



Interdisciplinary Centre For Mathematical and Computational Modelling
Warsaw University



www.eurogrid.org

Piotr Bała
WMIi UMK
Toruń



bala@mat.uni.torun.pl

Current situation of HPC

- High Performance Computing (HPC) systems are a critical resource for research and development
- Operation of HPC systems requires specialised centres
- European HPC centres offer a variety of HPC architectures from different vendors with frequent innovation
- Users want to focus on their science rather than becoming HPC specialists
- European HPC centers and users are connected by high-bandwidth networks



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**

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EUROGRID Goals

- Support the e-Science concept
- Integrate resources of leading European HPC centres into a European HPC GRID
- Develop new software components for GRID computing
- Demonstrate the ASP model for HPC access ('HPC portal')

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EUROGRID Partners

HPC Centres

- CSCS Manno (CH)
- FZ Jülich (D)
- ICM Warsaw (PL)
- IDRIS Paris (F)
- Univ Bergen (N)
- Univ Manchester (UK)

Users

- Deutscher Wetterdienst
- EADS
- debis Systemhaus
(Assistant Partner)

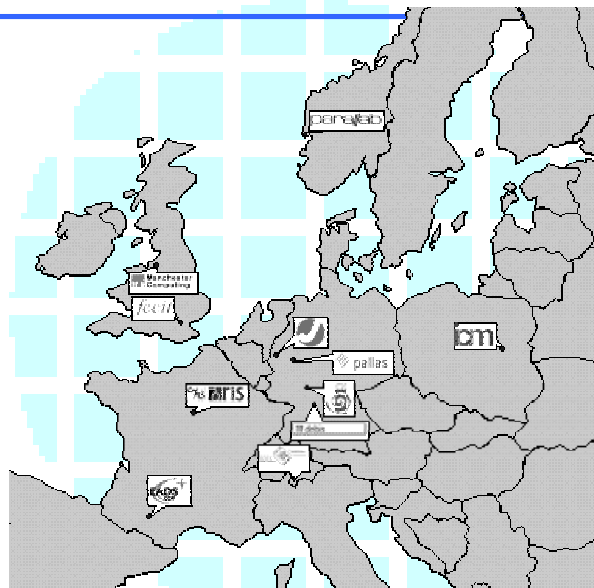
Integration

- Pallas (Project Coordinator)
- Fecit (Assistant Partner)

Volume: 33 person years, 2 MEuro funding
by European Commission Grant No. IST-1999-20247



EUROGRID Geography



Structure of the Work

- Application GRIDS:
application-specific interfaces, evaluation of GRID solutions
 - Bio-GRID
 - Meteo-GRID
 - CAE-GRID
- HPC GRID Infrastructure:
connect HPC centers using UNICORE technology
- Development and integration of new components
- Dissemination and exploitation

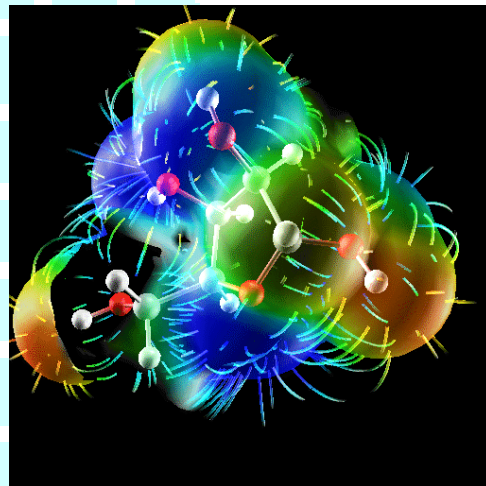
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Bio-GRID

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



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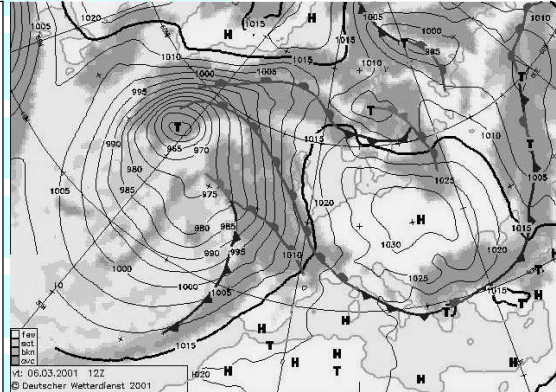
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Meteo-GRID

- Develop a relocatable version of DWD's weather prediction model
- Goal: 'Weather prediction-on-demand' as an ASP solution



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CAE-GRID

- Coupled simulations of aircrafts (e.g. structure and electromagnetics)
- Goal: internal HPC portal for EADS engineers



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CAE-GRID

- Provide HPC portal to engineers at Daimler-Chrysler and partners
- Develop GRID technology for computing cost estimates and billing









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HPC-GRID

- Demonstrate a European HPC GRID testbed
- Develop new GRID applications
- Enable sharing of competence and know-how
- Agree on security standards, certification, access policies, ...

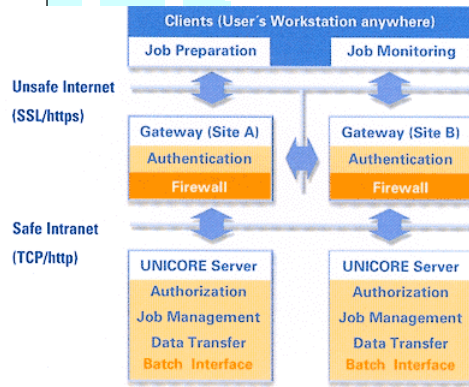
 <p>CRAY T3E 900 (32 PE) NEC SX4B/2A Linux Cluster (4 PE)</p>	 <p>SGI SGI O2000 (128 PE)</p>
 <p>Linux Intel Cluster (36 PE) CRAY T3E - 600 (512 PE) CRAY T3E - 1200 (512 PE)</p>	 <p>IBM SP3 (8 PE) NEC SX5 cluster (40 PE) IBM Power4 (256 PE, 1.3 TFLOPS) COMPAQ Linux Cluster (24 PE)</p>
 <p>CRAY T3E - 1200 (816 PE) FUJITSU VPP300 (8 PE) SGI O2000 (128 PE) SGI O3000 (256 PE)</p>	

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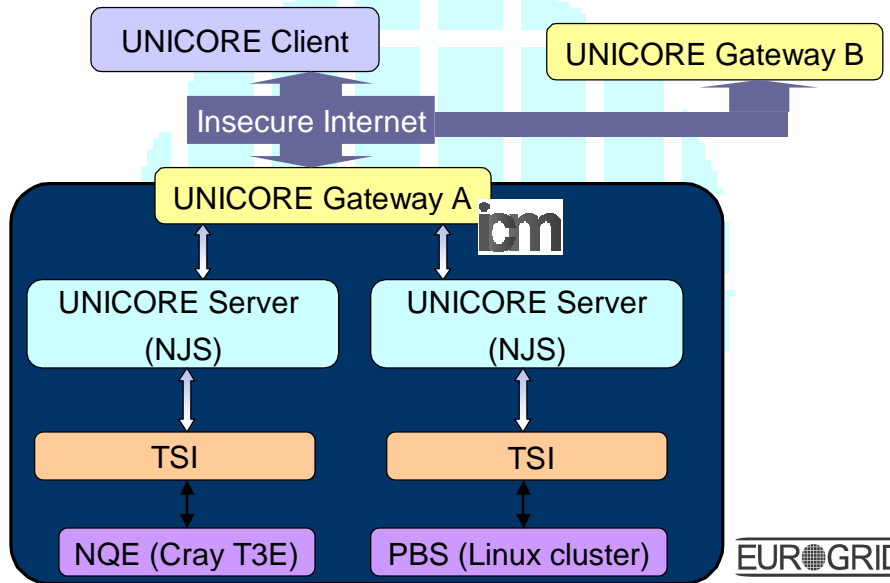
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EUROGRID Infrastructure and Components

- Based on UNICORE system
- Develop additional GRID components
 - efficient data transfer
 - ASP infrastructure
 - resource broker
 - application coupling
 - interactive access
- Integration of new components by Pallas and Fecit



UNICORE architecture



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 UADB database at each site
 - PKA mapped to user account (XLOGIN)
 - more than one certificate can map to xlogin
 - multiple CA allowed
 - Multiple certificates allowed

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UNICORE Security - Client

- User certificate
- Trusted CA

UNICORE: Certificates

User certificates

- pallas (Default)
- icm

Exports

Certificate

-Subject
Piotr Bała
Warsaw University
ICM
Warsaw
bala@icm.edu.pl

-Issuer
Pallas CA
Pallas GmbH
pst
Bruehl
support@pallas.com

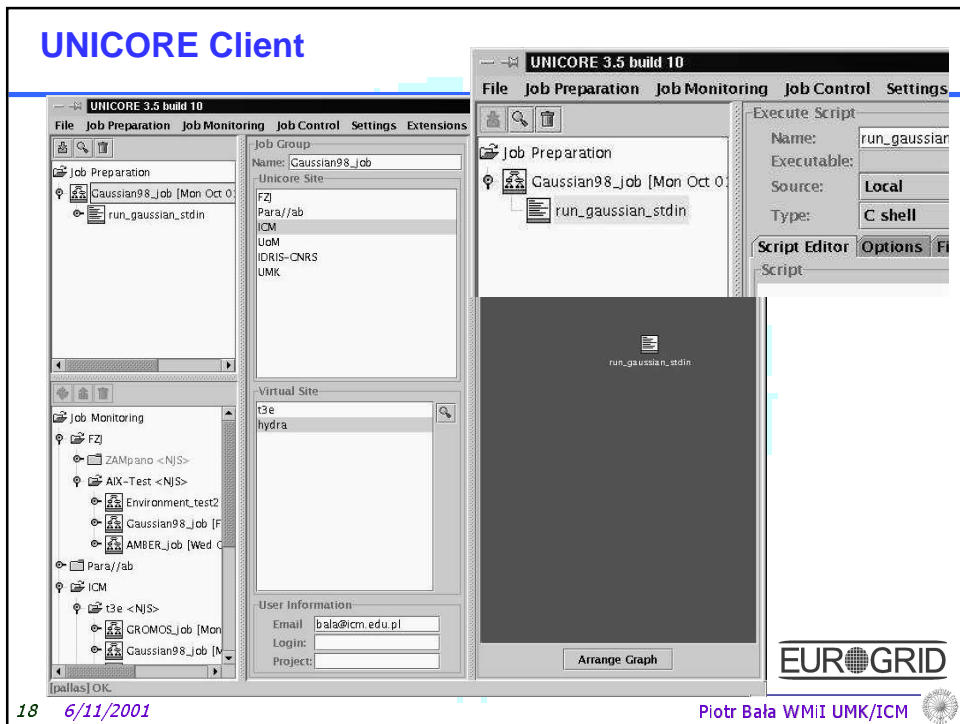
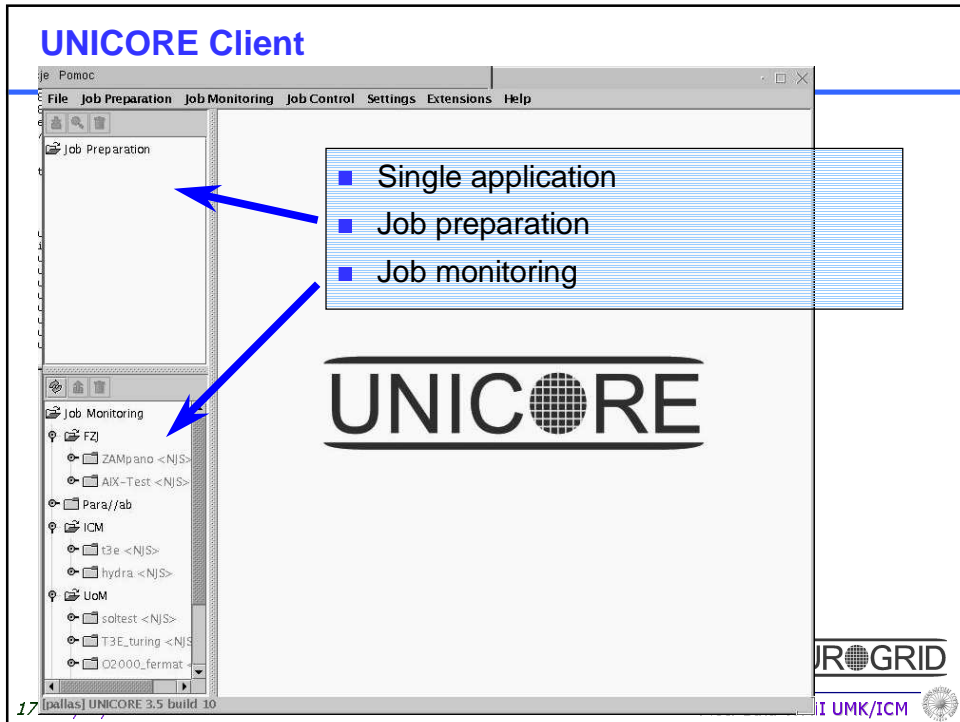
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Valid from Wed Apr 04 11:06:11 CEST 2001 to Thu Apr 04 11:06:11 CEST 2002

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EUROGRID



UNICORE Client

UNICORE: Resource Editor

Task Storage

- Memory: 128 Megabytes per node
- Nodes: 1 Nodes
- Processors: 1 Processors per node
- Run Time: 100 Seconds
- Priority: High

Buttons: Set to user defaults, Set to site defaults, Check values, Ok, Cancel

Script Editor content:

```
$GAUSS, E
# HF/6-31G(d)
water ener
O 1
O -0.464 0.177 0.0
H -0.464 1.137 0.0
H 0.441 -0.143 0.0
EOF
```

Put your input here

```
$GAUSS_EXEDIR/g98 << EOF
# HF/6-31G(d)
water energy
O 1
O -0.464 0.177 0.0
H -0.464 1.137 0.0
H 0.441 -0.143 0.0
EOF
```

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Current Status

- First year of project finished (Nov./Dec. 2001)
- Project web site: www.eurogrid.org
- EUROGRID-0 installed (Feb. 2001) and tested, requirements from different application areas defined.
 - UNICORE 3.1 software
- EUROGRID-0.5 installed (Sept. 2001)
 - UNICORE 3.5 software
 - UNICORE 3.5.10 client
 - Cooperation with UNICORE Plus project
 - UNICORE test site www.eurogrid.org

BioGRID biogrid.icm.edu.pl

- BioGRID extensions
 - Introduction of IDB entries for site dependent installation.
 - Abstract Job Objects (AJO) for biomolecular packages
 - Gaussian98
 - GROMOS96
 - AMBER
 - AJO independent on site configuration and differences in instalation directory
 - Plug-in for job and input preparation
 - preliminary version of Amber plug-in
 - first version of Gaussian98 plug-in (Unicore Client 3.1.4)
 - See biogrid.icm.edu.pl for downloads

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Gaussian plug-in

- BioGRID will developed plug-in's for various packages
- Gaussian98 plug-in for UNICORE Client 3.1.4
- User specifies input parameters with plug-in
- Job will be submitted through UNICORE client



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Gaussian *plug-in* (cont.)

The screenshot shows the UNICORE 3.1 build 4 interface. The main window is titled "Gaussian" and contains the following elements:

- File Menu:** Add Job Group, Add Script, Add Transfer, Gaussian Plugin, Remove, Submit, Check.
- Job Group:** Name: Gaussian
- Unicore Site:** ICM, UMK
- Virtual Site:** (Empty)
- Task Dependencies:** (Empty)
- Email:** pyciu@suleckiego.com
- Buttons:** Edit Dependencies, Apply, Reset.

At the bottom left, the text "OK." is visible. At the bottom right, there is a logo for "GRID" and the text "Piotr Bała WMII UMK/ICM".

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Gaussian *plug-in* (cont.)

The screenshot shows the UNICORE 3.1 build 4 interface. The main window is titled "Gaussian Script" and contains the following elements:

- File Menu:** Job Preparation, Job Monitoring, Job Control, Settings, Help.
- Job Preparation:** New job group, Job_name_1
- Job Name:** Job name 1
- Job Type:** Opt
- Parameter:** QST2
- Model:** Density Functional Methods
- Theory:** B3LYP
- Basis Set:** 6-21G
- Charge:** 1
- Multiplicity:** Doublet
- status:** molecule loaded successful
- Buttons:** Load a Molecule, Generate Gaussian Input, Apply, Reset.

The "Gaussian Input" section shows the following data:

```
# molecule data
O -0.464 0.177 0.0
H -0.464 1.137 0.0
H 0.441 -0.143 0.0
```

At the bottom left, the text "OK." is visible. At the bottom right, there is a logo for "GRID" and the text "Piotr Bała WMII UMK/ICM".

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Gaussian plug-in (cont.)

The screenshot shows the UNICORE 3.1 build 4 interface. The main window is titled 'Gaussian Script' and contains the following settings:

- Job Name: Job name 1
- Job Type: Opt
- Parameter: QST2
- Model: Density Functional Methods

A 'Load a molecule' dialog box is open, showing a file browser with the following contents:

- cert
- DOC
- PluginsExample35
- UNICORE_Client_3.1.4
- UnicoreDoc
- Version35
- Client35BetaDoc.tar.gz
- molekula.bt

The 'File name' field is set to 'molekula.bt' and the 'Files of type' is set to 'All Files (*.*)'. The 'Generate Gaussian Input' button is visible at the bottom of the dialog.

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Gaussian plug-in (cont.)

The screenshot shows the UNICORE 3.1 build 4 interface with updated settings in the 'Gaussian Script' window:

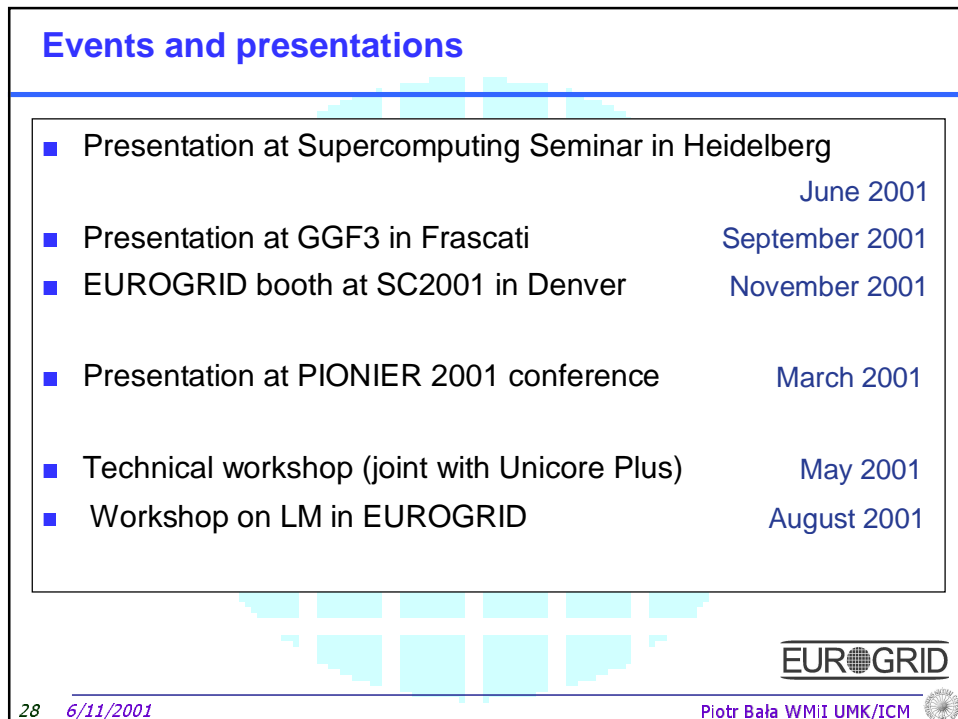
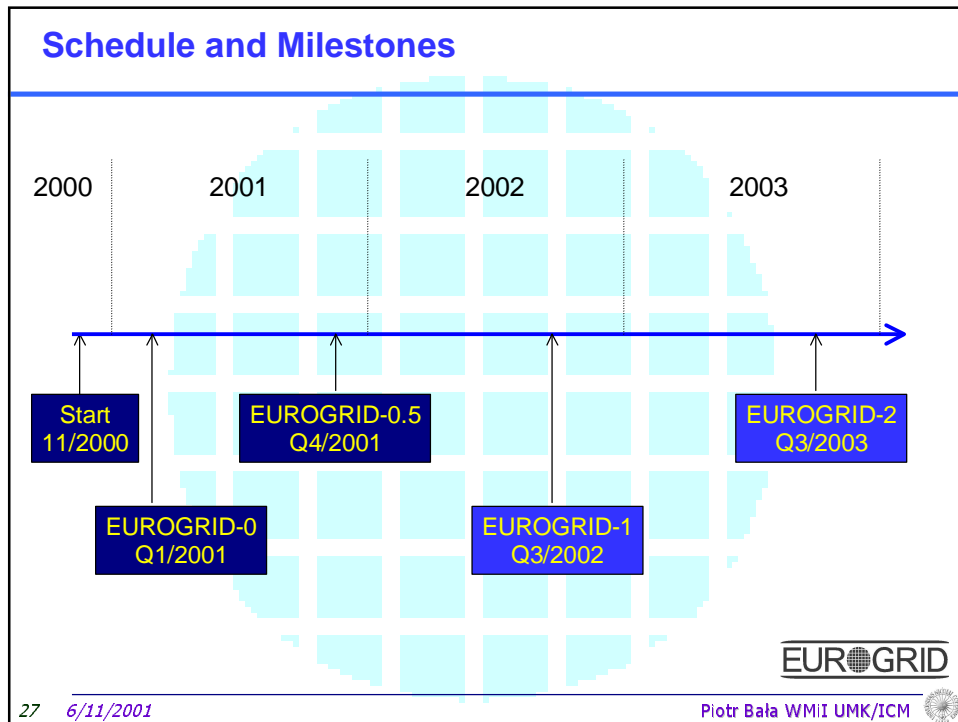
- Job Name: Job name 1
- Job Type: Opt
- Parameter: SP
- Model: Opt
- Theory: Freq
- Opt Freq
- Basis Set: NMR
- Charge: 1
- Multiplicity: Doublet
- status: input generated successful

The 'Load a Molecule' dialog box is open, showing the generated Gaussian input script:

```
# B3LYP/6-21G Opt=QST2
Job name 1
1 2
O -0.464 0.177 0.0
H -0.464 1.137 0.0
H 0.441 -0.143 0.0
```

The 'Generate Gaussian Input' button is visible at the bottom of the dialog.

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GRIP Project

Extend EUROGRID to cooperativity with globus middleware.

Provide UNICORE users with access to resources available through globus.

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GRIP Goals

- Increase UNICORE functionality
- Demonstrate inter-grid operability
- Open field to integrate resources of leading European HPC centres (EUROGRID) with US centers.
- Develop new software components for GRID computing
- Increase European activity in world wide grid activities (GGF)

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GRIP Partners

HPC Centres

- FZ Jülich (D)
- ICM Warsaw Univ (PL)
- Univ Bergen (N)
- Univ Manchester (UK)
- Univ Southampton (UK)

Integration

- Pallas

Users

- DWD (D)

Volume: 24 person years, 2 year project (2002-2003)
European Commission Grant Proposal

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- www.eurogrid.org
- biogrid.icm.edu.pl
- www.polgrid.pl

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