



A European Grid Middleware

<http://www.unicore.eu>

History Lesson

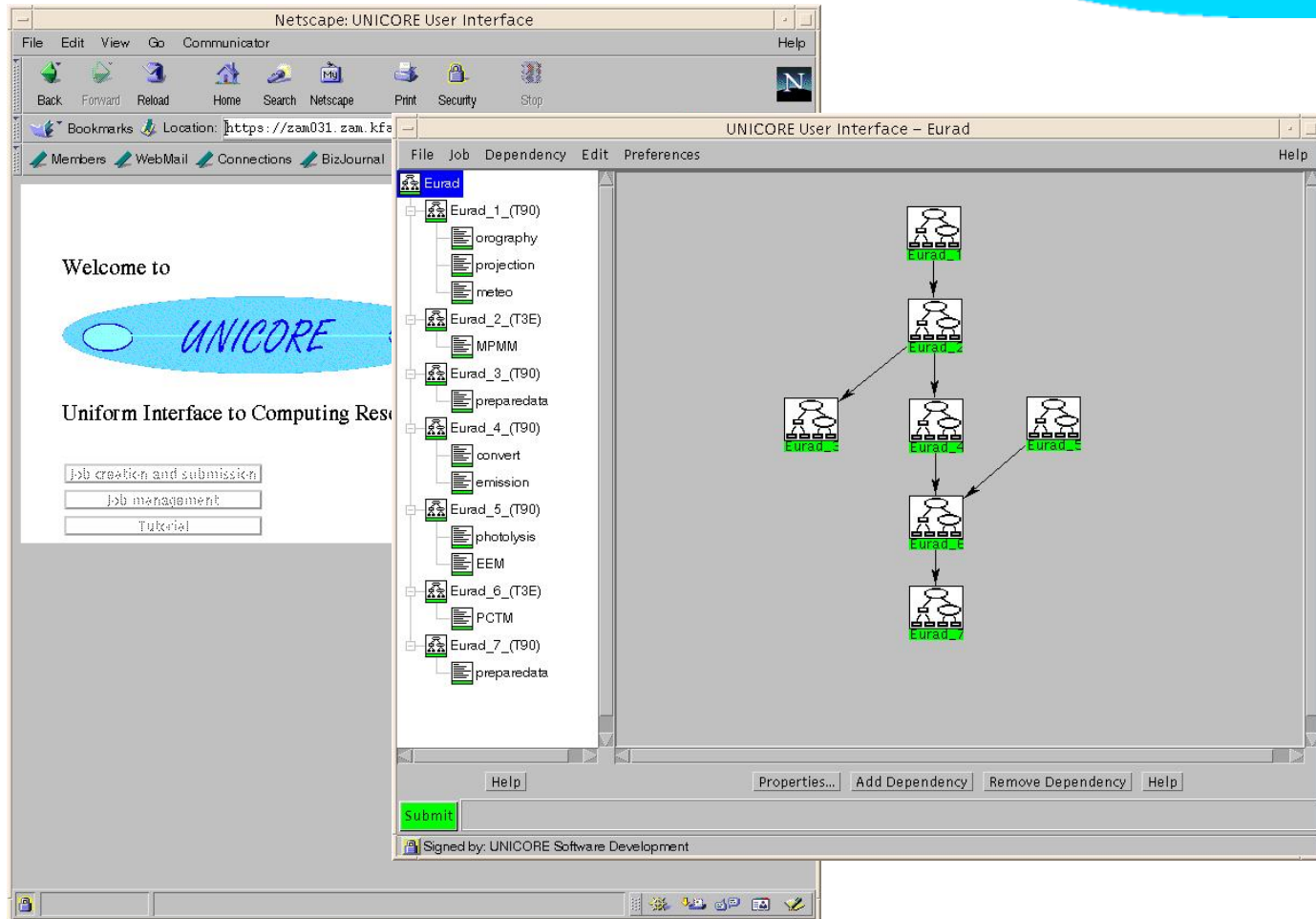


1996/1997

- ▶ 2nd – 6th September 1996: summer school in Jülich about “partial differential equations in numerics and applications”
- ▶ 3rd September 1996: round table with users, supercomputer centres, competence centres, vendors
 - ▶ discussion: “what prevents an efficient use of distributed supercomputers?”
 - ▶ results: seamless, secure and intuitive to use access
- ▶ December 1996: UNICORE project idea submitted to BMBF
- ▶ Spring 1997: UNICORE project proposal developed and submitted to BMBF
- ▶ 1st of August 1997: start of the German UNICORE project

1998

► UNICORE – applet client



1999

► UNICORE – compile, link & run task

The screenshot displays the UNICORE User Interface running in a Netscape browser window. The main interface shows a welcome message and a list of buttons: "Job creation and submission", "Job management", and "Tutorial". A blue oval with the word "UNICORE" is overlaid on the welcome message.

An "Edit job properties" dialog box is open, showing the following fields:

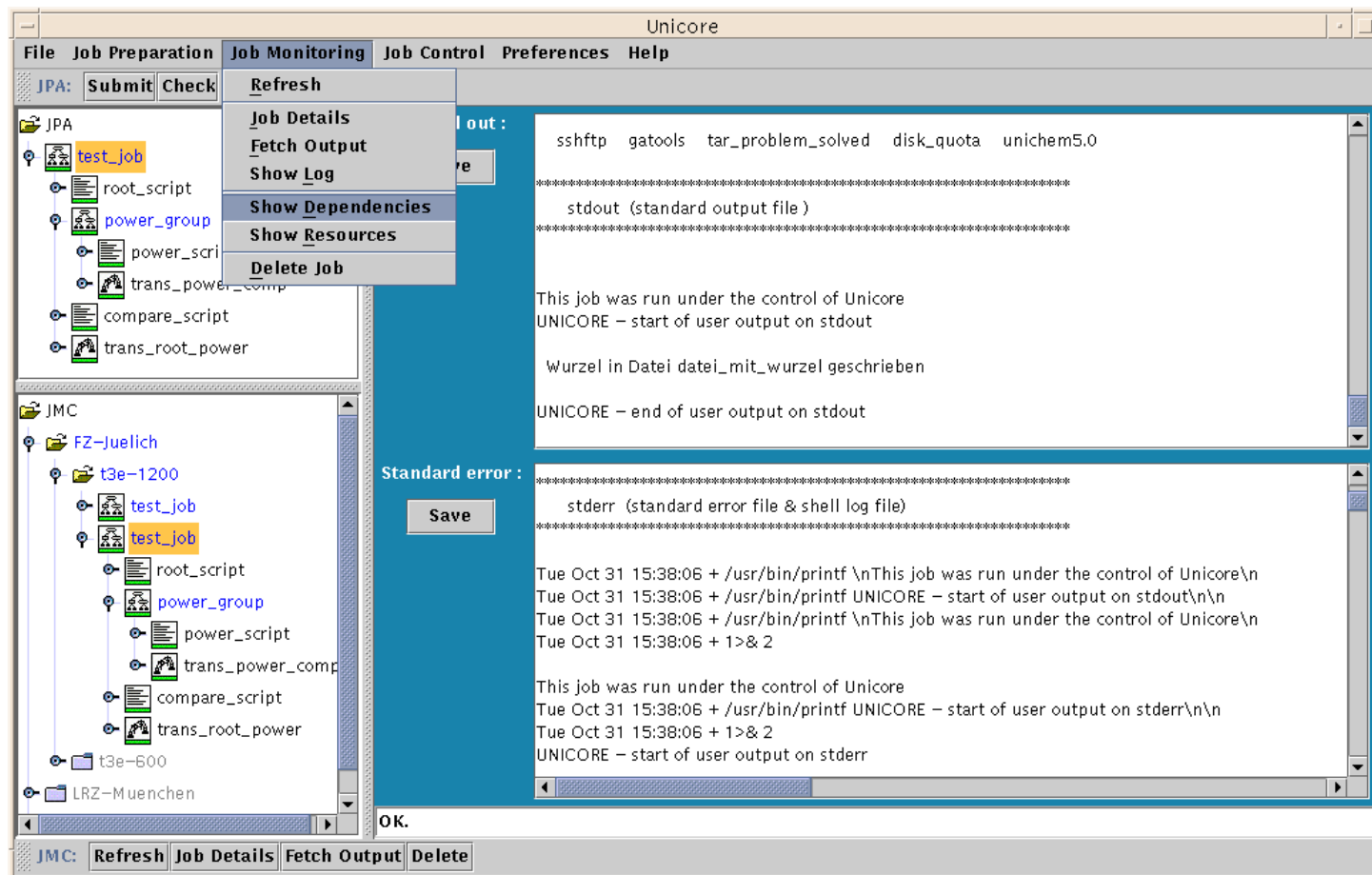
- Job Group Name: UNI_Job_MR
- Destination: T3E-600@FZ Juelich
- Account: SP-Test002@RUKA
- Your email: T3E-1200@FZ Juelich

The dialog box also includes "Ok", "Cancel", and "Help" buttons. Below the dialog box, a section titled "Choose destination system and site" shows a signed certificate: "Signed by: UNICORE Software Development's Pallas GmbH Certificate".

The bottom of the browser window shows a status bar with the text "Applet unicore.clients.Wrapper running".

2000

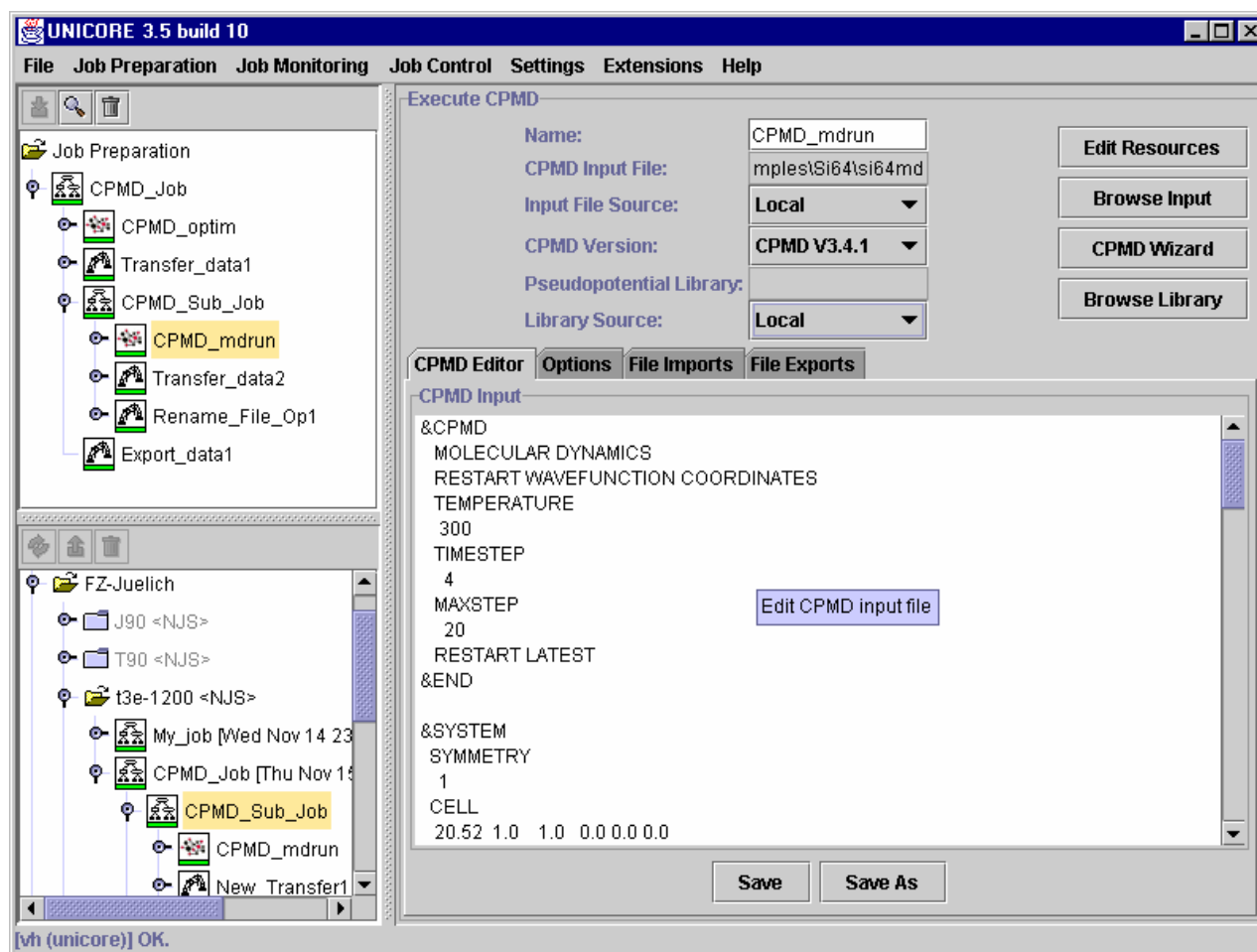
► UNICORE Plus – First Application Client



2001

► UNICORE Plus – CMPD plugin

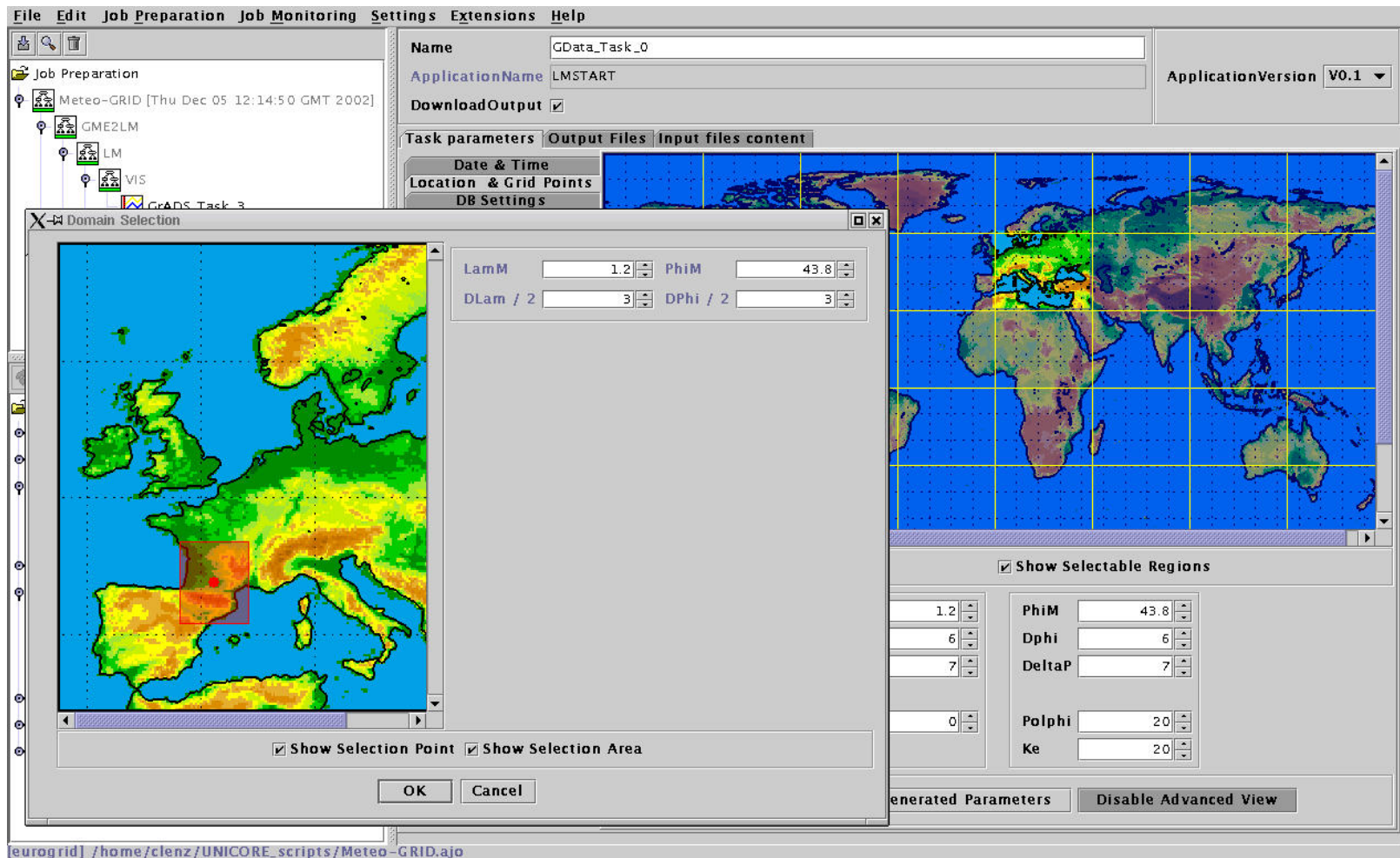
UNICORE



2002

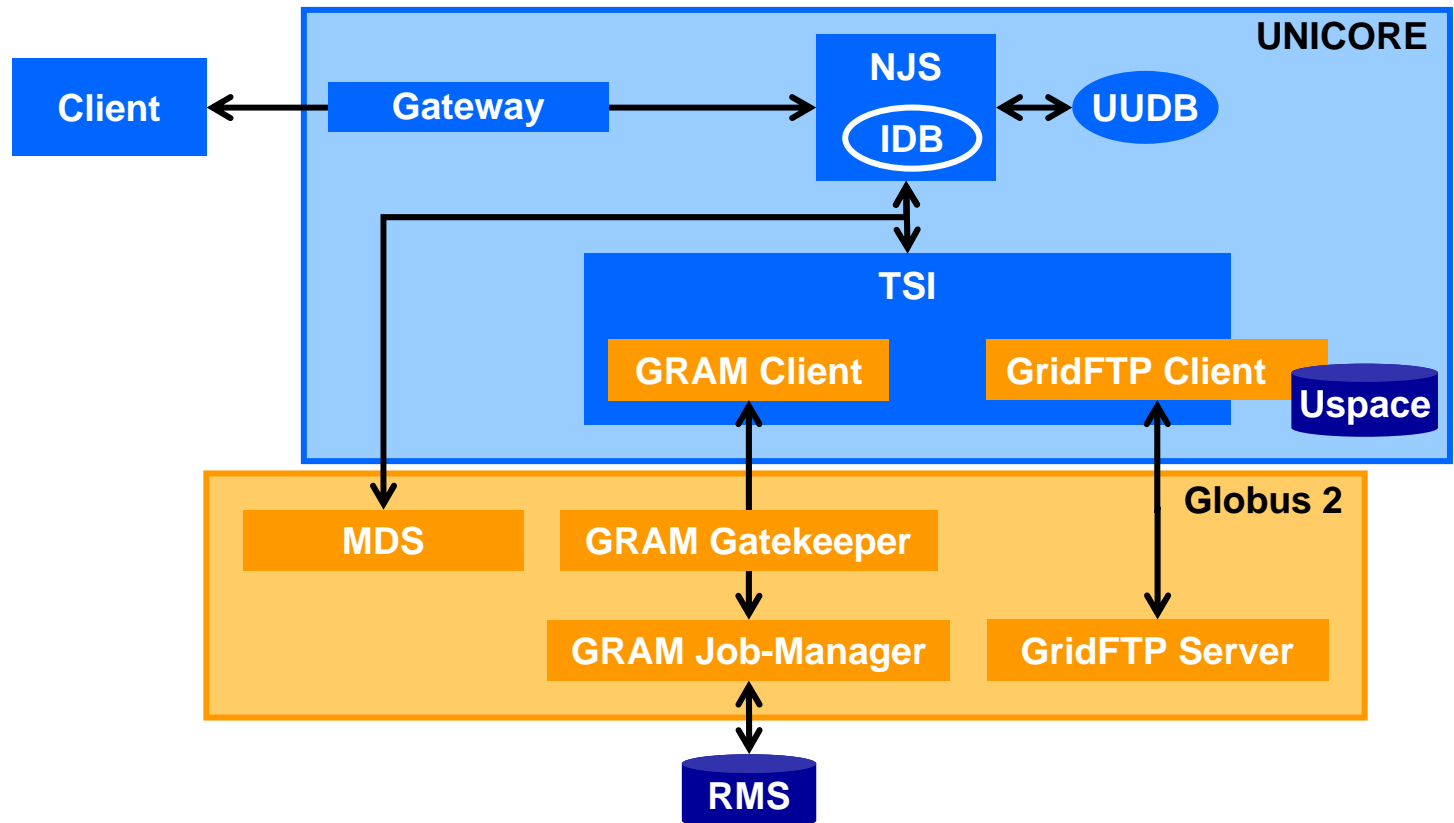


► Application Testbed for European GRID Computing



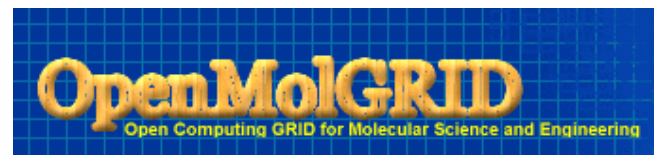
2003

- ▶ Running UNICORE jobs on Globus 2.4 managed resources



2004

► Workflow automation & speed-up



UNICORE Client

File Job Preparation Job Monitoring Settings Extensions Help

Job Preparation

- New_Workflow1 [10:02:38 09/28/2005]
 - Query_Database
 - Query_Database
 - Structure_file_preparation
 - Property_file_preparation
 - Auto_Transfer
 - 3D
 - Convert_2D_to_3D
 - Auto_Transfer
 - Distributed_Structure_optimization
 - Auto_SplitInputData
 - Auto_Transfer
 - Execute1
 - Structure_optimization_1
 - Auto_Transfer
 - Execute2
 - Structure_optimization_2
 - Auto_Transfer
 - Auto_Join_Data
 - DC
 - Codessa_CD
 - Model_building
- Globus_Job [09:53:27 09/28/2005]

Job Monitoring

- DEISA_BSC
- DEISA_Cineca

OpenMolGRID Workflow Control

Workflow control: UNICORE job control: XML Workflow: To do:

File Edit

```
<?xml version="1.0"?>
<workflow xmlns="http://www.openmolgrid.org/namespaces/2004/WorkflowDescription"
  xmlns:rd="http://www.openmolgrid.org/namespaces/2004/SimpleResources">
  <group type="subjob" identifier="Query Data" id="1" export="false" split="false">
    <task name="DataBaseRequest" identifier="Query Data" id="1" export="false" split="false">
      <option name="query" value="
        SELECT chemical.moldw_id,chemical.structuretype,chemical.molecularstructure,
        property.propertyid,property.propertyname,property.logid
        FROM (chemical LEFT JOIN property ON chemical.moldw_id=property.moldw_id)
        WHERE chemical.molecularstructure!='' and property.propertyname='Multi-Drug'
      "/>
    </task>
  </group>
  <task name="DataBaseRequestToPLF" identifier="Property file preparation" id="3" export="false" split="false"/>
  <task name="DataBaseRequestToSLF" identifier="Structure file preparation" id="2" export="false" split="false"/>
  <resourceRequest>
    <rd:node usite="Ulster OMG" vsite="MOLDW" id="1" export="false" split="false"/>
  </resourceRequest>
  </group>
  <task name="2Dto3Dconversion" identifier="Convert 2D to 3D" id="21" export="false" split="false"/>
  <task name="SemiempiricalCalculation" identifier="Structure optimization" id="25"
    export="false" split="true" splitterTask="SplitStructureList"
    joinerTask="JoinStructureLists">
    <option name="keywords" value="AM1 PRECISE 1SCF NOINTER"/>
  </task>
  <task name="DescriptorCalculation" identifier="Codessa CD" id="29" export="false" split="false"/>
  <task name="ModelBuilding" identifier="Model building" id="40" export="false" split="false">
    <resourceRequest>
      <rd:resources runtime="3600"/>
    </resourceRequest>
  </task>
  <dependency pred="11" succ="2"/><!-- db request to structure extract-->
  <dependency pred="11" succ="3"/><!-- db request to property extract-->
  <dependency pred="3" succ="40"/><!-- property extract to model building -->
  <dependency pred="2" succ="21"/><!-- struct extract to 2d to 3d -->
  <dependency pred="21" succ="25"/><!-- 2d to 3d to semiempirical-->
</workflow>
```




automatic split-up of data-parallel task

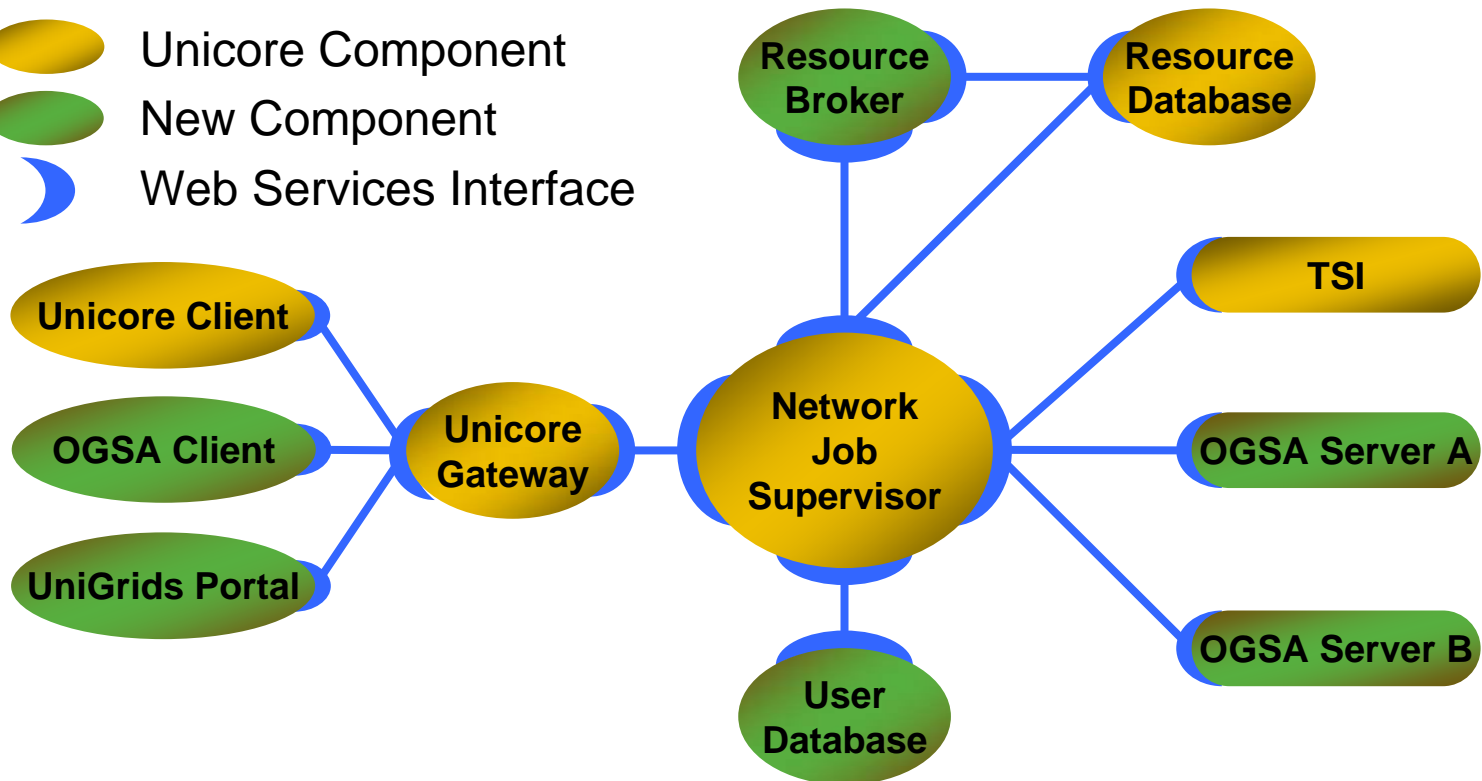
2005

► Web Services enabled UNICORE



Unicore/GS Architecture

-  Unicore Component
-  New Component
-  Web Services Interface

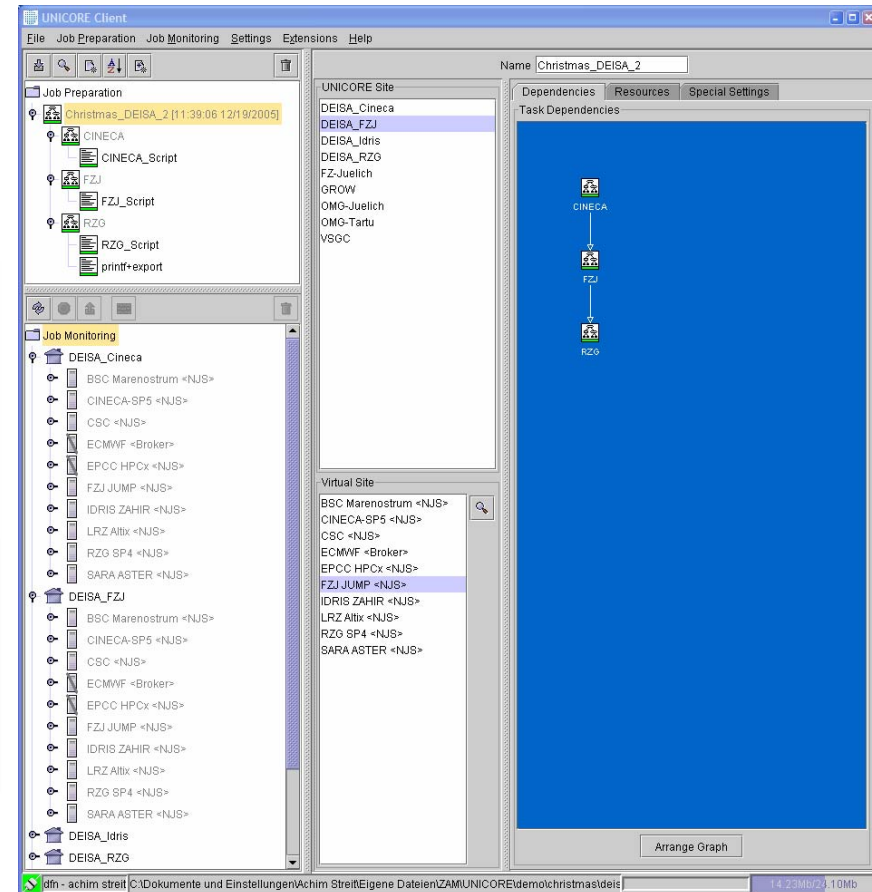
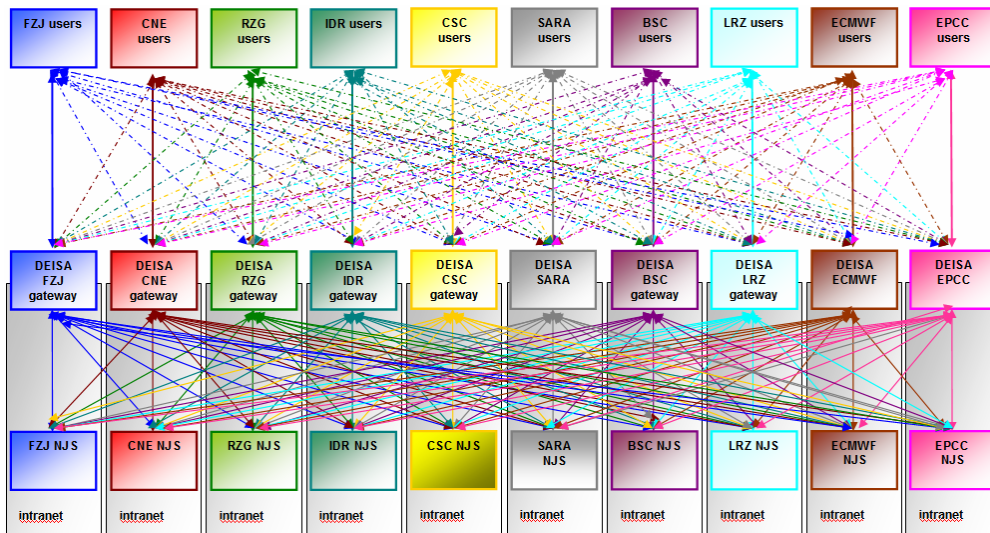


2006

► Accessing the DEISA infrastructure with UNICORE



UNICORE





2007

UNICORE 6.0

11. January	6.0 alpha5
30. April	6.0 beta
3. July	6.0 RC1
21. July	6.0 RC2
13. August	6.0 final

By 30. September	6.0.5
By 31. December	6.1

Some Technical Details of UNICORE 6.0

Design Principles

- ▶ Service-oriented, web services foundation
- ▶ Integrated, complete stack
- ▶ Strong security
- ▶ Easy installation and configuration
- ▶ Excellent application support
- ▶ Workflows
- ▶ Support for many operating and batch systems
 - ▶ Existing TSI installation can be reused
- ▶ Open, extensible, interoperable
- ▶ Easy to use clients
 - ▶ Graphical and command line clients
 - ▶ Portal, RCP-based
- ▶ Open Source under BSD license

CINECA
Consorzio Interuniversitario

icm

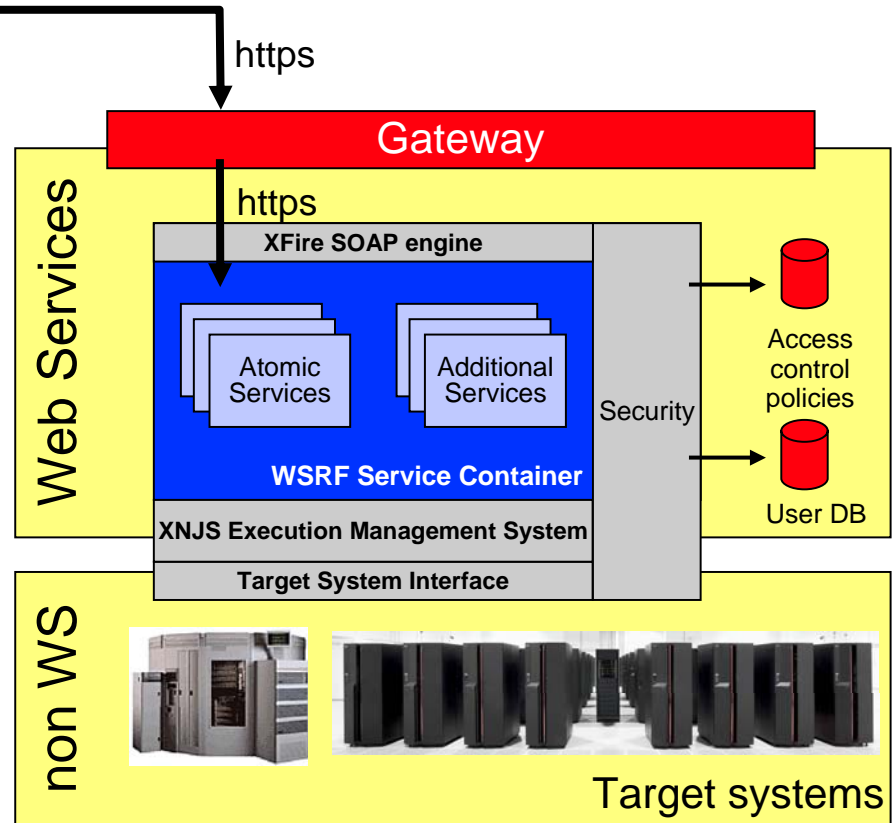
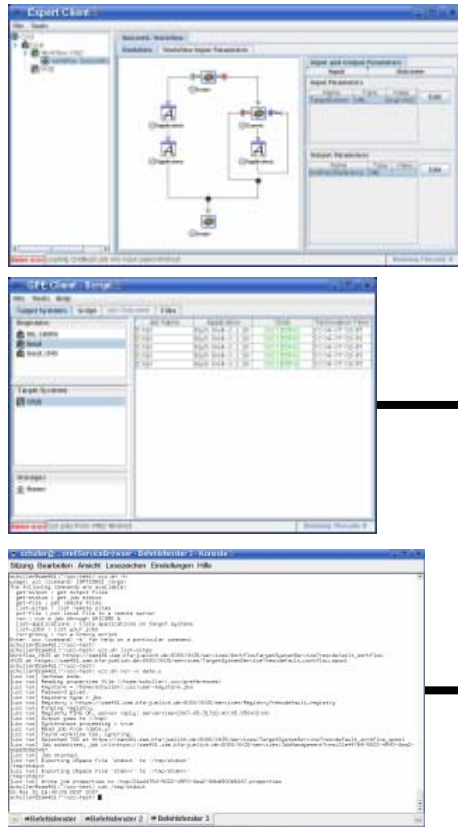
intel.

FUJITSU



Architecture

Clients
e.g. graphical, portal, command line



Technical Features

- ▶ **Standards-compliant**

- ▶ OASIS WSRF 1.2
- ▶ OGF JSDL 1.0

- ▶ **Pluggable file transfer mechanisms**

- ▶ OGSA Bytelo as default
- ▶ Others are pluggable

- ▶ **State of the art software**

- ▶ High-performance SOAP stack (XFire)
- ▶ Jetty 6 web server
- ▶ Java 5

- ▶ **Security**

- ▶ X.509
- ▶ Support for proxy certificates
- ▶ XACML 1.0 authorisation policies
- ▶ Web-services based user database
- ▶ Pluggable extensions for VO management

- ▶ **Configuration, management and administration**

- ▶ All components are pluggable
- ▶ Support for Java management extensions (JMX)

<http://www.unicore.eu>

Please send support-requests to:
unicore-support@lists.sourceforge.net