



Enabling Grids for E-science

Charon Extension Layer

Modular environment for Grid jobs and applications management

Jan Kmuníček

CESNET NA4 effort

www.eu-egee.org



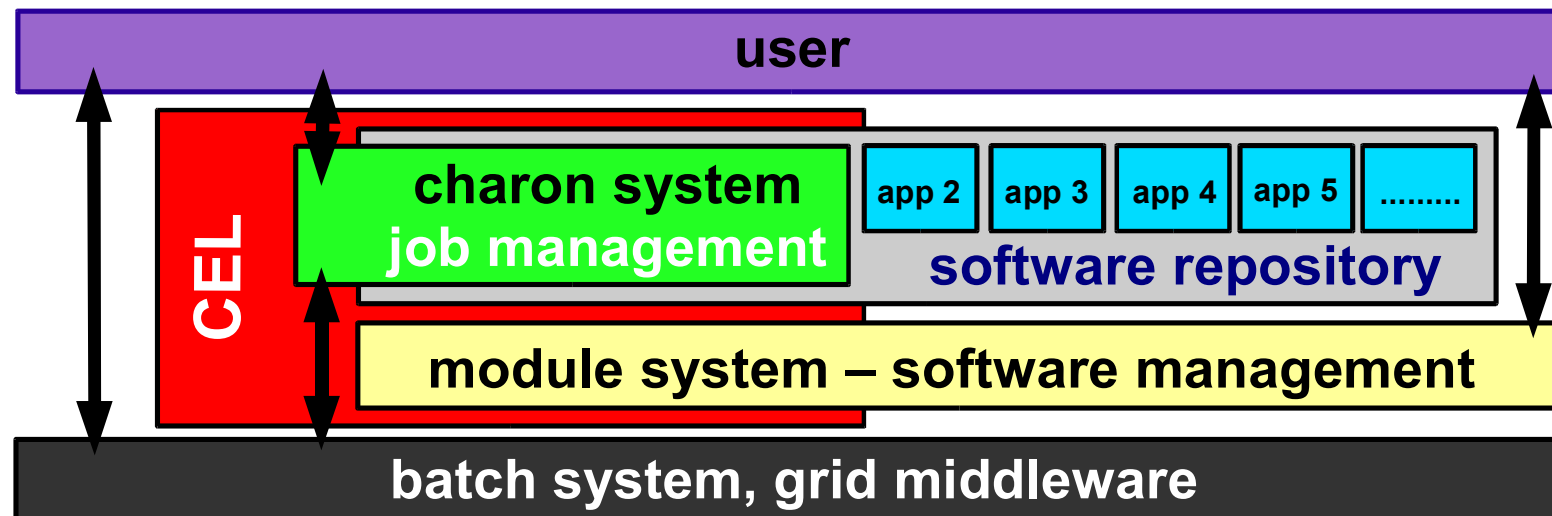
- **Introduction**
- **Charon Infrastructure**
- **Applications Management**
- **Jobs Management**
- **Conclusions**



- **What is Charon Extension Layer?**
 - 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 Extension Layer?**
 - 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



- **Application management**
 - single/parallel execution without job script modification
- **Job management**
 - easy job submission, monitoring, and result retrieving
- **Command Line Interface (CLI) approach**

- **Requirements**

- easy application initialization
- version conflict handling
- inter-application conflicts and/or dependencies handling
- same usage in single/parallel execution
- different levels of parallelizations



Module System

- similar approach as in Environment Modules Project*
 - applications are activated by the modifications of shell environment (e.g. PATH, LD_LIBRARY_PATH, etc.)
- particular build of application is described by realization (e.g. by instructions, which describe shell environment modifications)
- realization is identified by name consisting from four parts:

name[:version[:architecture[:parallelmode]]]
- user can specify only part of realization, in that case, module system completes full name of realization in such a way that the application will best fit available computational resources

*) <http://modules.sourceforge.net/>

- **Commands of Module System**

module [action] [module1 [module2] ...]

- main command of Module System

actions:

- add (load), remove (unload)
- avail, list*, active, exported, versions, realizations
- disp, isactive

* list is default action

modconfig

- menu driven configuration of Module System
(vizualizations, autorestored modules, etc.)

- **Example of Module Activation**

```
$ module add povray
```

```
Module specification: povray (add action)
```

```
=====
WARNING: Nonoptimal architecture is used for module 'povray'
```

```
Cache type           : system cache
Architecture         : i786
Number of CPUs       : 1
Max CPUs per node   : 1
Exported module      : povray:3.6
Complete module      : povray:3.6:i386:single
```

- **Module Name Completion**

```
povray → povray:3.6:auto:auto → povray:3.6:i386:single
user   → default values       → resolved final name
```

- **Module Name Completion**

name - specified by user (it is mandatory)

version - specified by user / default

architecture - specified by user / default / automatically determined

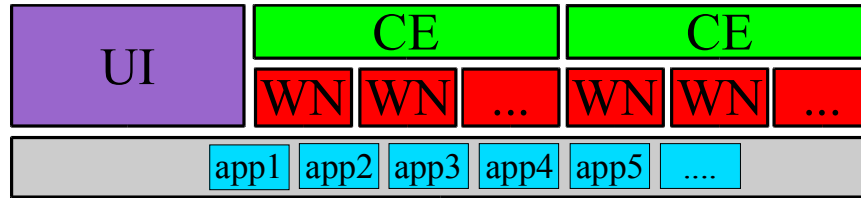
- Module System tries to find such realization, which is the closest to system architecture

parallelmode - specified by user / default / automatically determined

- para - always
- p4 - $N_{CPU} > MaxCPU_{s/node}$
- shmem - $1 < N_{CPU} \leq MaxCPU_{s/node}$
- node - $N_{CPU} \leq MaxCPU_{s/node}$
- single - $N_{CPU}=1$

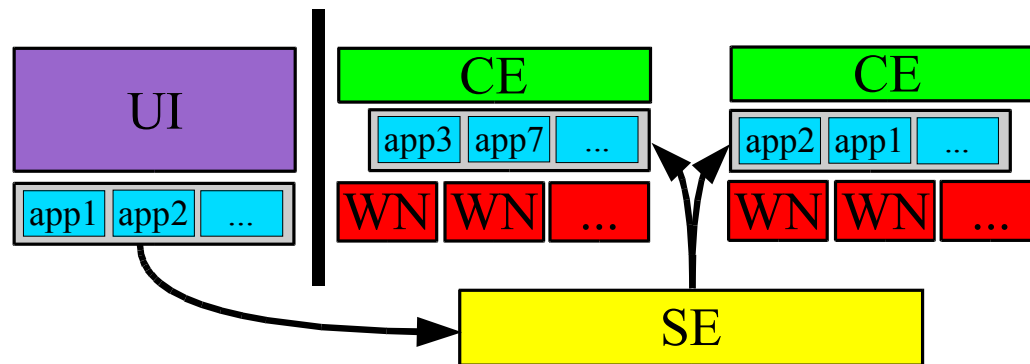
- **Current enhancements of Module System**
 - easy-to-use **configuration of user preferences** using configuration by a single command which is menu driven
 - user can setup the behavior of module name completion, visualization of listed modules
 - user is allowed to select modules to be automatically loaded during site activation
 - user can change priority between system and user module caches
 - **user modules**
 - user is permitted to extend available application portfolio by own module specifications

- **Model I - METACentrum (Czech national GRID)**



Applications are on shared volume available to all grid elements

- **Model II – EGEE GRID**



Legend:

- UI - user interface
- CE - computing element
- SE - storage element
- WN - worker node
- app - application

- applications cannot be shared with all grid elements
- their “sharing” is provided by their deployment to SE (once time)
- only required applications are then installed on CE during ever job execution

- **Interactive browser of the module database**
 - extension of Module system containing real-time list of available software realizations
 - this service can show the list of available applications with or without the accessible application versions
 - this information is integrated with the detailed description of applications (documentation of particular compilation and installation in the MediaWiki)



<http://troll.chemi.muni.cz/whitezone/development/charon/isoftrepo/>

Site Info - Mozilla Firefox

http://troll.chemi.muni.cz/whitezone/development/charon/isoftrepo/site.php?site=voce&type=cat&includeversions=no

iSoftrepo - Interactive Software Repository CEL - Charon Extension Layer

Site Info

sites / voce

Categories Categories (versions) List of realizations Tree of realizations

Molecular Mechanics and Dynamics

- autodock
- gromacs
- solvate

Quantum Mechanics and Dynamics

- abinit
- dalton
- pcgames
- uspp

Conversion and Analysis

- babel
- hull
- qhull
- cats
- octave
- retinal
- cpmd2cube
- openbabel
- wham
- hbplus
- pdb2pqr

Vizualization

- gnuplot
- povray
- grace
- raster3d
- ligplot
- molscript

Nuclear Magnetic Resonance

- dasha

Physics, Astrophysics, Technical and Material Simulations

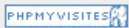
- gmsh
- getdp
- mpb
- octave

Compilers and Supporting Environment

- mpichrun

System

- charon
- hwtoken
- certificates
- ui-voce
- general
- voce
- glibc

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- **Requirements**

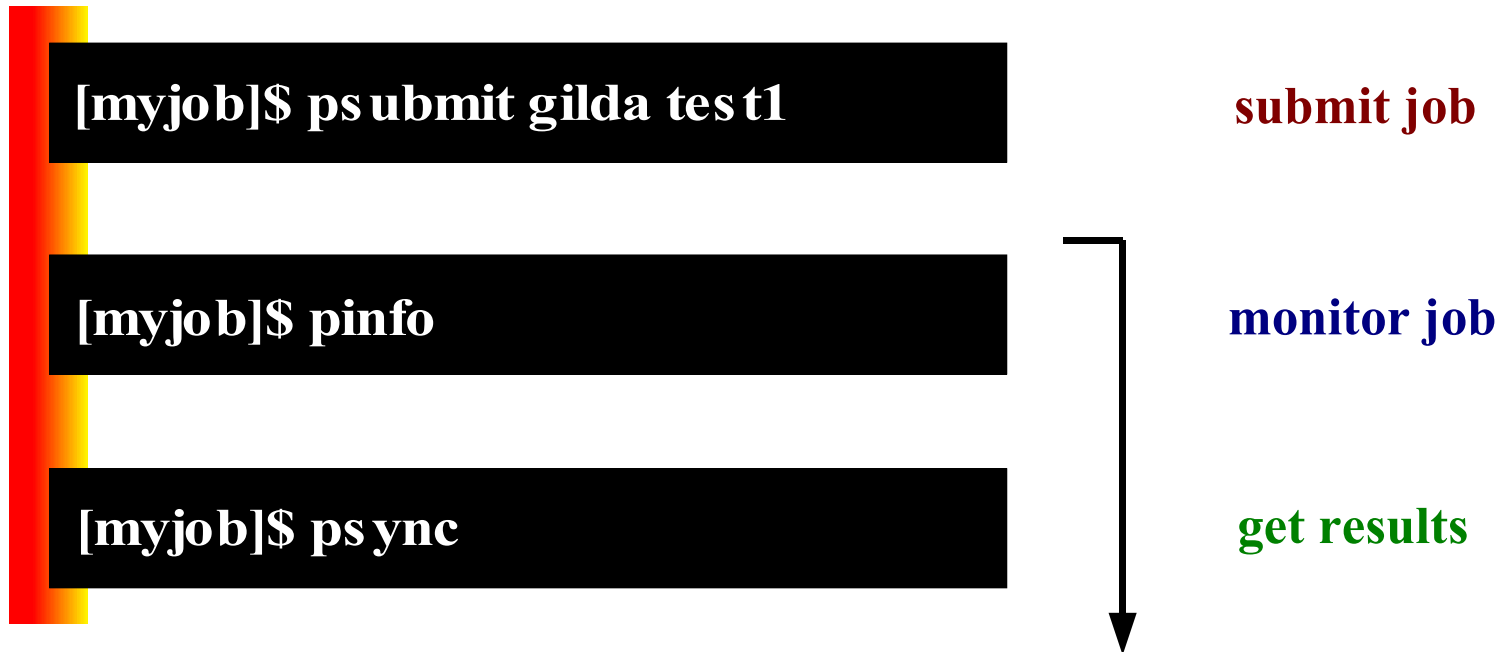
- easy job submission
- user should focus only on desired task not to all things related to submissions
- easy parallel executions of applications
- often repeated things should be process automatically
- keep information about job during execution and/or after execution



Charon System

- **Overview**
 - it is application in the context of Module System
 - it separates resources settings from job submission
- **Job Submission and Management**
 - **psubmit** <resources> <job_script> [NCPU] [syncmode]
 - **pinfo**
 - **psync**
 - **pkill**
 - **pgo** (does not work in EGEE GRID environment)
- **Charon Setup**
 - **pconfigure**

- **Typical job flow**



No additional arguments are required – all information about job is stored in control files in job directory.

- **Job Restrictions**

- job is described by script (specific input files can be autodetected)
- **each job has to be in separate directory** – control files need to be unique
- job directories must not overlap – because job directory is copied to WN and then back
- only relative paths to job directory contents have to be used in job script – only data from job directory will be present on WN
- software should be activated by Module System – only then best utilization of resources can be reached

- **Configuration**

- **Sync Mode** – option for data transfer between UI and WN
 - gridcopy
 - *all data within job directory as input and as as result*
 - stdout
 - *all data within job directory as input*
 - *only standard output as result (other data are discarded)*
- **Resources** – identification of particular CE
- **Properties** – fine grained selection of computational resources (through Requirements item in JDL)
- **Alias** – uniform combination of above setup items in a singleword

pconfigure menu driven command for configuration

- **Currently implemented features**
 - multi-grid (sites) approach
 - **virtual encapsulation of computational resources**
 - support for Job Provenance service
- **Planned features**
 - advanced job statistics
 - workflow support (DAG jobs)
 - access through graphical user interface

- **Single job management**
 - **encapsulation of a single computational job**
 - minimization of overhead resulting from direct middleware usage(JDL file preparation, etc.)
 - easy submission and navigation during job lifetime
- **Application management**
 - **powerful software management** and administration
 - comfortable enlargement of available application portfolio

- **Uncover all details!**
 - visit available web pages at

<http://egee.cesnet.cz/en/voce/Charon.html>