User friendly high level application support for EGEE/gLite

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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**

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<th>Total Slots</th>
<th>Max Run</th>
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</tbody>
</table>

- 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
    
  
  – documentation
    
  
  – request tracking
    
    ▪ send requests to [voce@cesnet.cz](mailto:voce@cesnet.cz)
Application support - CHARON

• **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

  \[\text{name}[:\text{version}[:\text{architecture}[:\text{parallelmode}] alleged])]\\

  - 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
  - visualizations
    - Grace, PovRay, Raster3D, Molscript

- planned programs to be ported (based on users feedback)
  - Abinit, Dalton, Gromacs
  - Corsika (astrophysics), image processing tools
Provided services

- Application areas
• **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*
Application support - CHARON

- input

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

```bash
# 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 ... 
Submiting job ... 

Job was successfully submitted to GRID environment.
```
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!
Application support - CHARON

Molecular Dynamics of Isomaltose

output

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

input files

control files

results

```
0  0
-50  0
-100  0
-150  0
-200  0

<p>| |</p>
<table>
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<tr>
<th></th>
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<tbody>
<tr>
<td>time [ps]</td>
</tr>
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</table>

<p>| |</p>
<table>
<thead>
<tr>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>[-50,-100 ]</td>
</tr>
<tr>
<td>myjob.rst</td>
</tr>
</tbody>
</table>
```

INFSO-RI-508833

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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
Application support - CHARON

• 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**
• 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)