



Enabling Grids for E-science

IBCP - CNRS STATUS

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Lyon - France

5th Quattor workshop - Bologna - 17/03/2008

www.eu-egee.org



- **Institute of Biology and Chemistry of Proteins**



- Dir. Prof. G. Deléage, <http://www.ibcp.fr>, LYON, FRANCE
- Associated to CNRS and Univ. Lyon1

- **Study of proteins in their biological context**

- Approaches used include : integrative cellular (cell culture, various types of microscopies) and molecular techniques, both experimental (including biocrystallography, and nuclear magnetic resonance) and theoretical (structural bioinformatics)



- **3 departments, 13 groups**

- Topics such as cancer, extracellular matrix, tissue engineering, membranes, cell transport and signalling, bioinformatics and structural biology



What about the GPSA portal

- **Scientific objectives**
 - Molecular Bioinformatics: protein sequence analysis
 - Analyse data from high-throughput Biology: complete genome projects, EST, complete proteomes, structural biology,
 - Integration of biological data and tools
- **Method**
 - Provide Biologists with an usual Web interface: NPS@
 - ✦ NPS@ Web portal online since 1998
 - ✦ 46 tools & 12 updated databases
 - ✦ + **10,000,000 jobs** & 5,000 jobs/day
 - Ease the access to updated databases and algorithms.
 - Protein databases are stored on grid storage as flat files.
 - Legacy bioinformatics applications
 - ✦ Wrapping usual binary in grid environment
 - ✦ transparent remote access with local filesystem
 - Display results in graphical Web interface.
- **Status:** Production
- **Contact:** Christophe.Blanchet@ibcp.fr



NPS@ | BLAST Homology Search

http://gpsa-pbl.ibcp.fr/cgi-bin/npsa_automat.pl/page...

Pôle Bioinformatique Lyonnais
Network Protein Sequence Analysts

GPSA is the grid part of NPS@ from PBL/IBCP in Lyon, France

(HOME) (NPS@) (SRS) (HELP) (REFERENCES) (NPSA) (LANTHIBROT) (Geno3D) (SuMo) (Positions) (PBL)

February 27, 2006: First public release of GPSA@ online at <http://gpsa.pbl.ibcp.fr>
Take advantage of the EGEE Grid platform for your bioinformatic analysis on the NPS@ portal.

Work supported in part by projects: French ACI Grid GridPPS, EU-FP6 EGEE and EU-FP6 EMBRACE.

EGEE Enabling Grids for E-science

MBRACE Grid

BLAST search on protein sequence databank

(About) (FAQ) (Help) (Original server)

Programs:

Database:

Sequence name (optional):

Paste a protein/nucleic sequence below:

Use the GRID resources from EGEE

SUBMIT CLEAR

User: public@193.55.43.12. Last modification time: Fri Jul 12
This service is supported by *Ministère de la recherche (ACC-Alisa (Programme EMERGENCE))*. Comments

IBCP

PBL
ibcp.fr

- **OBJECTIVES OF THE IBCP'S EGEE NODE**
 - Provide resources to Biomed VO.
 - Operational site for testing our applications.
 - Different levels of expertise :
 - user,
 - administrator,
 - developer - grid applications port and support.

- **site IBCP-GBIO**
- **gLite 3.1**
- **COMPUTERS**
 - 1 CE : 1 GB ram, 1 CPU - SL 4.5 64 bits (virtual machine),
 - 1 SE : 2 GB ram, 2 CPU, 74 GB of storage (XSan) - SL 4.5 64 bits (virtual machine),
 - 18 WN (11) : 2 GB ram, 2 CPU - SL 4.4 32 bits.
- **Gigabit ethernet**
- **QWG templates - rev. 3054**

- **Automatised configuration for OS and gLite middleware.**
- **Compensation for the lack of human power.**
- **Focus on our job and objective : biology.**
- **Need an efficient tool : QUATTOR ?**

- **August 07** : Introduction of Quattor by Cal Loomis (Paris & Lyon) ⇒ creation of our repository.
- **From august 07 until now** :
Precious help from Michel Jouvin and Guillaume Philippon, other sites feedback.
- **Online documentation** :
 - <http://quattor.web.cern.ch/quattor/documentation.htm>
 - <https://trac.lal.in2p3.fr/LCGQWG>
 - <http://www.eu-egee.org/>
 - <https://twiki.cern.ch/twiki>
 - <http://www.ukiroc.eu/>
 - ...
- **Mailing lists** :
 - project-quattor@cern.ch, project-lcg-gdb-quattor-wg@cern.ch
 - EGEE-SA1-FR-L@in2p3.fr

⇒ **Site** : Being deployed from scratch since august 07.
Pending SA1 certification (invalid lcg tools).

- **gLite 3.0 : configuration of mysql database for apel accounting.**
- **QWG tpl rev 2847**
 - Missing of lcg-info-static-site.conf in /opt/glite/etc/gip
⇒ no publication of site information by the BDII.
 - Missing of gsi-authz.conf in /etc/grid-security
⇒ globus-gatekeeper not functional.
- **Missing of perl-DateTime package.**
- **Identification of these problems when machines are reinstalled and not just updated.**

- **Template `pro_site_system_filesystems` : sda/hda only.**

```

variable DISK_BOOT_DEV_B = {
  if (exists("/hardware/harddisks/sdb")) {
    return("sdb");
  };
};

variable DISK_PART_SDB ?= {
  if (exists(DISK_BOOT_DEV_B) && is_defined(DISK_BOOT_DEV_B)) {
    return(DISK_BOOT_DEV_B+"1");
  };
};

"/system/filesystems" =
if (exists(DISK_PART_SDB) && is_defined(DISK_PART_SDB)) {
  set_partitions(

```

⇒ **Modified to configure sdb when exists.**

- TFTP server ≠ RPM repository server
 - Template pro_site_global_variables

```
# Name of tftp server used by PXE installation
variable AII_OSINSTALL_SRV = "quattor.ibcp.fr";
```

- Template quattor/aii/config (in cfg/standard)

```
#
# Install type and URL (for http or https) or directory (for NFS)
# with the OS distribution
# For backward compatibility (deprecated), allow installtype to be defined explicitly
# rather than from AII_OSINSTALL_xxx variables.
#
"/system/aii/osinstall/options/installtype" ?= {
  if ( !exists(AII_OSINSTALL_PATH) || !is_defined(AII_OSINSTALL_PATH) ) {
    error("You need to define the variable AII_OSINSTALL_PATH or AII_OSINSTALL_ROOT "
      + "(OS distribution location on the Quattor server)");
  };

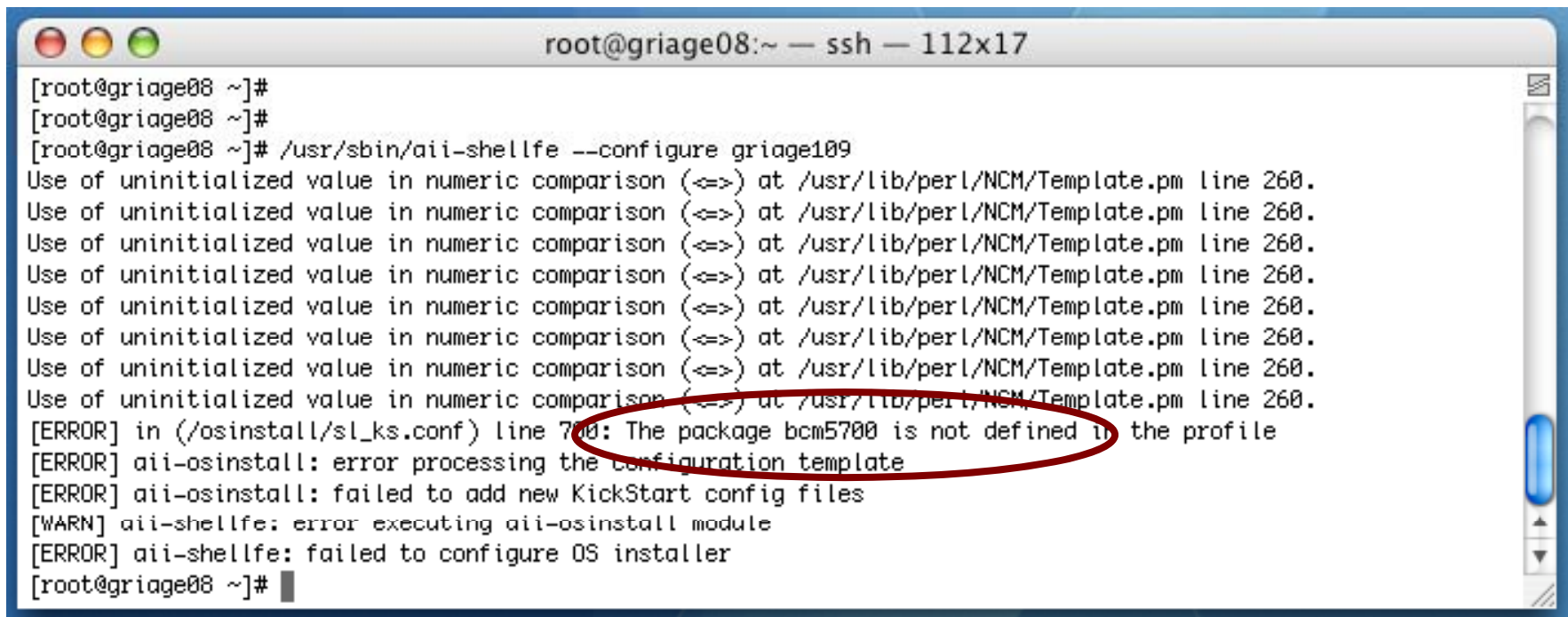
  if ( match(AII_OSINSTALL_PROTOCOL, "^https?") ) {
    return("url --url " + AII_OSINSTALL_PROTOCOL + "://" + AII_OSINSTALL_SRV + AII_OSINSTALL_PATH);
  } else if ( match(AII_OSINSTALL_PROTOCOL, "(?i)nfs") ) {
    return("nfs --server " + AII_OSINSTALL_SRV + " --dir " + AII_OSINSTALL_PATH);
  } else {
    error('Unsupported OS installation protocol: '+AII_OSINSTALL_PROTOCOL);
  };
};
```

⇒ **Redefine /system/aii/osinstall/options/installtype in each profile.**

- **CREATION OF KICKSTART FILE**

AII-SHELLFE --configure :

- Always the same errors (line 260).
- Nodes \neq TFTP server \Rightarrow missing module (package bcm5700).



```

root@griage08:~ -- ssh -- 112x17
[root@griage08 ~]#
[root@griage08 ~]#
[root@griage08 ~]# /usr/sbin/aii-shellfe --configure griage109
Use of uninitialized value in numeric comparison (<=>) at /usr/lib/perl/NCM/Template.pm line 260.
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Use of uninitialized value in numeric comparison (<=>) at /usr/lib/perl/NCM/Template.pm line 260.
[ERROR] in (/osinstall/sl_ks.conf) line 700: The package bcm5700 is not defined in the profile
[ERROR] aii-osinstall: error processing the configuration template
[ERROR] aii-osinstall: failed to add new KickStart config files
[WARN] aii-shellfe: error executing aii-osinstall module
[ERROR] aii-shellfe: failed to configure OS installer
[root@griage08 ~]#
  
```

- **CE - BDII**

```
[root@grive11 ~]# tail -f /opt/bdii/var/bdii.log
```

Error for mkdir /var/glite: Permission denied at /opt/glite/libexec/glite-info-provider-ldap line 86 ==> slapadd: could not parse entry (line=2)

```
[root@grive11 ~]# mkdir /var/glite
```

```
[root@grive11 ~]# chown edguser /var/glite
```

```
[root@grive11 ~]# chgrp edguser /var/glite
```

- **SE - DISK POOLS AND DPMMGR RIGHTS (dpm-qryconf)**

```
gridmac02:/Volumes/egEE/se01 root# mkdir biomed/vol
```

```
gridmac02:/Volumes/egEE/se01 root# mkdir biomed/perm
```

```
[root@grive12 ~]# dpm-addpool --poolname VBio --def_filesize 200M --def_pintime 600 --s_type V
```

```
[root@grive12 ~]# dpm-addpool --poolname PBio --def_filesize 200M --s_type P
```

```
[root@grive12 ~]# dpm-addfs --poolname VBio --server grive12.ibcp.fr --fs /gbiose01/biomed/vol
```

```
[root@grive12 ~]# dpm-addfs --poolname PBio --server grive12.ibcp.fr --fs /gbiose01/biomed/perm
```

- **Biomed site :**
 - Objectives
 - Provide resources to Biomed VO.
 - Operational site for testing our applications.
 - Different levels of expertise on EGEE grid.
 - Status of IBCP-GBIO site
 - Installation from scratch.
 - Deployed by bioinformaticians, not quattor developers.
 - Pending for certification.
- **Improve online documentation**
 - All configuration.
 - Python 32 bits for SL 64 bits.
 - Cohabitation of gLite 3.0 and 3.1.



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THANKS FOR YOUR ATTENTION