Interdyscyplinary Centre For Mathematical and Computational Modelling

Warsaw Uniwersity

EUROGRID

www.eurogrid.org

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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

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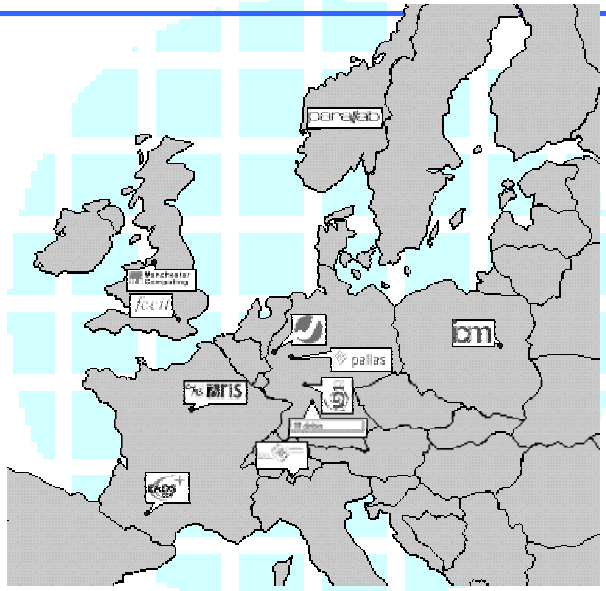
EUROGRID Geography



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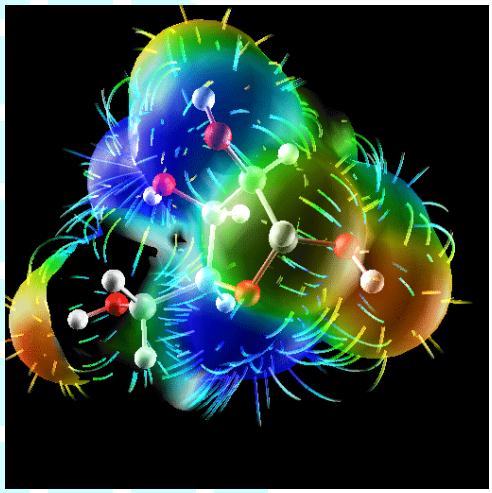
Structure of the Work

- 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

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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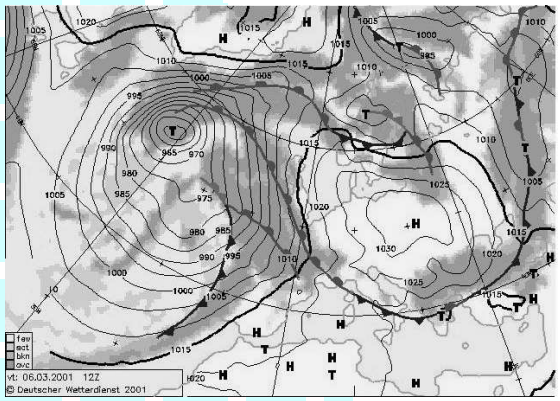
Meteo-GRID

- 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, ...

icm
CRAY T3E 900 (32 PE)
NEC SX4B/2A
Linux Cluster (4 PE)

paralab
SGI
SGI O2000 (128 PE)

FZJ
Linux Intel Cluster (36 PE)
CRAY T3E - 600 (512 PE)
CRAY T3E - 1200 (512 PE)

Manchester Computing
CRAY T3E - 1200 (816 PE)
FUJITSU VPP300 (8 PE)
SGI O2000 (128 PE)
SGI O3000 (256 PE)

IDRIS
IBM SP3 (8 PE)
NEC SX5 cluster (40 PE)
IBM Power4 (256 PE, 1.3 TFLOPS)
COMPAQ Linux Cluster (24 PE)

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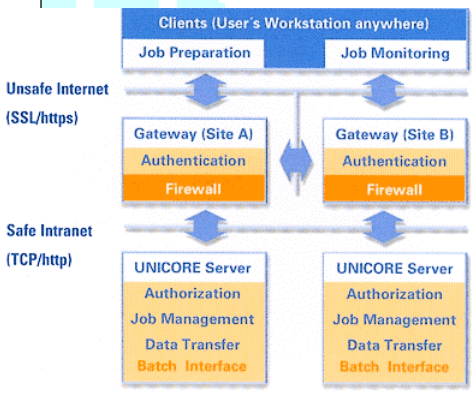
EUROGRID Infrastructure and Components

- 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



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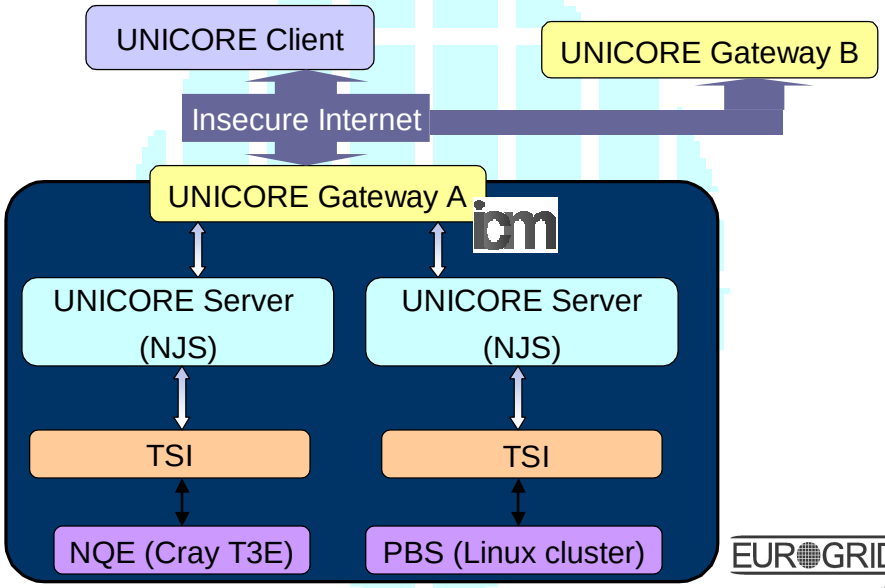
UNICORE architecture



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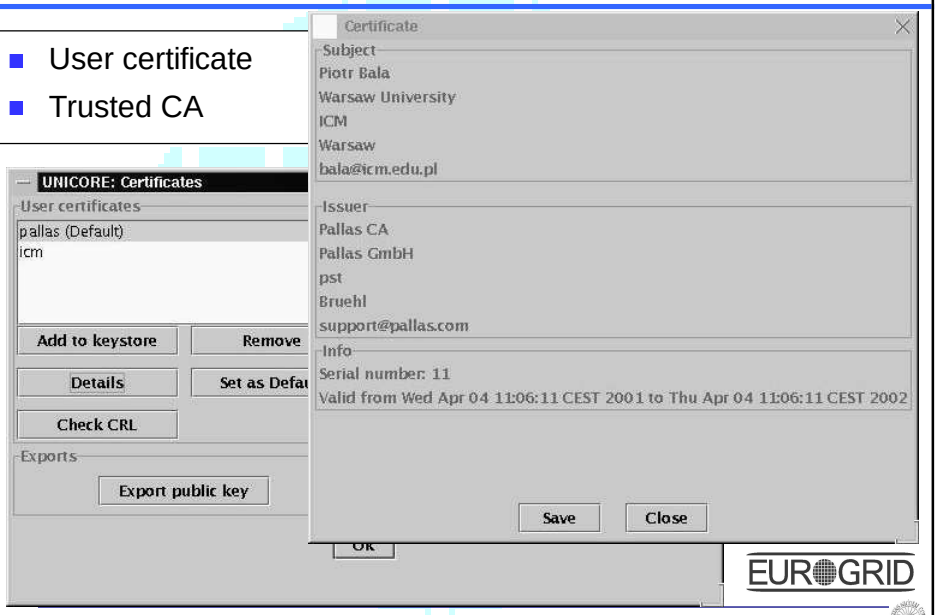
UNICORE Security

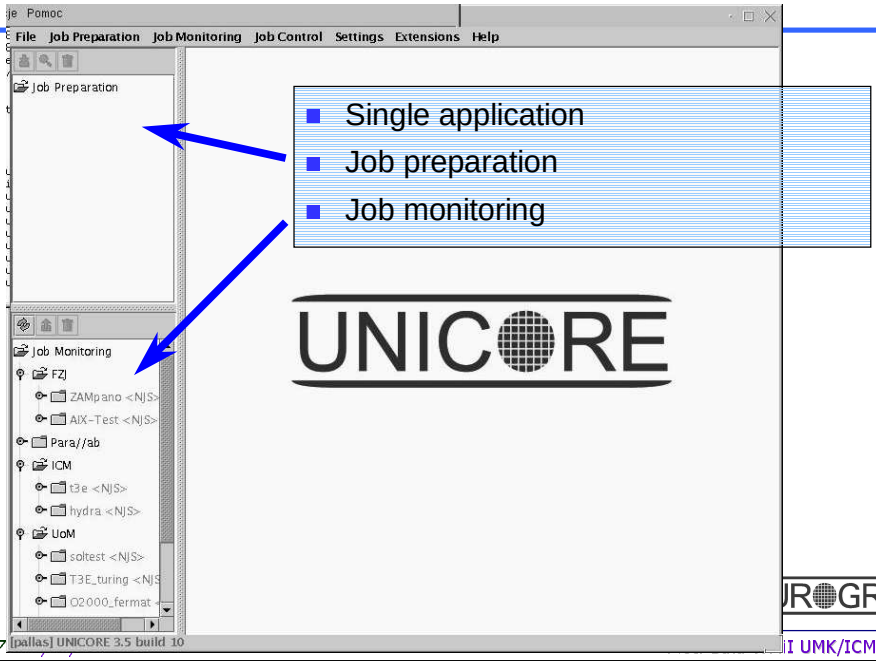
- Based on the PKA
- Industrial standard X509
- Secure communication
  - Gateway, NJS cetificates
  - Gateway, NJS check user certificate
  - Multiuple CA accepted
- User certificates
  - User certificate stored in client
  - Public key stored in UUDB database at each site
  - PKA mapped to user account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

UNICORE Security - Client

- User certificate
- Trusted CA



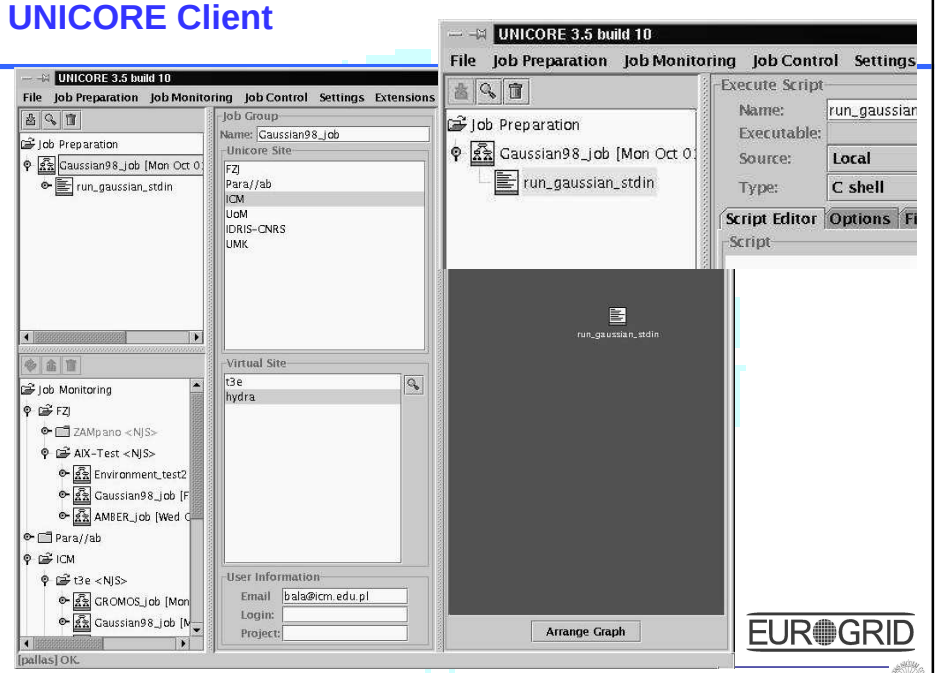
UNICORE Client



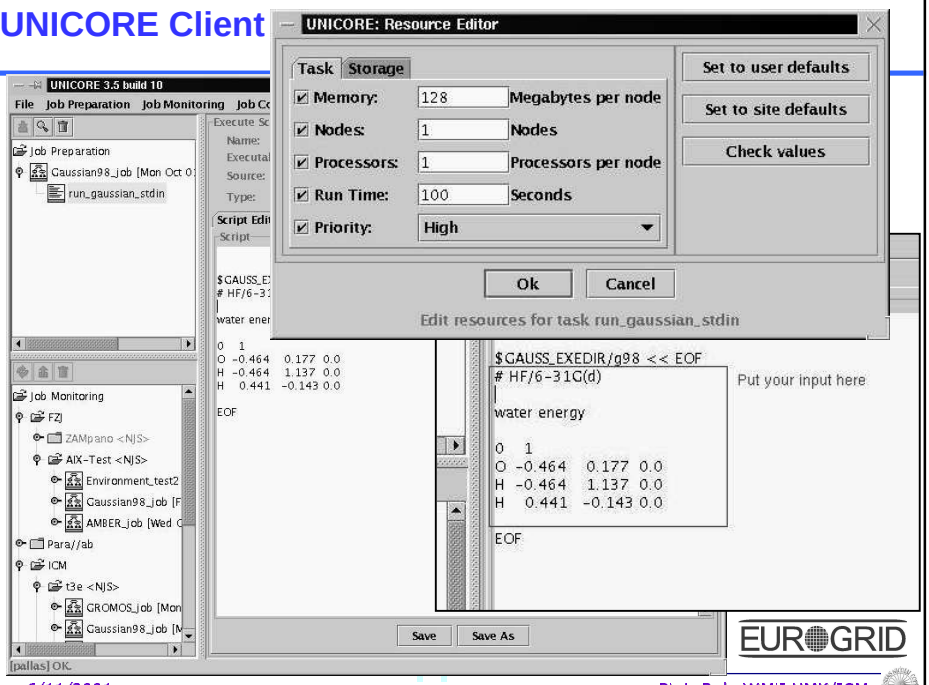
- Single application
- Job preparation
- Job monitoring

UNICORE

UNICORE Client



UNICORE Client



EUROGRID

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

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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 submited through UNICORE client

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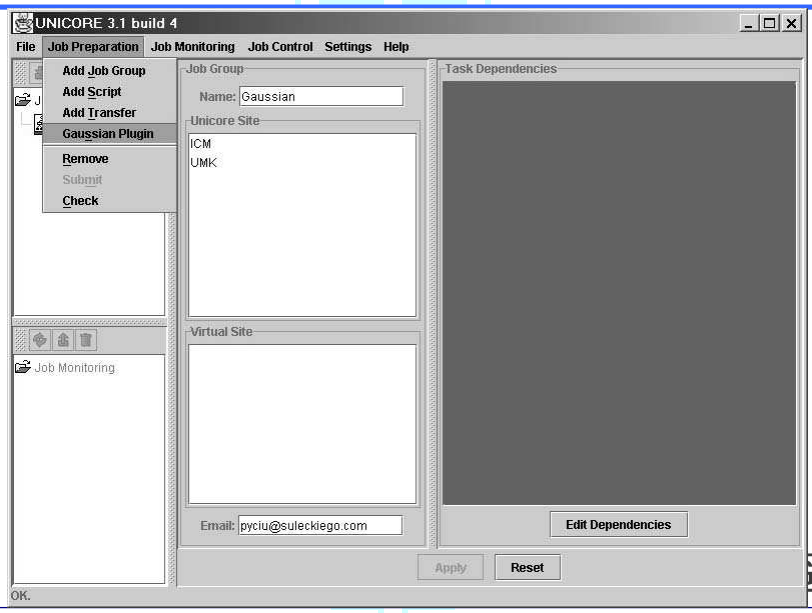
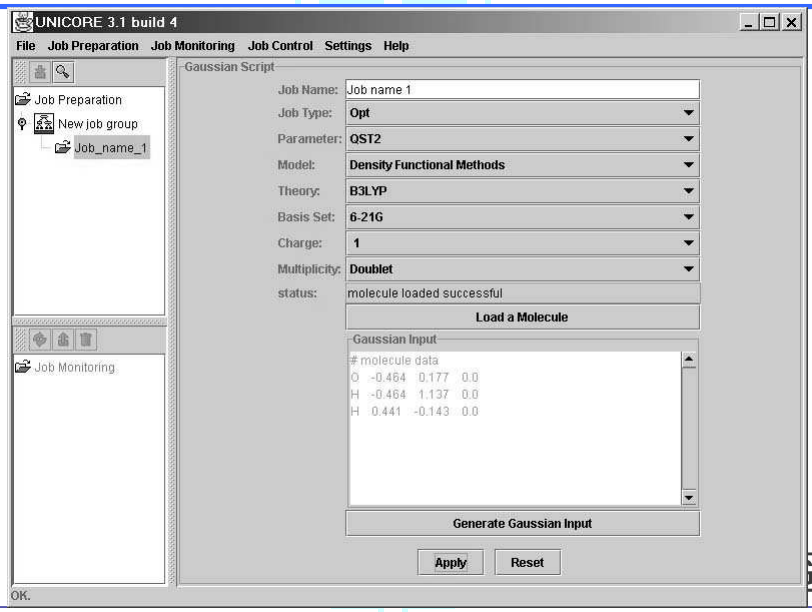
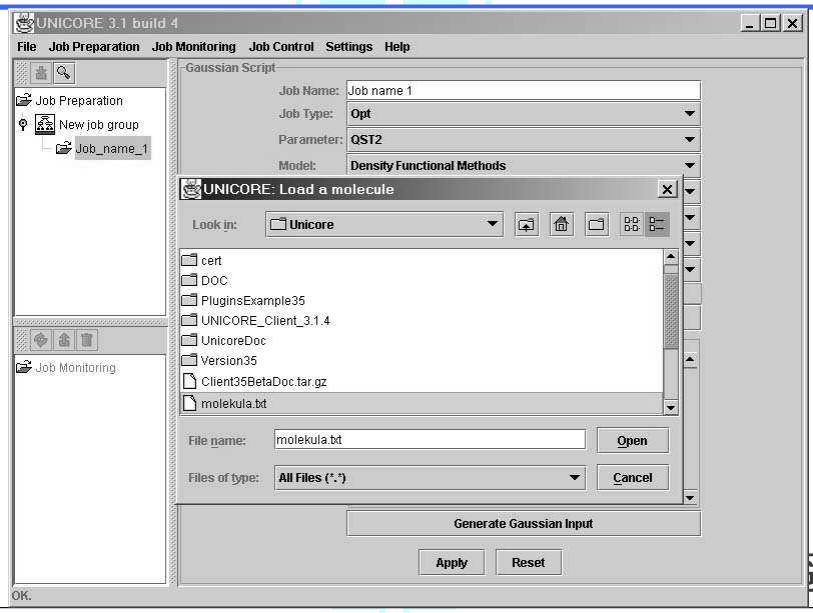
Gaussian *plug-in* (cont.)



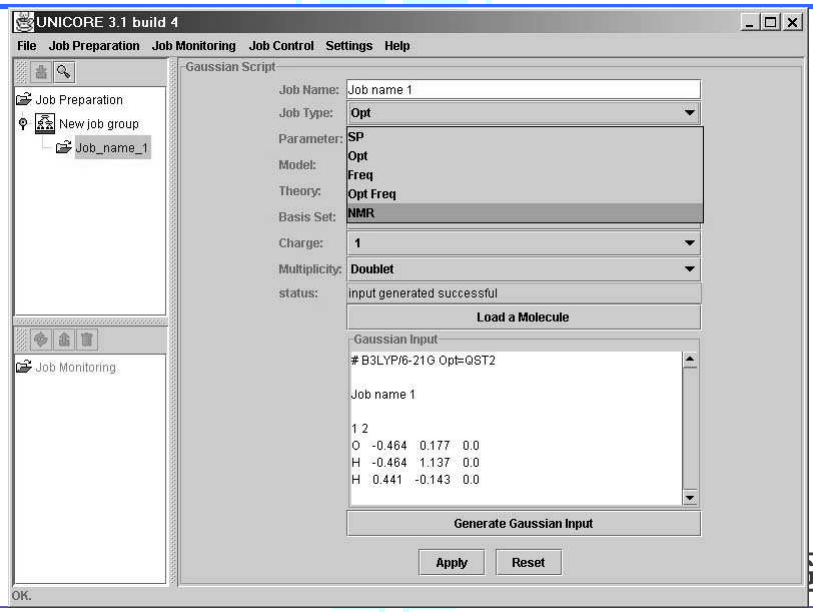
Gaussian *plug-in* (cont.)



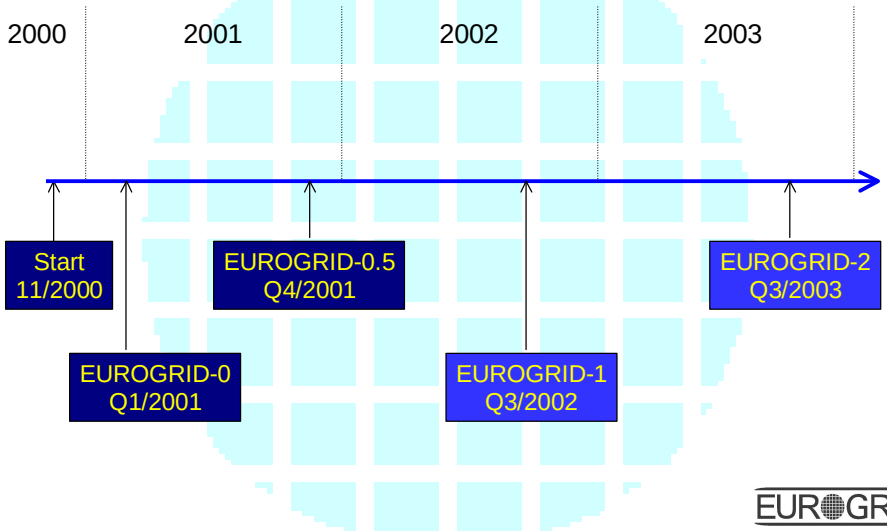
Gaussian *plug-in* (cont.)



Gaussian *plug-in* (cont.)



Schedule and Milestones



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Events and presentations

- Presentation at Supercomputing Seminar in Heidelberg — June 2001
- Presentation at GGF3 in Frascati — September 2001
- EUROGRID booth at SC2001 in Denver — November 2001
- Presentation at PIONIER 2001 conference — March 2001
- Technical workshop (joint with Unicore Plus) — May 2001
- Workshop on LM in EUROGRID — August 2001

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GRIP Project

Extend EUROGRID to cooperativity with globus middleware.

Provide UNICORE users with access to resources avaliable trough globus.

EUROGRID

GRIP Goals

- Increase UNICORE functionality
- Demonstrate inter-grid operatibility
- 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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