EUROGRID Vision

Build a European Grid infrastructure that gives users a seamless, secure access to High Performance Computing resources and that advances computational science in Europe

Piotr Bała
UNICORE architecture

UNICORE Client

UNICORE Gateway A

UNICORE Gateway B

UNICORE Server (NJS)

UNICORE Server (NJS)

TSI

TSI

NQE (Cray T3E)

PBS (Linux cluster)

Insecure Internet

UNICORE Security

- Based on the PKA
- Industrial standard X509
- Secure communication
  - Gateway, NJS certificates
  - Gateway, NJS check user certificate
  - Multiple CA accepted
- User certificates
  - User certificate stored in client
  - Public key stored in UUDB database at each site
  - PKA mapped to user account (XLOGIN)
    - more than one certificate can map to xlogin
    - multiple CA allowed
  - Multiple certificates allowed
EUROGRID resources

- European HPC GRID testbed
- Agreement on security standards, certification, access policies etc.

**UNICORE Client**

- Single application
- Job preparation
- Job monitoring
UNICORE Client – Gaussian98 job preparation
UNICORE Applications

- Job files for user applications
  - script tasks
  - command tasks
  - file transfer tasks (client-vsite, vsite-vsite)

- Plug-in for job and input preparation

- User can run the same script at all VSITES
  - Introduction of IDB entries for site dependent installation
    GROMOS96=/pkg/gromos96; export GROMOS96
    GAUSS_EXEDIR=/pkg/gaussian/g98; export GAUSS_EXEDIR
    AMBERHOME=/pkg/amber6; export AMBERHOME
    CHARMM=/pkg/charmmb2/exec/t3e/charmmb; export CHARMM
BioGRID

- UNICORE Client (ver 3.6.7) unix and Windows
  - Easy installation (www.unicore.org)
- Example jobs:
  - Gaussian98
  - Amber
  - Gromos
- Plugins
  - Gaussian98
  - AMBER
  - CPMD (Unicore Plus project)
  - PDB Search
  - List Jobs

Gaussian98 plugin

Input preparation reads existing input, recognizes keywords

Molecule coordinate editor formats:
- XYZ
- Z-matrix
- text
Gaussian98 plugin

CPU time estimate based on known algorithm scaling $O(N^4)$

Checks program availability

Prepares and transfers files for visualization
Gaussion98 plugin

Output

Amber 6.0 plugin

Input preparation
Amber 6.0 plugin

Input can be edited by user

Errors are marked in red

Panel for each group of options

Default options

Help window

Flag for the removal of translational and rotational motion at the beginning of the simulation.

-0: The translational and rotational motion about the center of mass is not removed (default).

=1: The above motion is removed once time at the beginning of the simulation.
Amber 6.0 plugin

CPMD plugin

Find parameter button

CPMD input
CPMD plugin

Job submission

CPMD plugin

Output window
- text
- tables
- graphs
PDB search plugin

Lite search

Enter a PDB ID or keyword: 

- query by PDB id only
- match exact word
- remove sequence homologues

PDB search plugin

Advanced search

PDB Identifier:

Citation Author:

Authors of primary citation only!

Compound Information:

Title:

PDB HEADER:

Exp. Technique: – select one –

Text Search:

Select a subset of results with sequence homologues removed

- 50% sequence identity

Library Plugin

Piotr Bala
PDB search plugin

User can use different mirrors
The best one is selected (fastest answer)

Visualization with external packages
List All Jobs Plugin

<table>
<thead>
<tr>
<th>User</th>
<th>Video</th>
<th>Job name</th>
<th>Status</th>
<th>Date</th>
<th>ID</th>
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<tbody>
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<td>PZJ</td>
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BioGRID

- Operate a GRID for biomolecular simulations
- Develop interfaces to existing biological and chemical codes
- Web site: biogrid.icm.edu.pl
Web site

Information on software
- info
- home page
- local info
- VSITEs
- USITEs

Web site

Step by step user guides
GRIP Project

Extend EUROGRID to cooperativity with globus middleware.
Provide UNICORE users with access to resources available through globus.

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biogrid.icm.edu.pl
www.eurogrid.org
www.grid-interoperability.org

Funding by European Commission Grant No. IST-1999-20247 (EUROGRID) and IST-2001-32257 (GRIP)