EUROGRID - Seamless Access to Computer Resources with Unicore

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

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
UNICORE architecture

UNICORE Client

UNICORE Gateway A

UNICORE Gateway B

Insecure Internet

UNICORE Server (NJS)

UNICORE Server (NJS)

TSI

TSI

NQE (Cray T3E)

PBS (Linux cluster)

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

The image shows the UNICORE Client software interface with a focus on job preparation. The interface includes options for job submission, monitoring, and settings. The highlighted section is titled "Script Editor" with a sample script for Gaussian98 job preparation.

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UNICORE Client – edit resources for job

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/charmm/c27b2/exec/t3e/charm; export CHARMM
Gaussian98 in EUROGRID

- Easy installation ([www.unicore.org](http://www.unicore.org))
- Example jobs:
  - Gaussian98
  - Amber
  - Gromos
- Plugins:
  - Gaussian98
  - AMBER
  - CPMD (Unicore Plus project)
  - PDB Search
  - List Jobs
  - Local Model (DWD, SCSC)
  - Crash code (T-Systems)
  - Electromagnetic code (EADS)
  - Fluent (Unicore Plus project)
  - Nastran (Unicore Plus project)

BioGRID

- UNICORE Client (ver 3.6.7) unix and Windows
  - Easy installation ([www.unicore.org](http://www.unicore.org))
Gaussian98 plugin

Input preparation reads existing input, recognizes keywords

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

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

Checks program availability
Gaussian98 plugin

Prepares and transfers files for visualization.

Gaussian98 plugin

Output

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Amber 6.0 plugin

Input preparation

Input can be edited by user

Errors are marked in red
Amber 6.0 plugin

Panel for each group of options

Default options

Help window

Plug 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 one time at the beginning of the simulation.

Find parameter button

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CPMD plugin

CPMD input

PDB search plugin

Lite search
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>File</th>
<th>User</th>
<th>Job name</th>
<th>Status</th>
<th>Date</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>PZI</td>
<td>1-aFT</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
</tr>
<tr>
<td>PZI</td>
<td>2-aFT</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
</tr>
<tr>
<td>UOM</td>
<td>1-aFT</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
</tr>
<tr>
<td>Parnas</td>
<td>Parnas</td>
<td>New_job1</td>
<td>?</td>
<td>?</td>
<td>15/05/2019</td>
</tr>
<tr>
<td>UOM</td>
<td>2-aFT</td>
<td>New_job1</td>
<td>?</td>
<td>?</td>
<td>15/05/2019</td>
</tr>
<tr>
<td>UOM</td>
<td>3-aFT</td>
<td>Environment_test1</td>
<td>SUCCESSFUL</td>
<td>13/06/2019 19:33:10</td>
<td>22570503</td>
</tr>
</tbody>
</table>

File filter plugin

Pick up job from JMC
Define file to process
Submit job
**BioGRID**

- Operate a GRID for biomolecular simulations
- Develop interfaces to existing biological and chemical codes
- Web site: biogrid.icm.edu.pl
UNICORE 4.0

- UNICORE 4.0
  - Loops, conditional execution
- Plugins available for 4.0
  - List All Jobs Plugin
  - PDB Search Plugin
  - Gaussian98 Plugin
  - CPMD Plugin (V. Huber)
- Work in progress:
  - Amber plugins should be available soon
  - Text and graphical postprocessing
  - Resource Broker (UoM)
  - Interactive Access (Parallab)

GRIP Project

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

  *Web based system for wavepacket dynamics*
  *Lecture Notes in Computer Science* 2329, pp. 552-561

- J. Pytliński, Ł. Skorwider, P. Bała, M. Nazaruk, K. Wawruch
  *BioGRID - uniform platform for biomolecular applications*
  *Lecture Notes in Computer Science* 2400, pp 881-884

- J. Pytliński, Ł. Skorwider, K. Bednarczyk, V. Huber, P. Bała
  *UNICORE - An Uniform Platform for Chemistry on the Grid*
  *Journal of Computational Methods in Science and Engineering* 2 (3s-4s) p. 369-376

- P. Bala, B. Lesyng, D. Erwin
  *EUROGRID – European Computational Grid Testbed*
  *Journal of Parallel and Distributed Computing (in press)*

- J. Pytliński
  Master degree in computer science thesis, UMK 2002

- Ł. Skorwider
  Master degree in computer science thesis, UMK 2002

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**biogrid.icm.edu.pl**
**www.eurogrid.org**

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Funding by European Commission Grant No. IST-1999-20247 (EUROGRID)
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