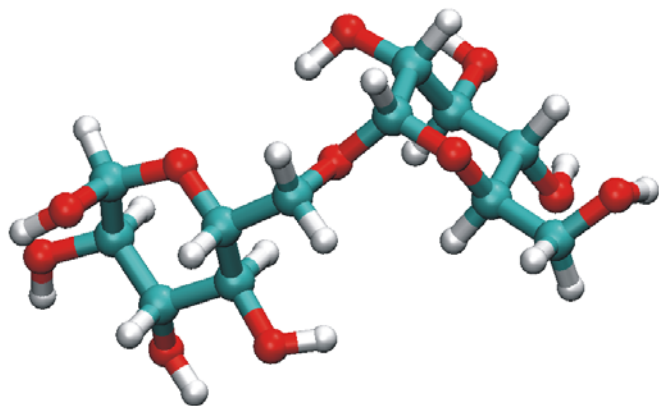
- **Charon system – Job Flow**
 - simplifies navigation through job life cycle to the maximum (critical added value especially for Grid newcomers)
 - in principle only **three simple commands** are needed for the complete manipulation with a computational job
 - compared to **GUI (portals)**
 - *higher flexibility in reconfiguration by user him/herself*
 - compared to **native CLI**
 - *smoother job management*

- input

```
[jobdir]$ ls
equi.rst  isomaltose.top  myjob  prep.in
```

```
# sander calculation on VOCE
module add amber
sander -O -i prep.in \
        -p isomaltose.top \
        -c equi.rst -o prep.out \
        -x prep.traj -r prep.rst
```

Molecular Dynamics of Isomaltose



- **psubmit**

```
[jobdir]$ psubmit voce myjob
```

```
Job name      : myjob
Grid job name : myjob (Job type: generic)
Job directory : skurut4.cesnet.cz:/home/kulhanek/jobdir
Job project   : -none-
=====
Alias         : -none-
Organization  : voce
Profile      : default
-----
NCPU         : 1
Resources    : -job match-
Properties   : -none-
Sync mode    : gridcopy
-----
Start after   : -not defined-
=====
Do you want to submit job to GRID environment (YES/NO) ? YES

Please wait packing data ...
Submitting job ...

Job was successfully submitted to GRID environment.
```

- **pinfo**

```
[jobdir]$ pinfo
```

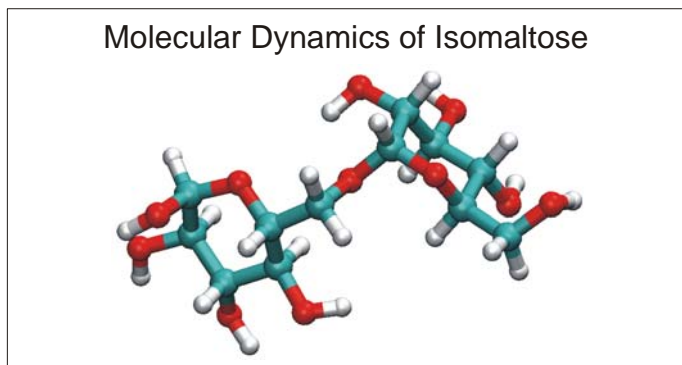
```
Job name      : myjob
Job ID       : https://skurut3.cesnet.cz:9000/bx06C-R9mB5uquZarwpCPQ
Grid job name : myjob (Job type: generic)
Job directory : skurut4.cesnet.cz:/home/kulhanek/jobdir
Job project  : -none-
=====
Alias        : -none-
Organization : voce
Profile      : default
-----
NCPU         : 1
Resources    : -job match-
Properties   : -none-
Sync mode    : gridcopy
-----
Start after  : -not defined-
=====
Job was submitted at      : 2005-10-12 14:16:28
  and was queued for     : 0d 00:04:28
Job was started at       : 2005-10-12 14:20:56
  and was running for    : 0d 00:02:12
Job was finished at      : 2005-10-12 14:23:08
```

- **psync**

```
[jobdir]$ psync
```

```
Starting synchronization procedure.  
  downloading sandbox ...  
  completing data ...  
  downloading data from SE ...  
  unpacking result archive ...  
  cleaning ...  
Synchronization was successfully finished !
```

- output

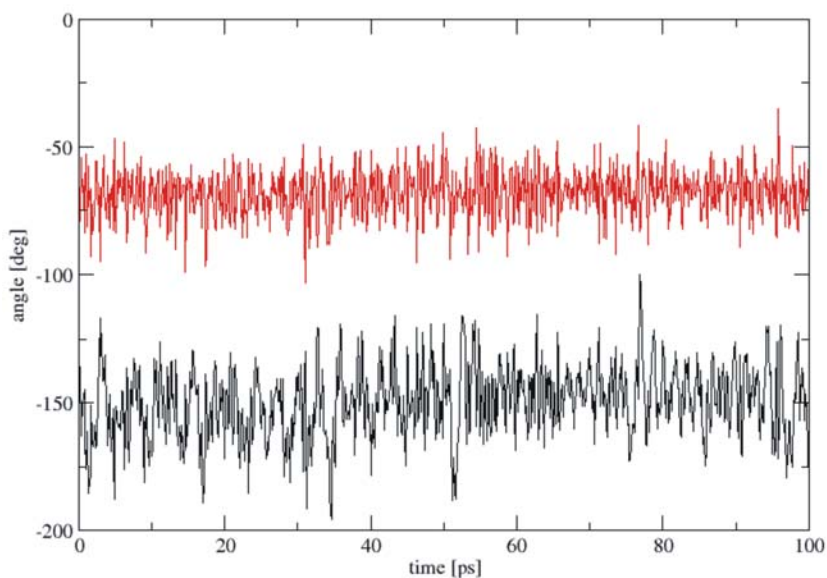


```
[jobdir]$ ls
equi.rst      myjob.ces      myjob.stdout
prep.in       myjob.cesout   mdinfo
isomaltose.top myjob.jdl      prep.traj
myjob         myjob.info     prep.rst
              prep.out
```

input files

control files

results



- **Main features**

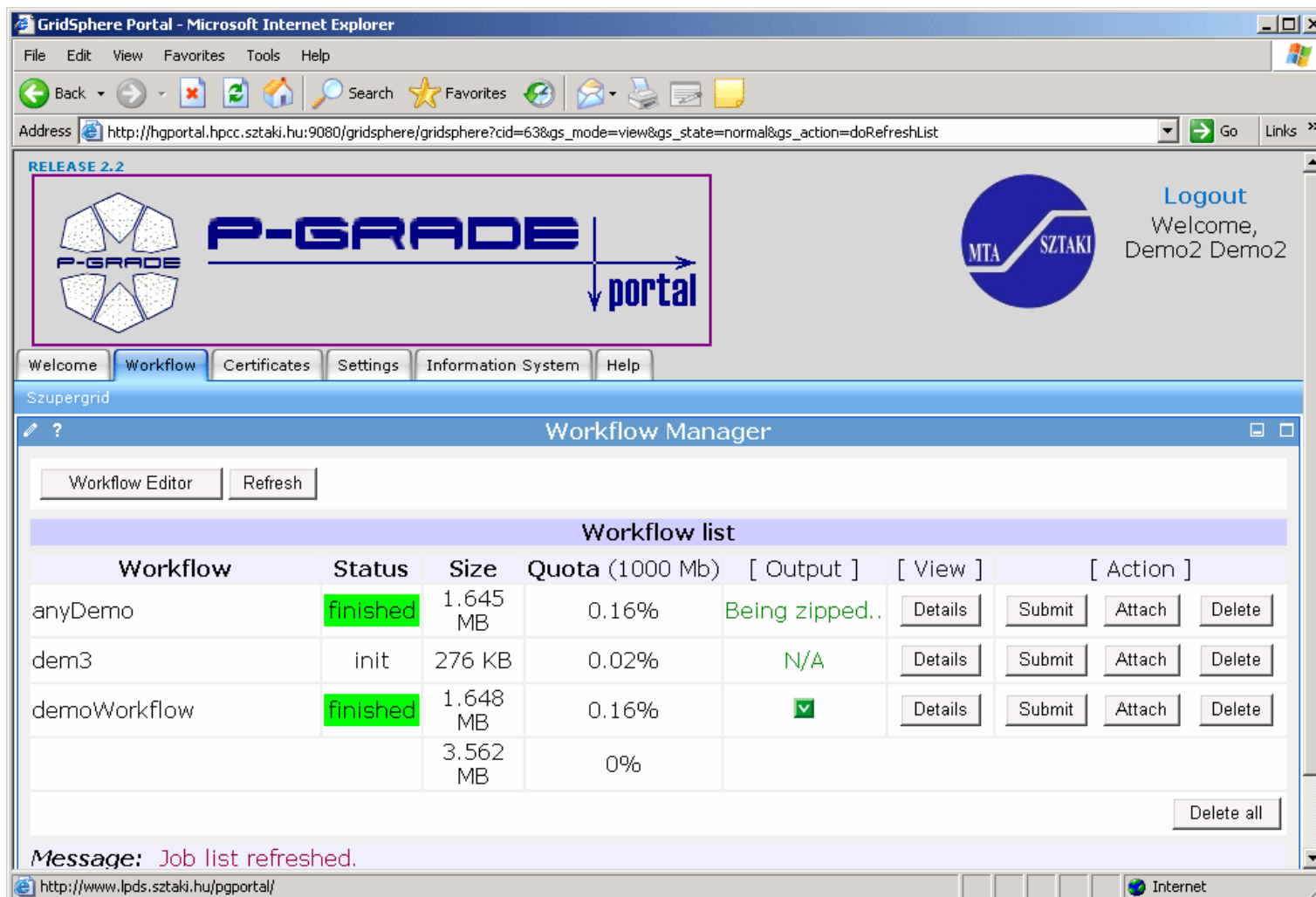
- **Grid middleware neutrality, multi Grid approach**
- single job management
 - encapsulation of a single computational job
 - minimization of overhead resulting from direct middleware usage (no JDL file preparation, *etc.*)
 - easy submission and navigation during job lifetime
- application programs management
 - powerful software management and administration
 - comfortable enlargement of available application portfolio
- documentation
 - CHARON info <http://egee.cesnet.cz/en/voce/Charon.html>

- **Issues to be addressed concerning CHARON**
 - **licensed software**
 - *using ACLs at dedicated application software repository SE*
 - production of **CHARON installer**
 - preparation of LightweightUI
 - *future distribution of CHARON as part of a LightweightUI*
 - support for DAG jobs
 - interconnection between EGEE / VOCE Grid (prototype utilization, guaranteed support) and local national grid environment (experimental utilization, best effort support)

- **P-GRADE – GUI to access VOCE**
 - basic facts
 - **official portal to access VOCE** infrastructure
 - main features
 - general purpose, **workflow-oriented computational Grid portal**
 - supports development and execution of workflow-based Grid applications
 - support for multi-grid workflows ⇔ **multi-Grid approach**
 - GridSphere based
 - *easy to expand with new portlets (application-specific portlets)*
 - *easy to be tailored according to end-user needs*

- **P-GRADE – GUI to access VOCE**
 - provided services
 - easy-to-use workflow concept for solving complex problems
 - fast development of Grid applications
 - integrating various components into large Grid applications:
 - **sequential codes**
 - **MPI codes**
 - **legacy codes**
 - application monitoring, performance visualization, guaranteed correctness

- P-GRADE – GUI to access VOCE



Workflow Manager

Workflow Editor Refresh

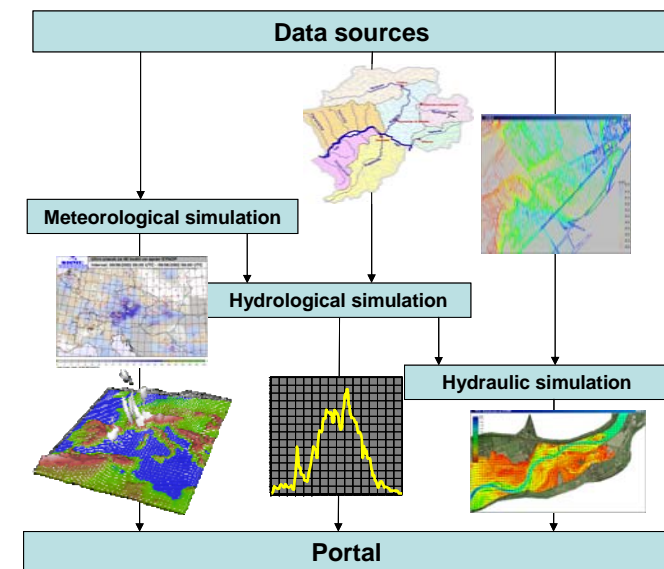
Workflow	Status	Size	Quota (1000 Mb)	[Output]	[View]	[Action]
anyDemo	finished	1,645 MB	0.16%	Being zipped..	Details	Submit Attach Delete
dem3	init	276 KB	0.02%	N/A	Details	Submit Attach Delete
demoWorkflow	finished	1,648 MB	0.16%	✓	Details	Submit Attach Delete
		3,562 MB	0%			

Delete all

Message: Job list refreshed.

- **ESR VO portal**

- **flood application** for forecasting floods using advanced technologies in computer science
- flood application consisted from several components
 - numerical models for **meteorology, hydrology, hydraulics**
 - workflow and data management modules
 - visualization and collaboration modules
 - portal itself
- built using generic portal components
 - portal framework together with management and collaboration modules are applicable for other applications



- **Regional middleware extensions**
 - CE software RPM repository at CYFRONET
 - apt/yum compliant
 - Read/Write access for local certification teams
 - currently available packages
 - OCM-G application monitoring system
 - GLOGIN certificate-based shell access
 - MPICH-P4 tested at CYFRONET
 - flood application ongoing migration

- **How to proceed further?**
 - expand **computational resources** in VOCE
 - utilize VOCE / CHARON / P-GRADE **training infrastructure**
 - extend **application portfolio**
 - migrate towards new application-centric CE VO based on VOCE production experience (e.g. specific MMCC VO)