UNICORE

TUTORIAL

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August 2006

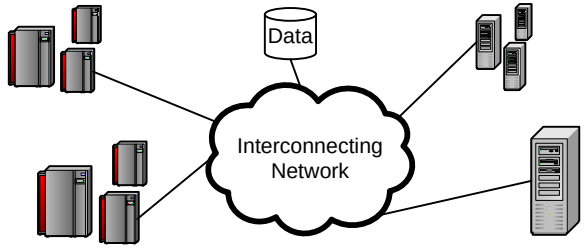
UNICORE SUMMIT 2006

Outline

- Motivation & History
- Production UNICORE 5
  - Features
  - Architecture
  - Example deployments within DEISA and T-Systems
- UNICORE 6
  - Improved Features
  - Architecture & Higher Level Services
  - Future Developments
- UNICORE as Open Source
- UNICORE Forum
- Summary

Motivation: Scientists & Parallel Computing

- Scientists need computational and storage related resources



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Motivation: Scientists & Parallel Computing

- Supercomputers are managed by Resource Management Systems (RMSs) that handle the scheduling
- But: There are many RMSs available
- All proprietary way of job submit
  - IBM Loadleveler → **`llsubmit`**…
  - Torque Resource Manager → **`qsub`**…
  - Different job description languages… (# of nodes, memory requirements,…)

Resource Management System

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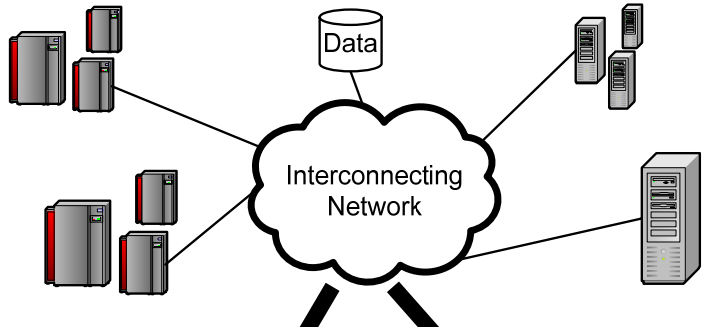
Motivation: Scientists & Parallel Computing

- Solution: Grid System UNICORE



- Define job workflows in abstract manner
- Immediate portability of job definitions for other systems with other architectures
- No ‘learn overhead’ if a new RMS is used
- Applications across multiple supercomputers/clusters → ‘going meta’

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Initial UNICORE developments

- UNICORE 08/1997-12/1999
- UNICORE Plus 01/2000-12/2002
- EUROGRID 11/2000-01/2004
- GRIP 01/2002-02/2004
- OpenMolGRID 09/2002-02/2005





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From Testbed to Production

2002

- Different communities
- Different computing resources (super computers, clusters, …)
- Know-how in Grid middleware

2006

Success factor: VERTICAL INTEGRATION

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UNICORE in (mostly) European Projects

Information Society Technologies

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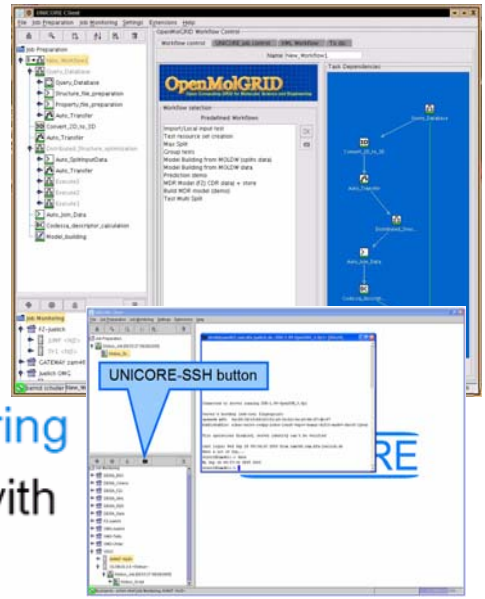
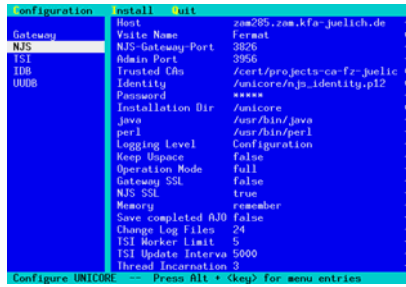
Production UNICORE Features

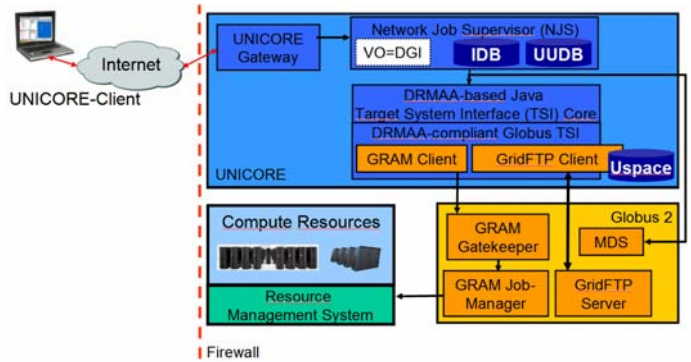
- A vertically integrated Grid middleware system
- Provides seamless, secure, and intuitive access to distributed resources and data
- Used in production and projects worldwide
- Features
  - intuitive GUI with single sign-on
  - X.509 certificates for AA and job/data signing
  - only one opened port in firewall required
  - workflow engine for complex multi-site/multi-step workflows
  - extensible application support with plug-ins
  - matured job monitoring
  - interactive access with UNICORE-SSH
  - integrated secure data transfer
  - resource management
  - full control of resources remains
  - production quality, ...

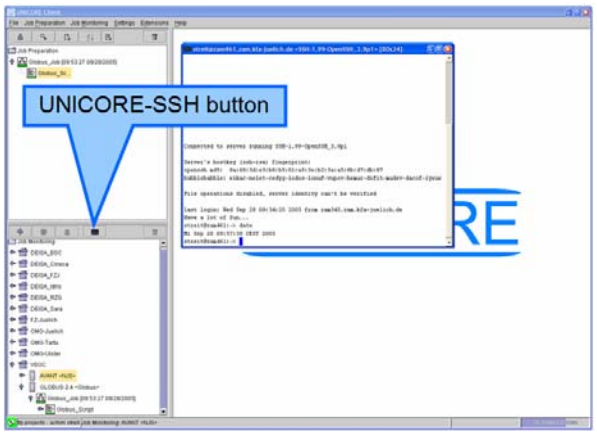


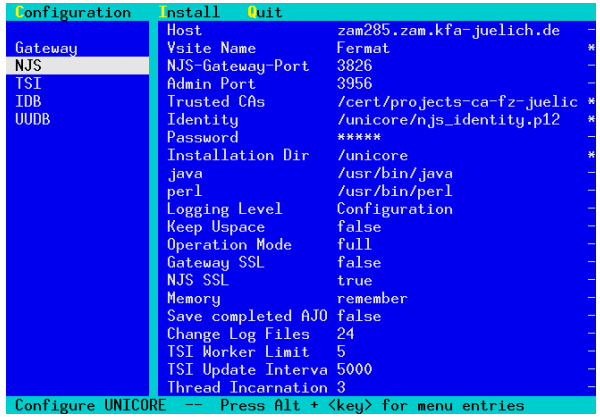


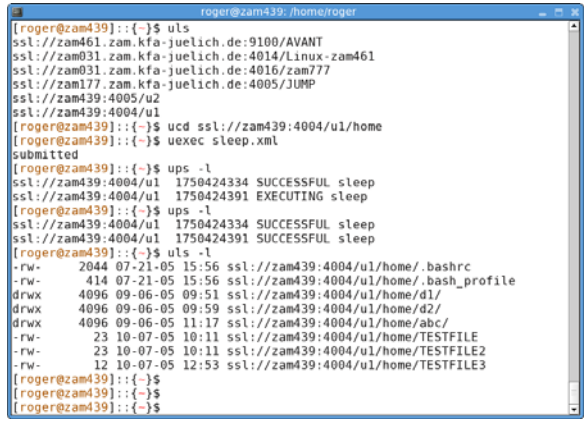
Recent Developments

- OGSA-based and WSRF-compliant UNICORE 6 alpha
- Interactive access → UNICORE-SSH
- High-level API for programming Grids
- DRMAA-based access to RMSs
- Comfortable configuration tool

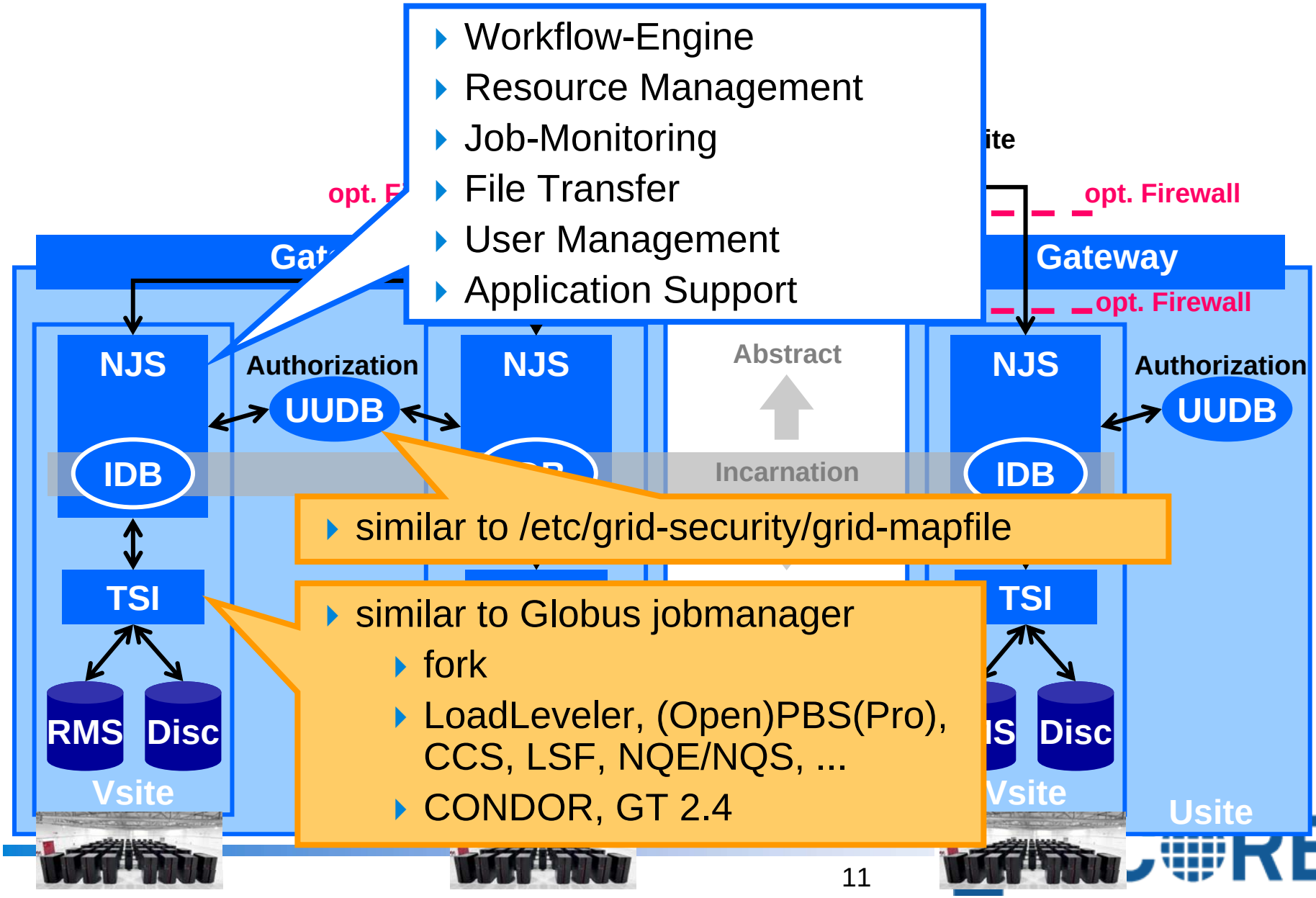




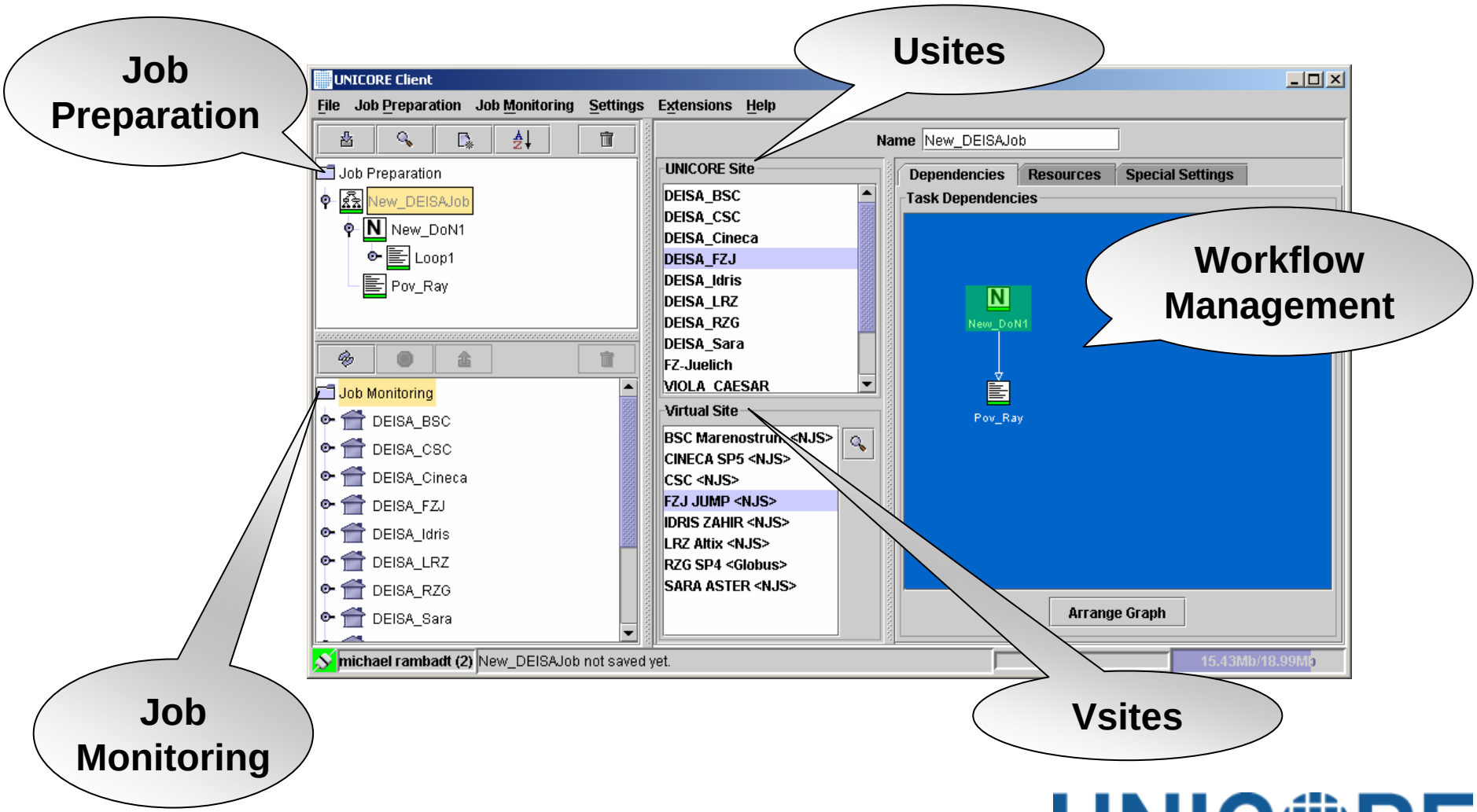




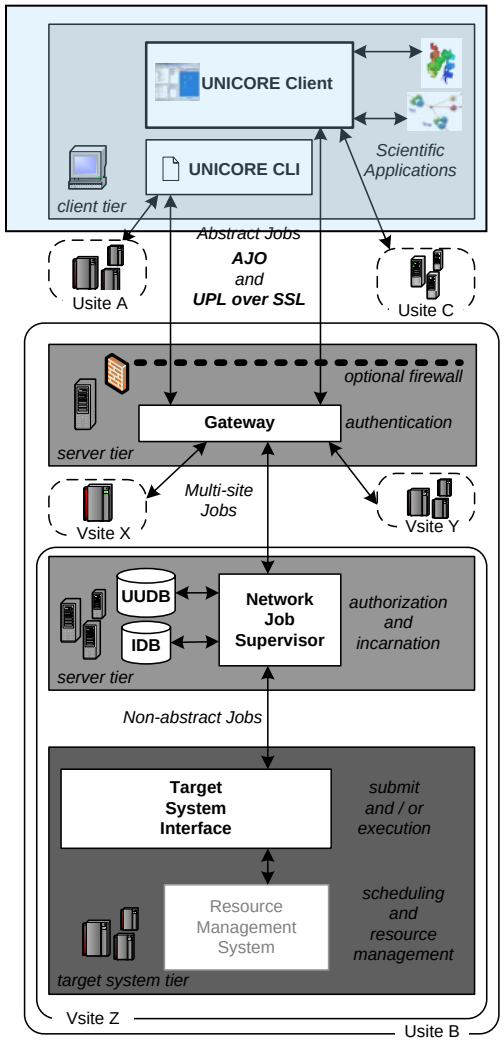
UNICORE Architecture Overview



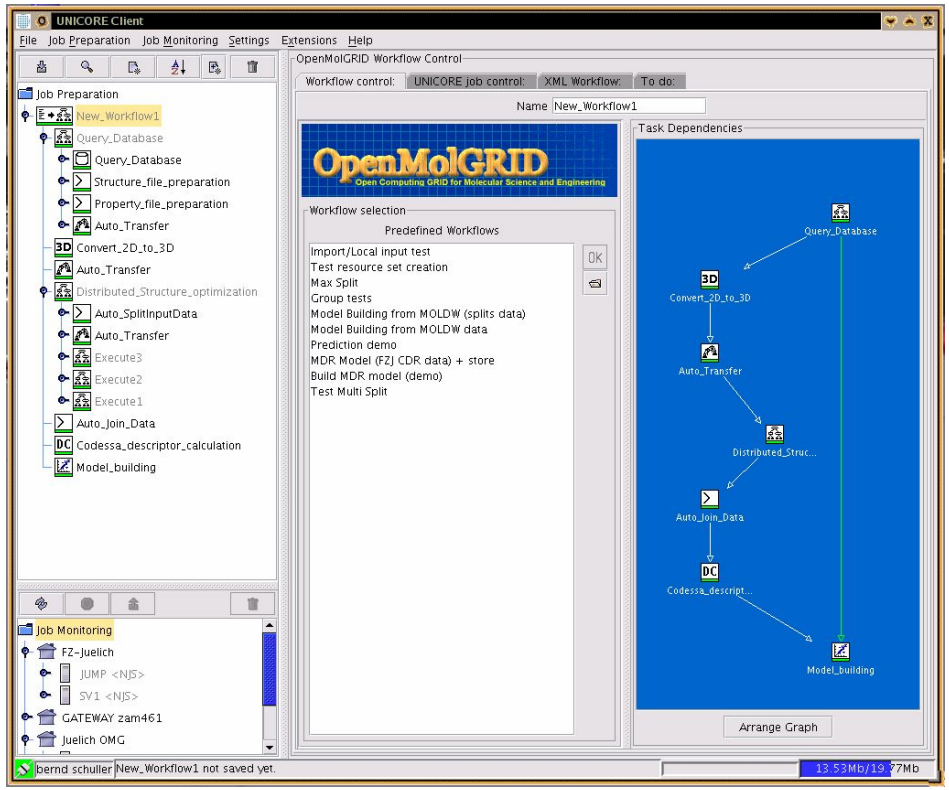
UNICORE Client



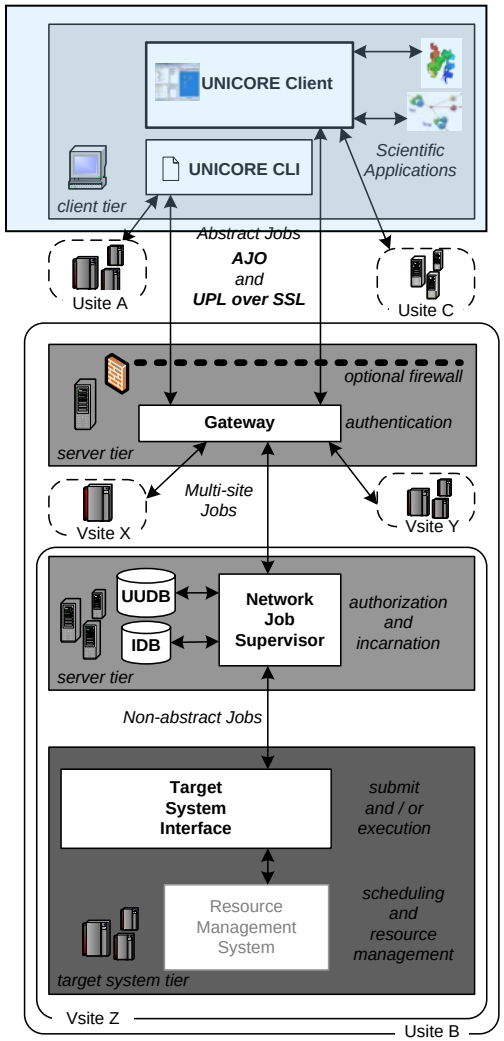
UNICORE 5 Architecture (1)



- Definition of abstract Jobs (not machine-specific)
- Creation of complex workflows (e.g.multi-site jobs for geographically dispersed supercomputers)



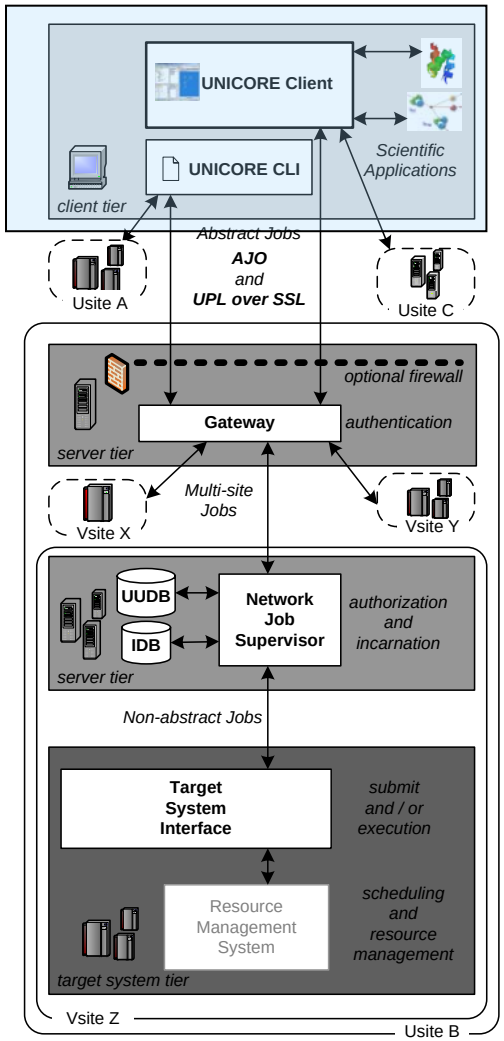
UNICORE 5 Architecture (2)

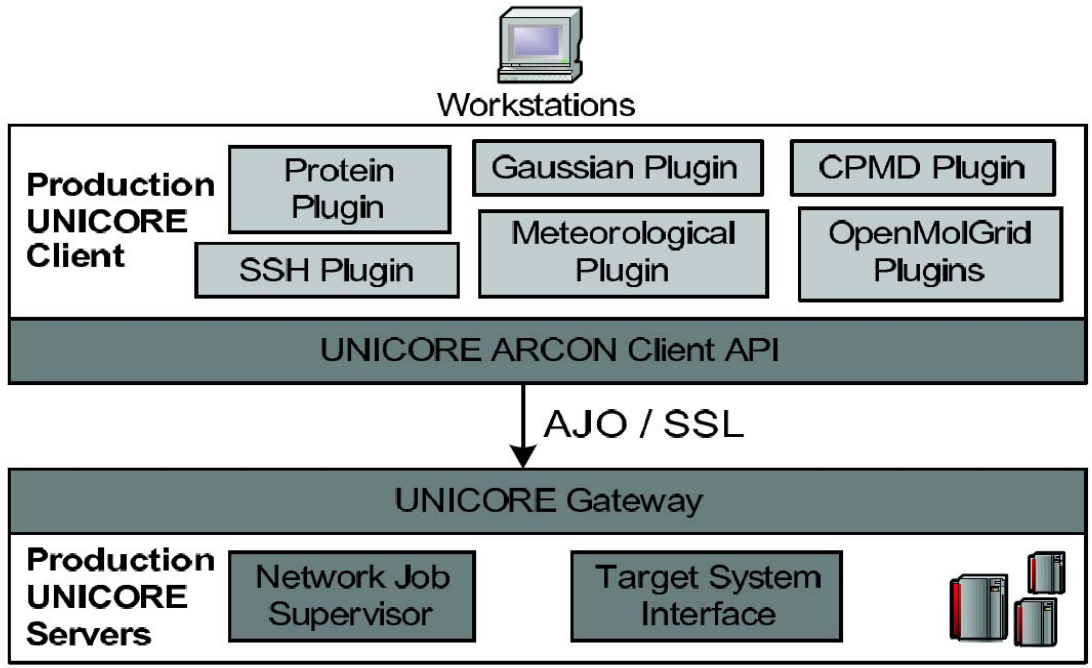


- Client extensions via application-specific plugins
  - Car-Parrinello Molecular Dynamics Plugin (speed up quantum chemical computations)
  - Fluent, Gaussian, MSC Nastran Plugins
  - OpenMolGrid – Plugins (Molecular Science)
- UNIX-Style Command-Line Interface (CLI)

```
[roger@zam439]::{~}$ uls
ssl://zam461.zam.kfa-juelich.de:9100/AVANT
ssl://zam031.zam.kfa-juelich.de:4014/Linux-zam461
ssl://zam031.zam.kfa-juelich.de:4016/zam777
ssl://zam177.zam.kfa-juelich.de:4005/JUMP
ssl://zam439:4005/u2
ssl://zam439:4004/u1
[roger@zam439]::{~}$ ucd ssl://zam439:4004/u1/home
[roger@zam439]::{~}$ uexec sleep.xml
submitted
[roger@zam439]::{~}$ ups -l
ssl://zam439:4004/u1  1750424334 SUCCESSFUL sleep
ssl://zam439:4004/u1  1750424391 EXECUTING sleep
```

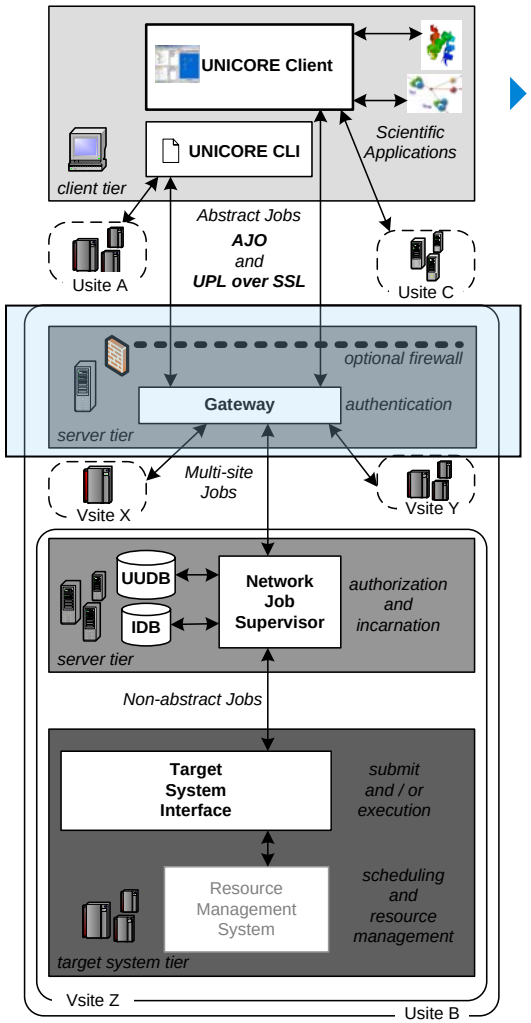
UNICORE 5 Architecture (3)



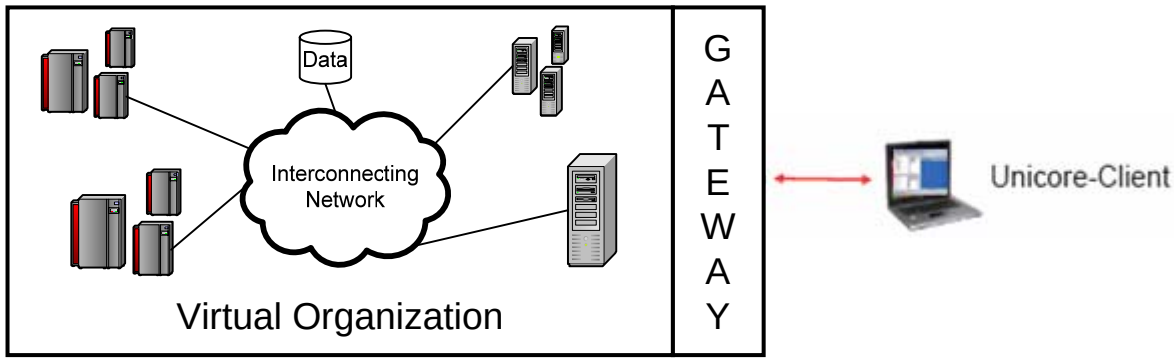


- Various plugins have been developed the last years
- Base upon the Arcon Client API (Java - API)

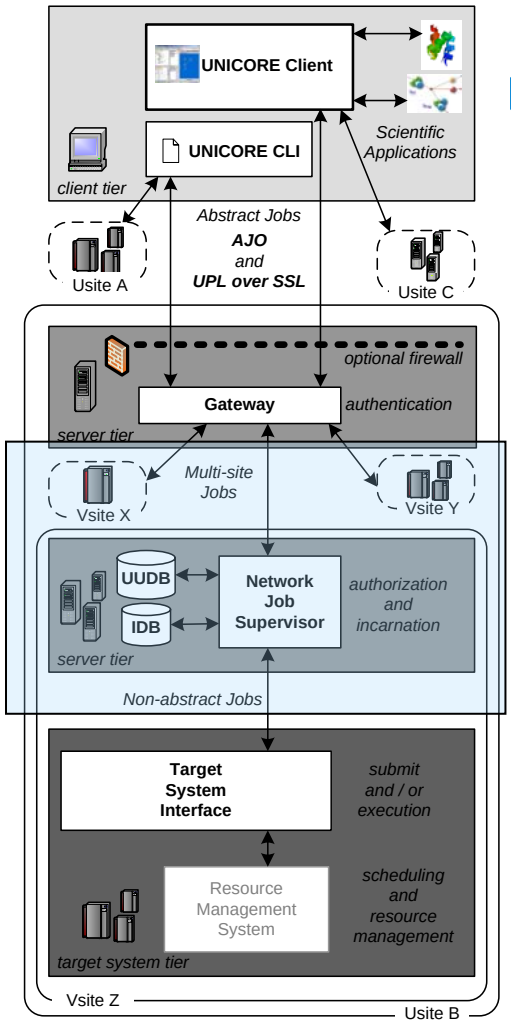
UNICORE 5 Architecture (4)



- Gateway
  - Single entry-point for UNICORE Sites (Usites)
  - Contains n Virtual Sites (Vsites)
    (e.g. provides access to n supercomputers)
  - Only ONE OPEN PORT in firewall
  - Authentication of users via X.509 certificates
  - Perfect base to group resources and access within Virtual Organizations (VOs)

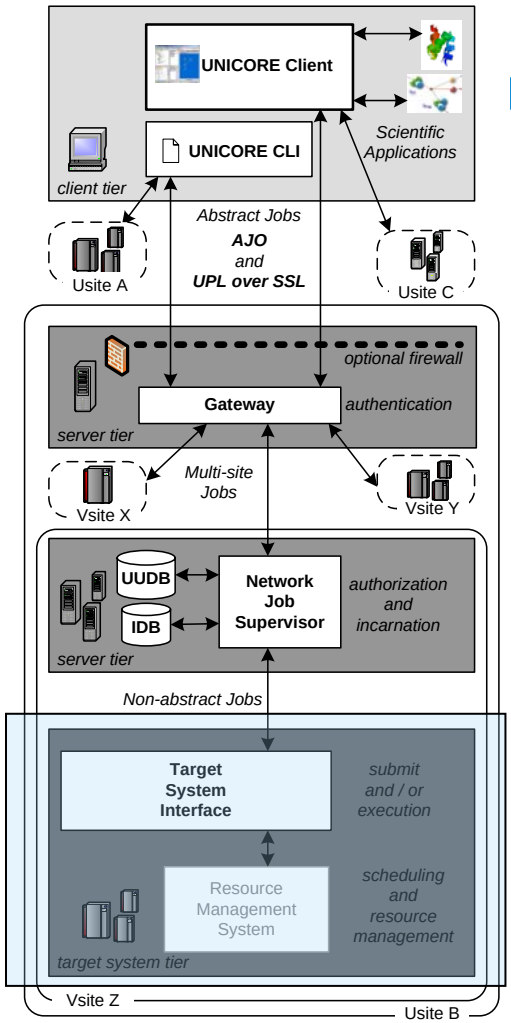


UNICORE 5 Architecture (5)



- Network Job Supervisor (NJS)
  - Analyse defined Workflows (workflow engine)
    - Multi-site, multi-step Jobs
    - Directed Acyclic Graphs
  - Submit of sub-jobs to other sites over Gateway
  - Job Incarnation via Incarnation Database (IDB)
    - turn abstract-jobs into machine-specific jobs
    - E.g. location of preinstalled software packages
  - Authorization via Unicore User Database (UUDB)
    - turn X.509 user certs to users xlogin of machine
    - The complete certificate is checked (not only DN)

UNICORE 5 Architecture (6)

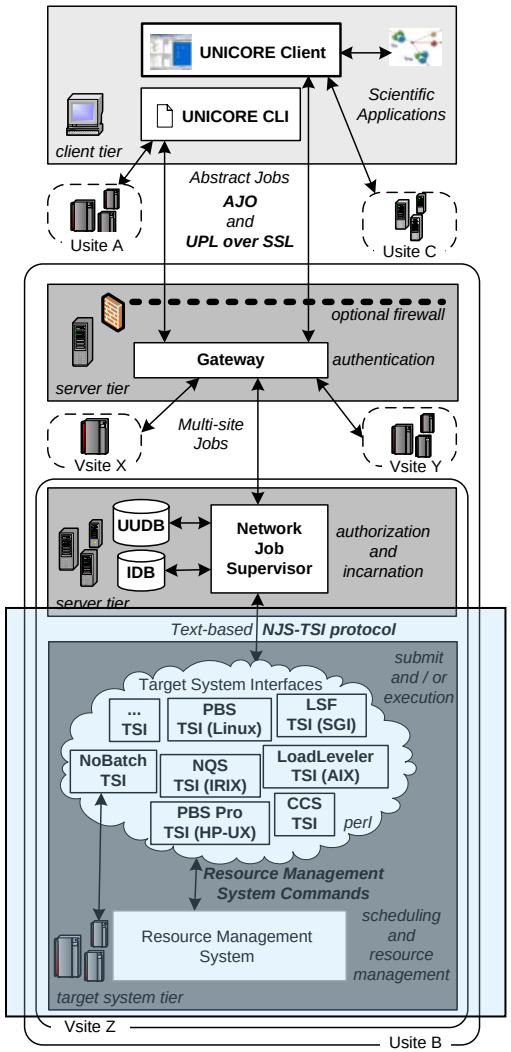


- Target System Interface
  - Represents a real Target System (e.g. a supercomputer or storage server)

  - Interaction with Resource Management Systems
    - Torque, PBS Pro, Load Leveler, (UNIX fork), …
    - Job submit to Resource Management System
    - Scheduling via Resource Management System
    - Retrieve job results and job output
    - Manage workspace

  - Access to pre-defined Applications
    - e.g. a massive parallel simulation for collaborative visualization & steering via UNICORE

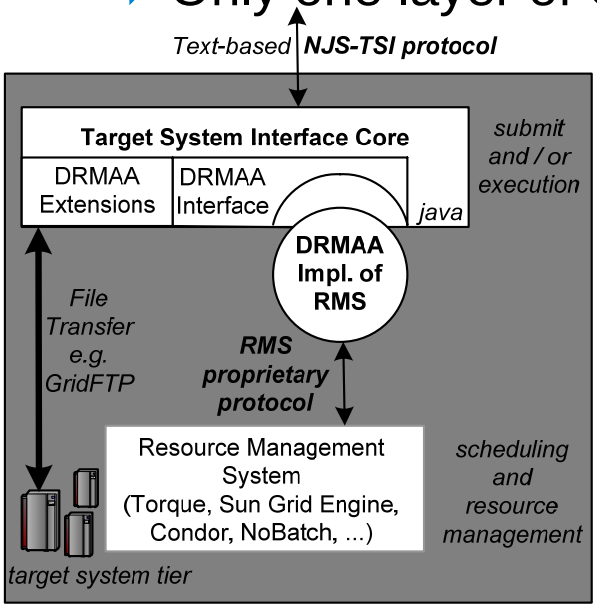
TSI & Resource Management



- Target System Tier
  - Consists of one Target System Interface
  - Interactions with underlying RMSs
- Target System Interface
  - Each supported RMS is used in conjunction with a target system-specific TSI impl. in perl
  - Perl TSI implementations are stateless daemons
  - Statically configured before startup (RMS admin)
  - Various TSI implementations
    PBS TSI (Linux), LSF TSI (SGI), PBS-Pro (HP-UX), NQS (IRIX), LoadLeveler TSI (AIX), …

TSI Framework using DRMAA

- Base upon Open Source SUN Grid Engine DRMAA impl.
  - Java Bindings of DRMAA specification are used
- Java-Based Target System Interface Core
  - Only one layer of UNICORE is exchanged → protocols still the same



- Platform & RMS command independent
- DRMAA - API “only” provides Interfaces for job submission & management
  - Additional DRMAA Extensions for file transfer
  - Transfer over Unicore Protocol Layer (UPL)
  - Optional transfer over GridFTP
- UNICORE 5/6

UNICORE in DEISA (1)

Distributed European Infrastructure for Supercomputing Applications

- Consortium of leading national HPC centers in EU

IDRIS – CNRS, France
FZJ, Jülich, Germany
RZG, Garching, Germany
CINECA, Bologna, Italy
EPCC, Edinburgh, UK
CSC, Helsinki, Finland
SARA, Amsterdam, NL
HLRS, Stuttgart, Germany
BSC, Barcelona, Spain
LRZ, Munich, Germany
ECMWF, Reading, UK

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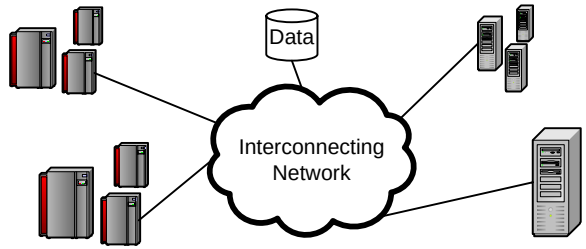
UNICORE in DEISA (2)

Distributed European Infrastructure for Supercomputing Applications

- **Deploy and operate a persistent, production quality, distributed, heterogeneous supercomputing environment**



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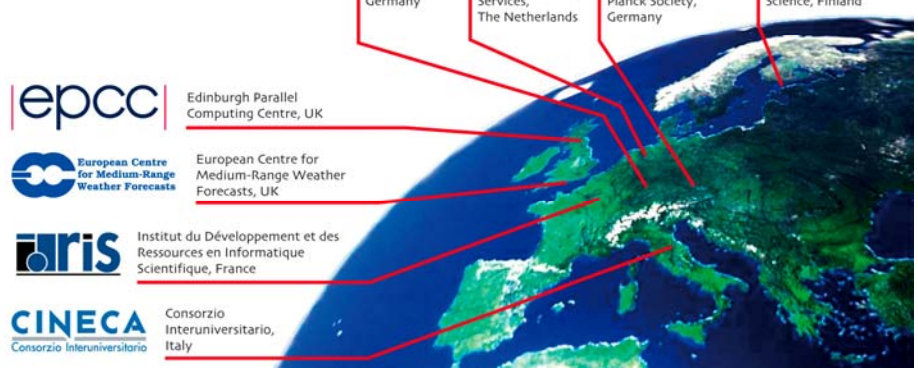
GEANT

Forschungszentrum Jülich in der Helmholtz-Gemeinschaft — Forschungszentrum Jülich, Germany

sara — SARA Computing and Networking Services, The Netherlands

RZG IPP — Rechenzentrum Garching of the Max Planck Society, Germany

CSC — Finnish Information Technology Centre for Science, Finland



epcc — Edinburgh Parallel Computing Centre, UK

European Centre for Medium-Range Weather Forecasts — European Centre for Medium-Range Weather Forecasts, UK

IDRIS — Institut du Développement et des Ressources en Informatique Scientifique, France

CINECA Consorzio Interuniversitario — Consorzio Interuniversitario, Italy

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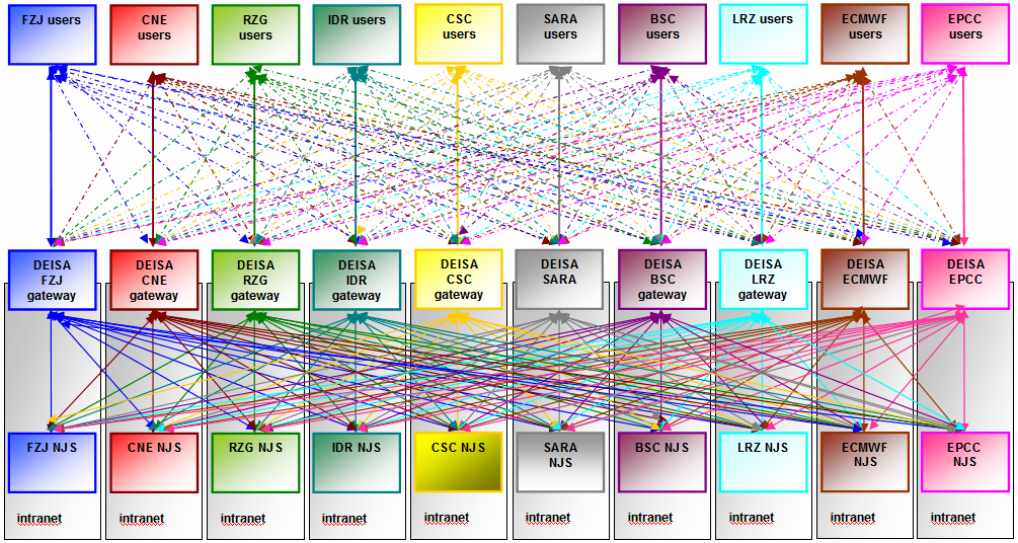
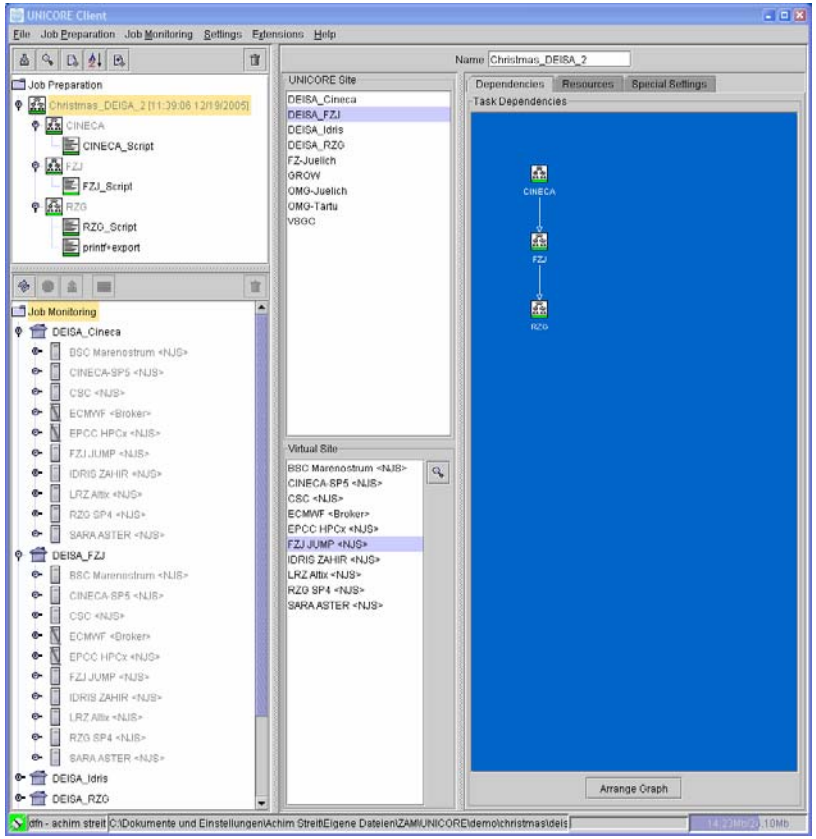
UNICORE in DEISA (3)

Distributed European Infrastructure for Supercomputing Applications

- Fully-meshed UNICORE infrastructure among partners
- Complex multi-site workflows easily possible
- Heavily used by DECI projects





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UNICORE based Access to Computing-Resources.
Delivery-Model for DWD, GRS and Team Shosholoza

UNICORE in Business scenarios

Deutscher Wetterdienst

Unicore Users

Deutscher Wetterdienst

TI

Service-Management

User Help Desk

T-Systems

SCAI

System-Management

Customer-Training

T-Systems

2nd Level Support

SCAI

2nd Level Support

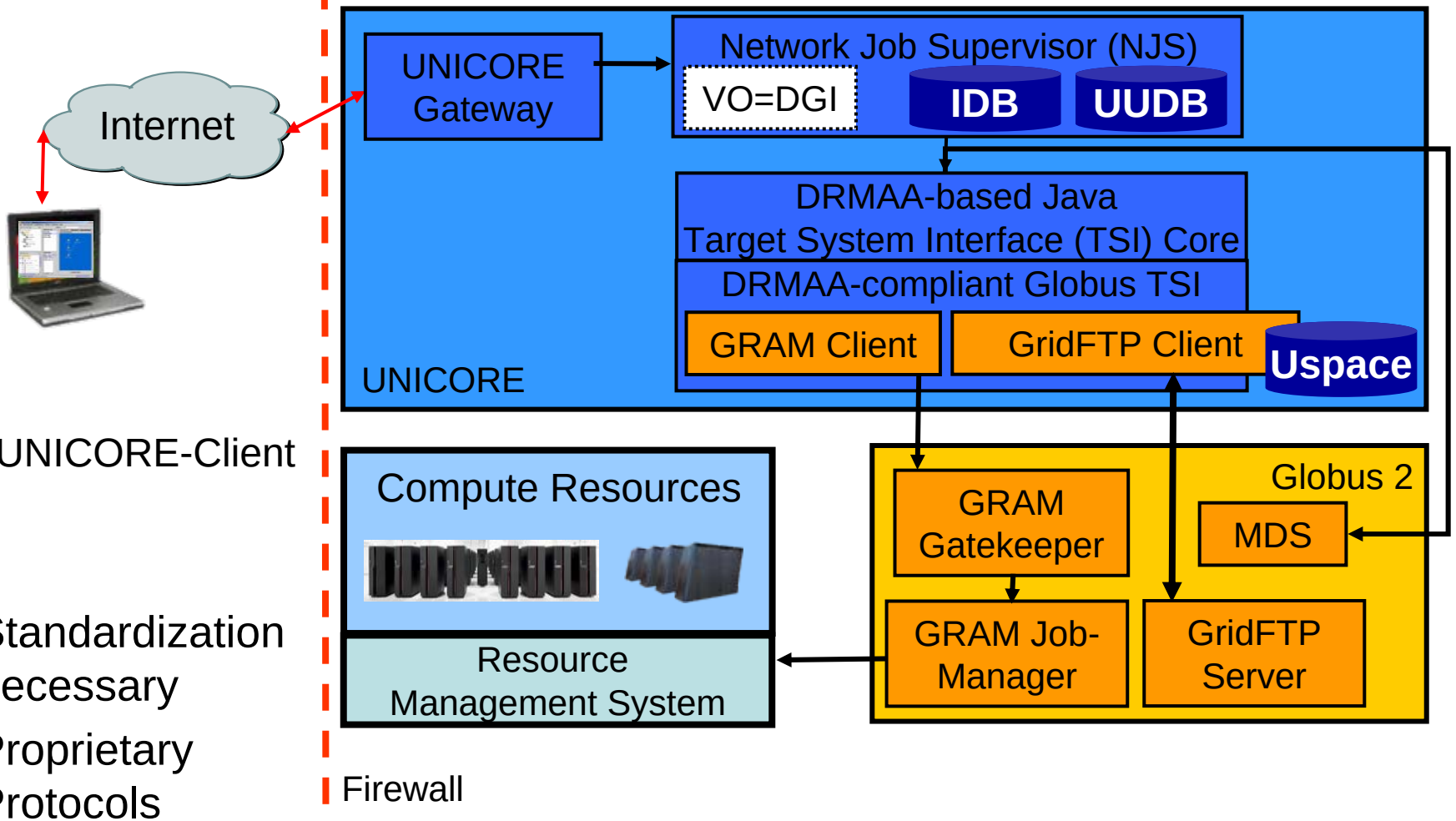
3rd Level Support by Developpers

UNICORE - LIFE - CD

- Complete “out-of-the-box” usage of UNICORE 5
- Bootable Linux OS with UNICORE 5 pre-installed
- Does not harm your system → Sandbox scenario
- For testing, evaluating, …

AVAILABLE HERE AND AT THE GRID VILLAGE UNICORE BOOTH

Initial Interoperability UNICORE & Globus 2.4



- Standardization necessary
- Proprietary Protocols
  - UNICORE AJO/UPL, Globus RSL

Emerging Grid Standards (1)

- OGSA – Open Grid Services Architecture
  - “The Physiology of the Grid”, GGF - GFD30
  - Resources shared via services in Grids
  - Lifecycle management for Web Services necessary

- OGSI – Open Grid Services Infrastructure
  - Globus Toolkit 3 provides early implementation
  - (US Projects using Globus are better funded by US – Gov)

- WS-RF - Web Services Resource Framework
  - Re-factors and evolves OGSI to exploit WS-* technologies
  - Same functionality as OGSI, but separated Specifications

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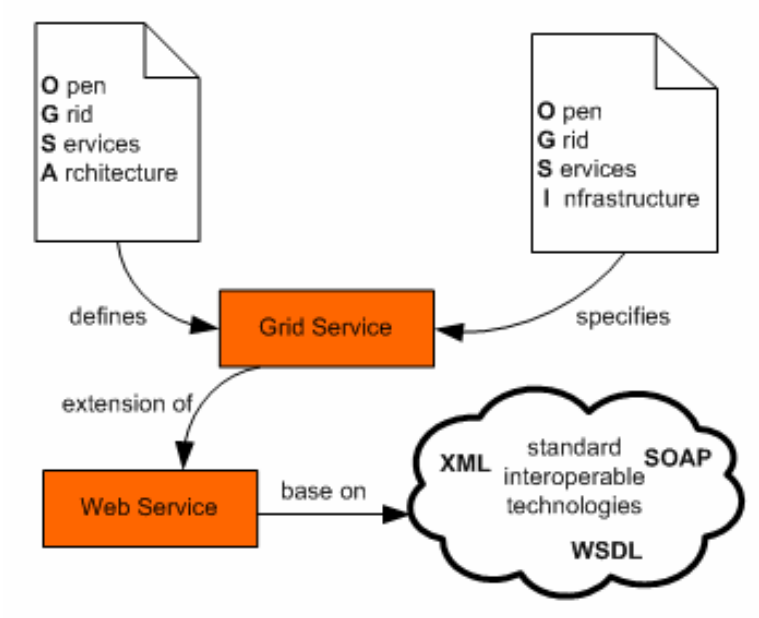
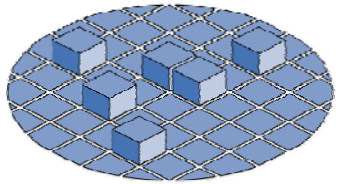
Emerging Grid Standards (2)

- Change of Terminology
  - From ***Grid Services*** …



  - …to ***stateful Web Services***

UNICORE 6



UniGrids

- Development of next generation of UNICORE called UNICORE 6 based on OGSA and compliant with WS-RF
  - Broader vision of interoperability between different Grid middleware
  - Interoperable infrastructures through standards

Research Center Jülich (project manager)

Consorzio Interuniversitario per il Calcolo Automatico dell'Italia Nord Orientale

Fujitsu Laboratories of Europe

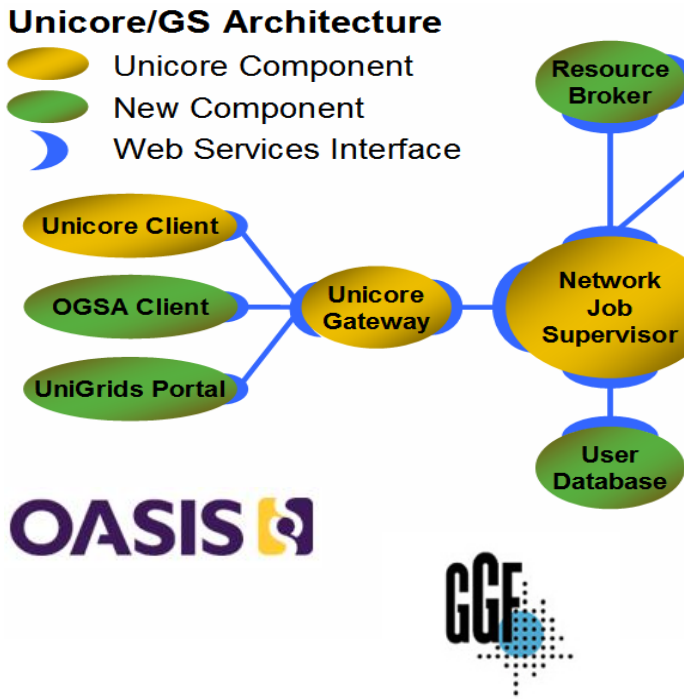
Intel GmbH

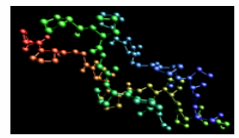
University of Warsaw

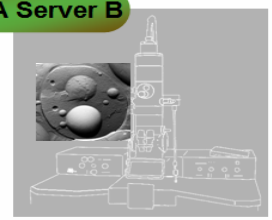
University of Manchester

T-Systems SfR

Funded by EU grant: IST-2002-004279







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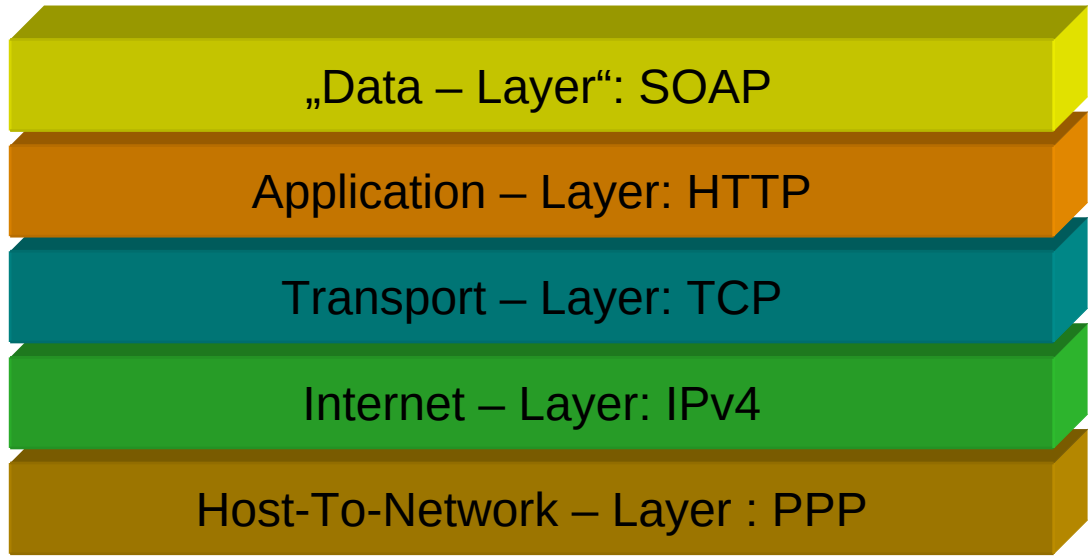
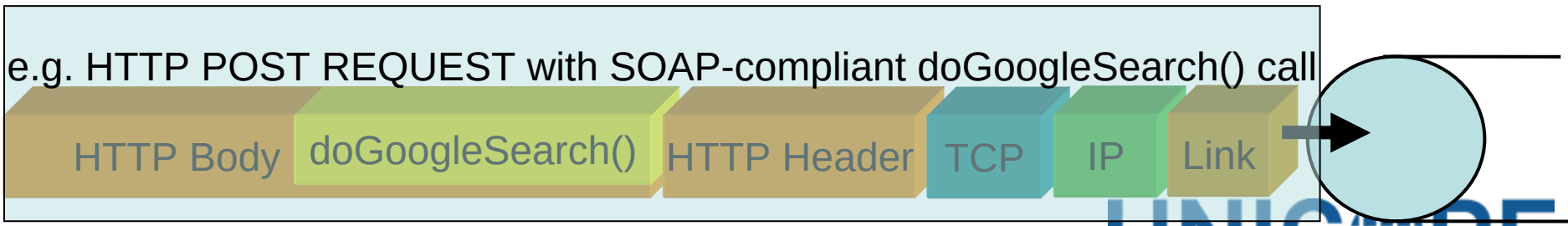
Understanding SOAP & WS-RF (1)

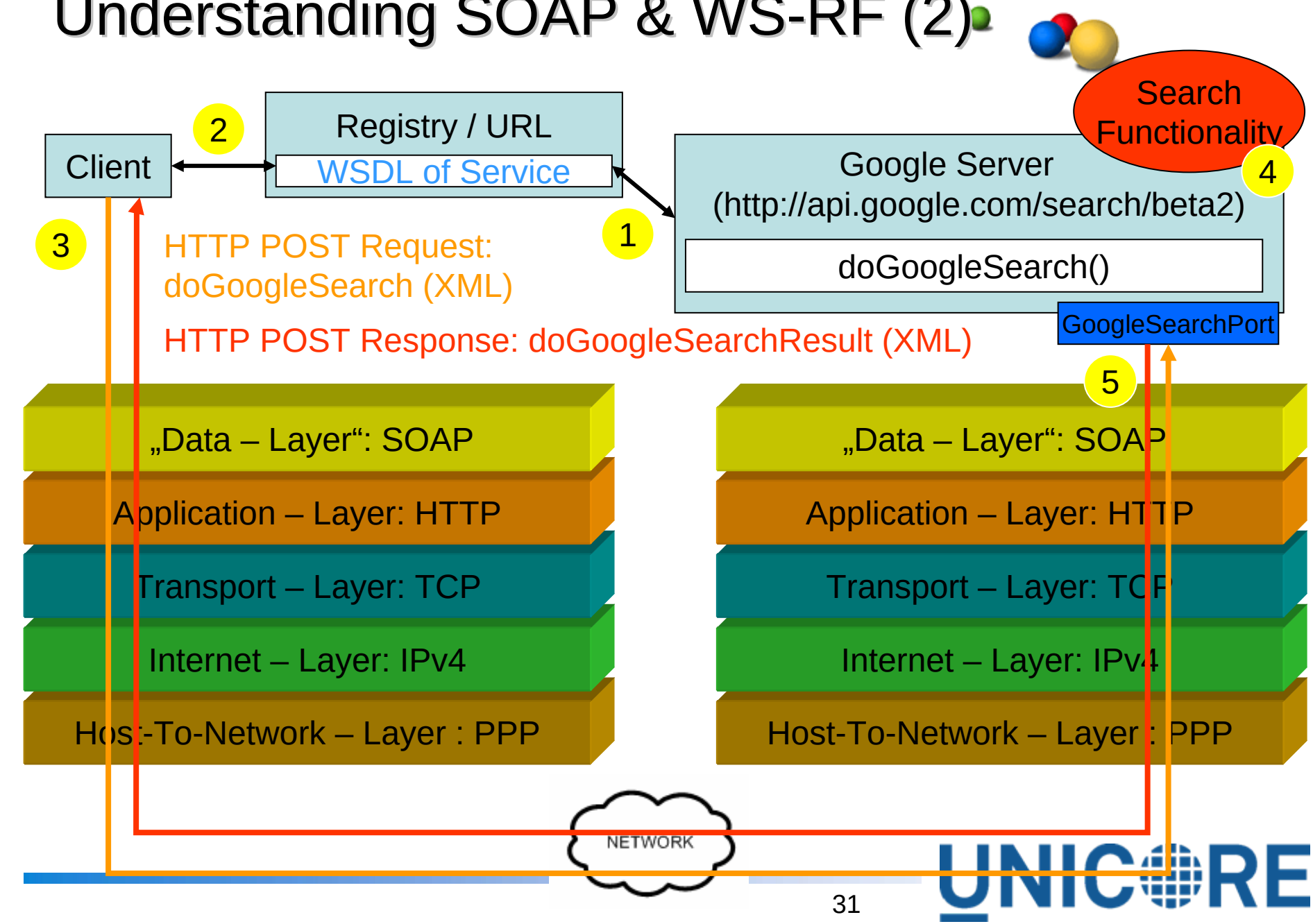
- Using WSDL description for XML tags of doGoogleSearch()

```
<soap>
<soap:header>
http://api.google.com/
search/beta2
</soap:header>
<soap:body>
doGoogleSearch( key = ‚Grid‘ )
</soap:body>
</soap>
```





Understanding SOAP & WS-RF (2)



Understanding SOAP & WS-RF (3)

Job Execution

Client

2

Registry / URL

WSDL of Service

UNICORE Server

(http://jump.kfa-juelich.de/TargetSystemService)

4

submit()

TargetSystemPort

1

3

HTTP POST Request:
submit (XML → JSDL)

HTTP POST Response: submitResult (XML)

5

„Data – Layer“: SOAP

Application – Layer: HTTP

Transport – Layer: TCP

Internet – Layer: IPv4

Host-To-Network – Layer : PPP

„Data – Layer“: SOAP

Application – Layer: HTTP

Transport – Layer: TCP

Internet – Layer: IPv4

Host-To-Network – Layer : PPP

NETWORK

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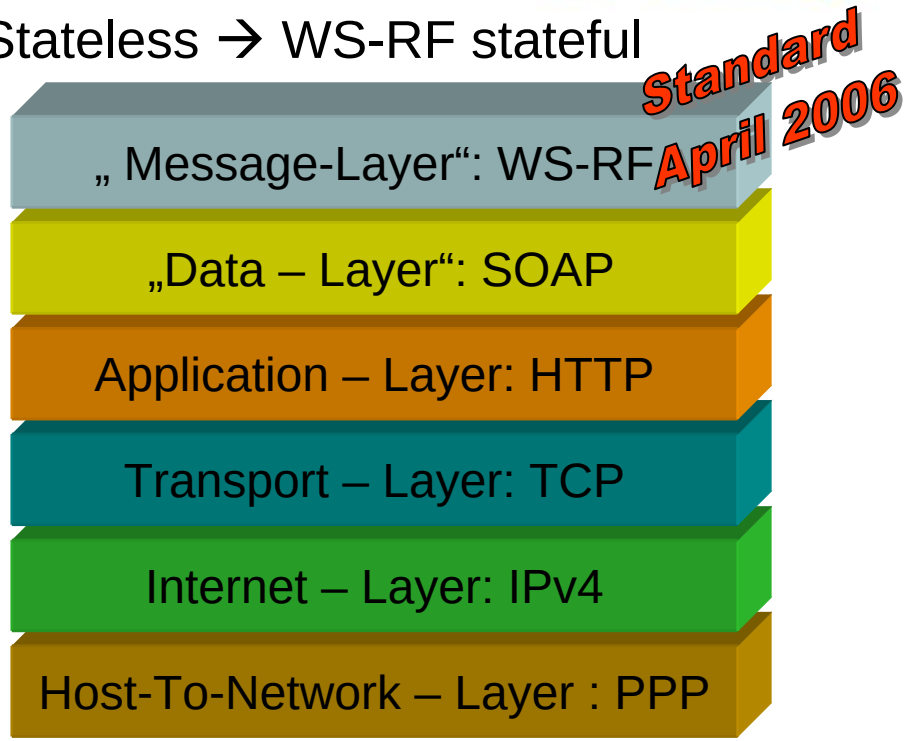
Standardization for interoperability

- Web Services Resource Framework (WS-RF) protocol
  - Add semantics & syntax to operations (GetResourceProperties)
    - Get a list of properties that the service is offering
  - A Web Service itself is typically Stateless → WS-RF stateful
  - Grids need access to stateful resources
    - jobs, supercomputers, telescope, collider,…
- Autonomic behaviour
  - Services know how they can interact
  - Standardized operations & properties

OASIS



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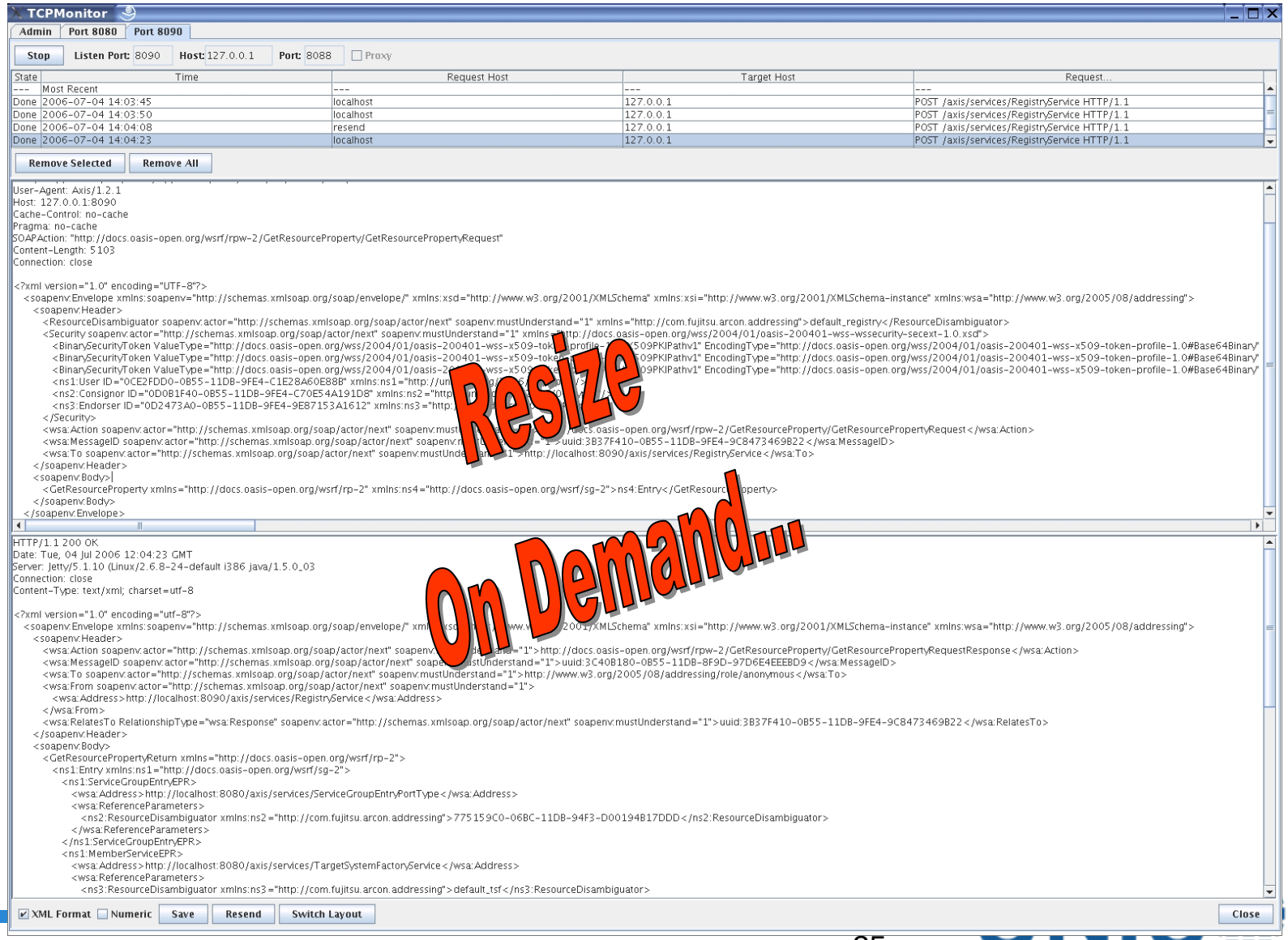
WS-RF Specifications

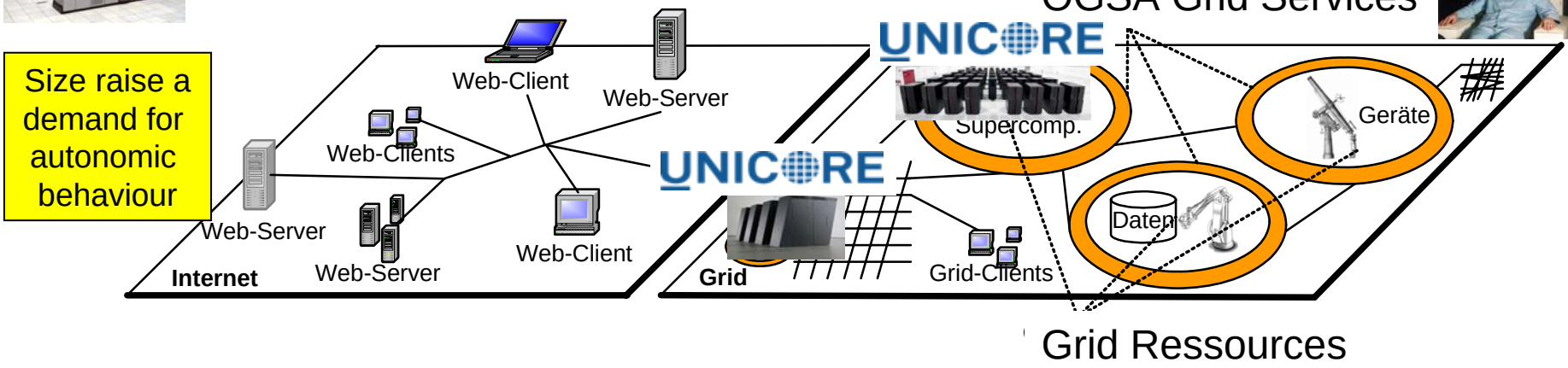
- Base for others WS-Notifications, WS-Agreement, …
- Five Specifications (public comment - Version 1.2)
  - WS - Resource
    - Relationship Web service and resource
  - WS – Resource Lifetime
    - Lifecycle of a WS-Resource, TerminationTime, etc.
  - WS – Resource Properties
    - Getters/Setters/Queries of Properties
  - WS - BaseFaults
    - Base set of information that appear in fault messages
  - WS – Service Groups
    - Collections of WS or WS-Resorces

A WS-RF message via SOAP (use of WS-Addressing&Security)



Stateful Web Services & Grids with UNICORE

- ‚Grid Services' – Web Services that implement Grid patterns
- Open Grid Services Architecture (OGSA)
  - WS-RF is one implementation of OGSA concepts
  - Access and management of Grid resources of interest
  - Web Services with standardized state interactions
    - State of a supercomputer (memory, applications, etc.)
    - State of submitted jobs on resources

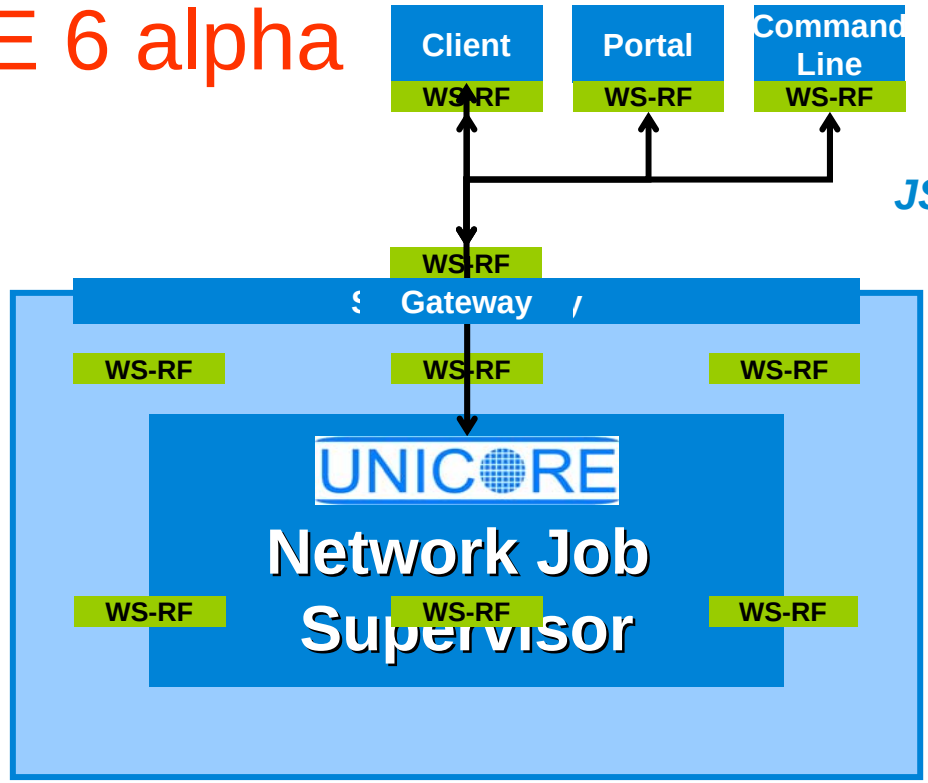


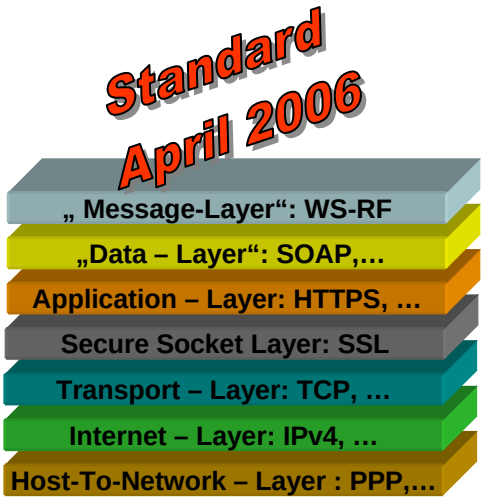
UNICORE

Transforming UNICORE

UniGrids

- Developments of
  UNICORE 6 alpha





OASIS

UNICORE

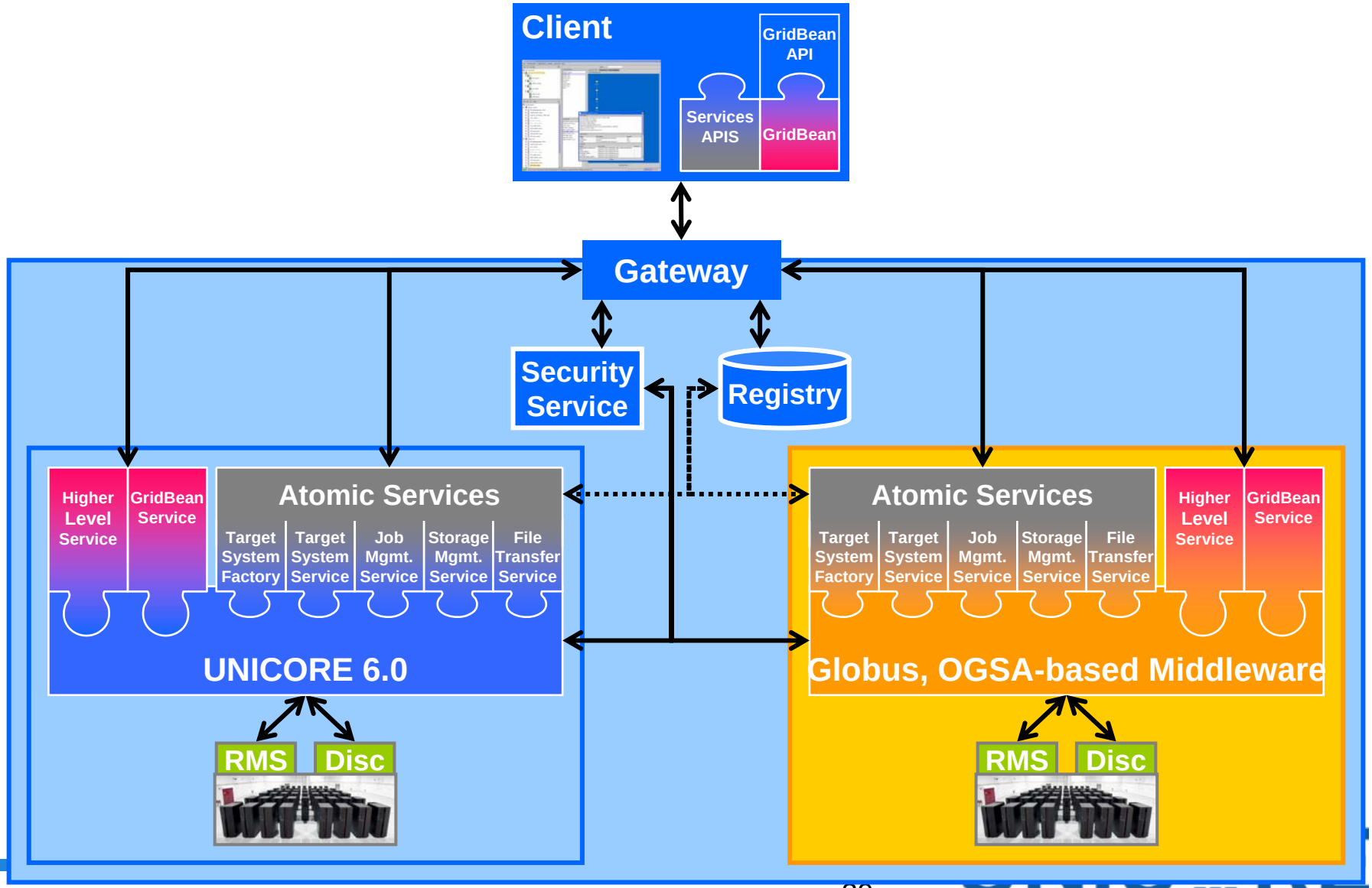
Job Submission Description Language Example

```
<?xml version="1.0" encoding="UTF-8"?>
<JobDefinition xmlns="http://schemas.ggf.org/jsdl/2005/11/jsdl">
  <JobDescription>
    <Application>
      <POSIXApplication xmlns="http://schemas.ggf.org/jsdl/2005/11/jsdl-posix">
        <Executable>/bin/echo</Executable>
        <Argument>hello world</Argument>
      </POSIXApplication>
    </Application>
 </JobDescription>
</JobDefinition>
```

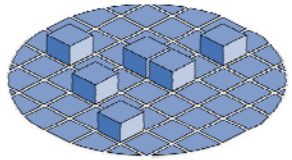
- JSDL Specification → GFD.56
  - November 2005 - Published as GGF Recommendation

Architecture of UNICORE 6.0

UniGrids

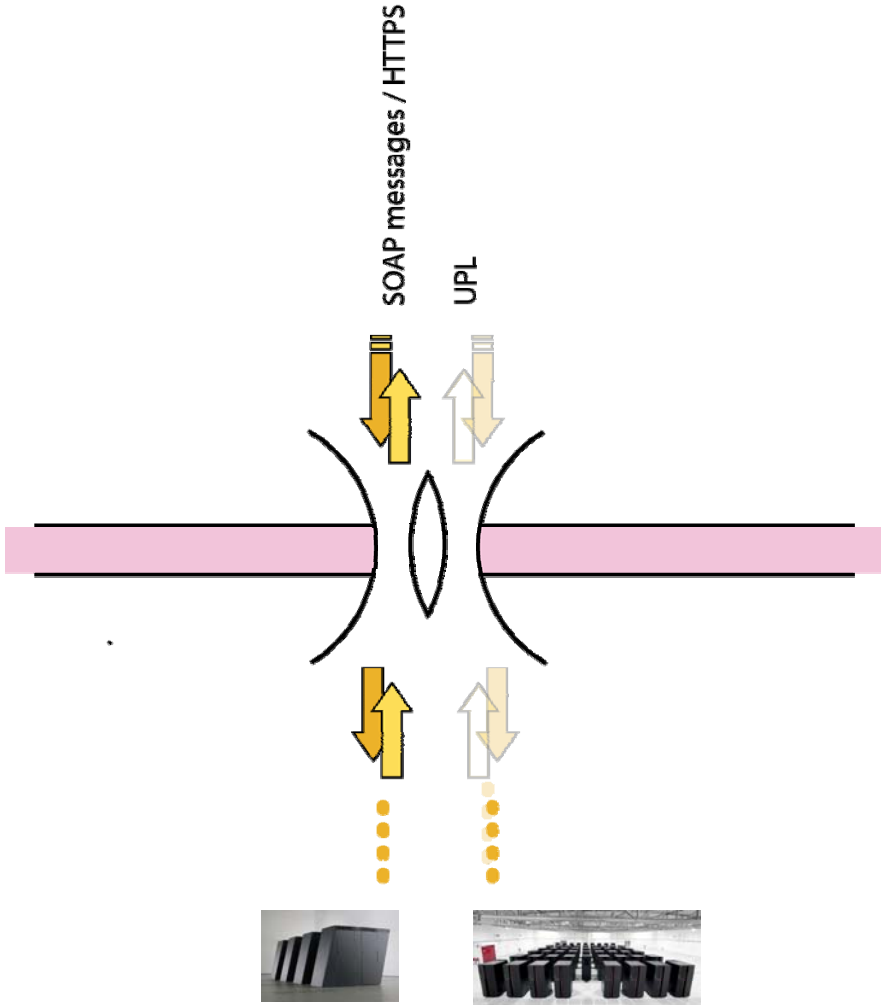


New Gateway of UNICORE 6



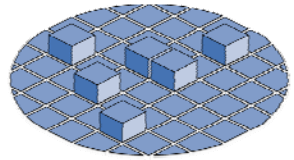
UniGrids

- Multiple Protocol Support
- Supports UPL
  - For Production UNICORE Installations
- Supports WS-* technologies
  - WS-Addressing
  - SOAP messages / HTTPS
- Retains Unicore Security (!)
  - Single point of entry
  - Client Authentication
  - SSL Connections



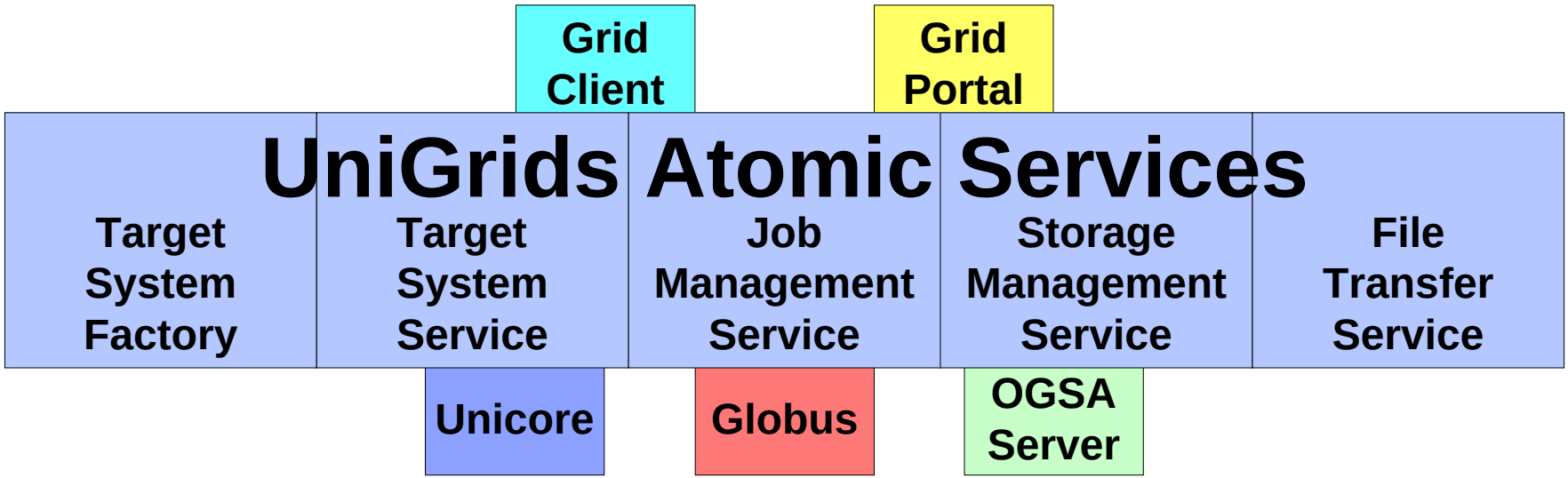
UNICORE

UniGrids Atomic Services



UniGrids

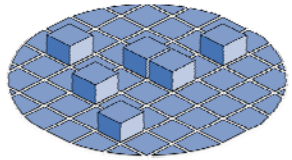
- Interoperability between OGSA based Grid systems
- Cross–authentication for UNICORE and Globus



- Enable cross–Grid resource brokering
- Workflows over different Grid Systems

UNICORE

Interoperability & Standards



UniGrids

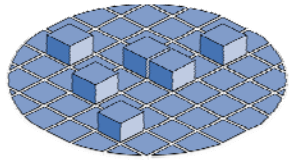
UniGrids Atomic Services				
Target System Factory	Target System Service	Job Management Service	Storage Management Service	File Transfer Service

UNICORE and Globus developers

- Feed in standardisation process of GGF via OGSA Basic Execution Services (BES) Working Group

UNICORE

Job Submission Standards



UniGrids

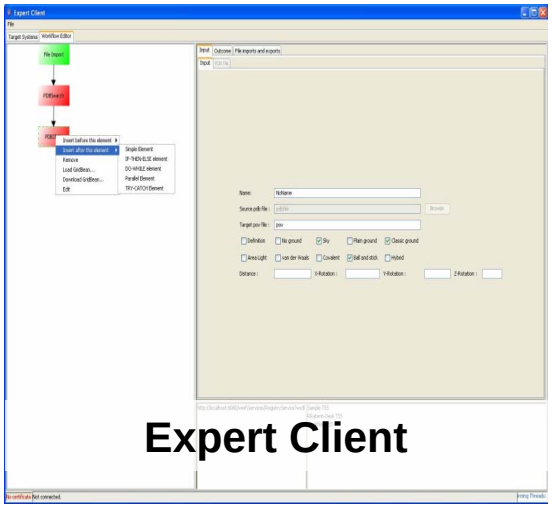
- OGSA - Basic Execution Services (BES)
- Unigrids (Uniform Interface to Grid Services)
  - Developed WS-RF- based UniGrids atomic services (UAS)
  - UAS: basic interfaces for job/file management in UNICORE 6 alpha

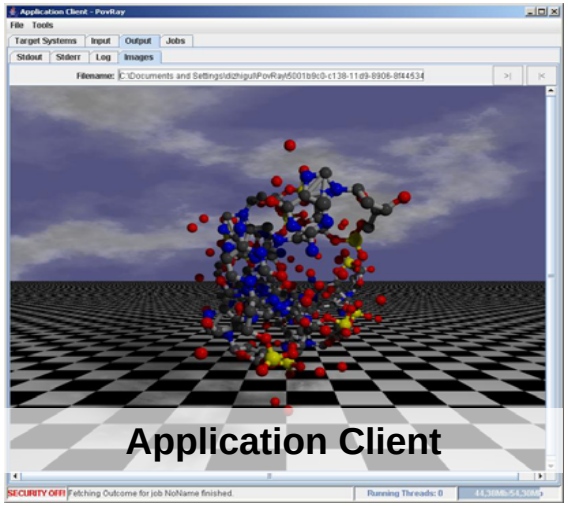
Target System Factory	Target System Service	Job Management Service	Storage Management Service	File Transfer Service

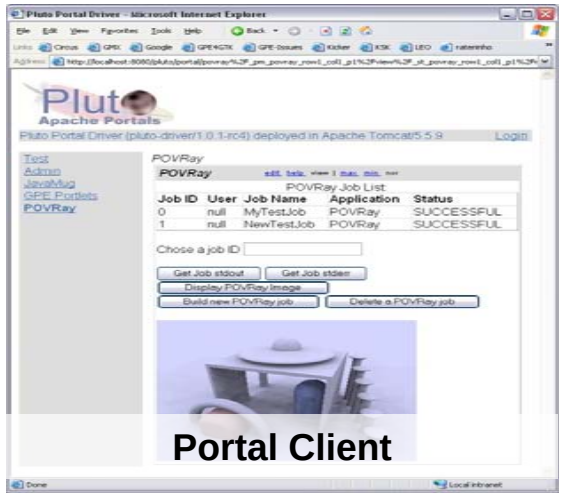
- Execution Services Interface
  - Draft by Argonne (Globus) and Fujitsu (UNICORE)
  - Consists of UAS input and Globus GRAM demands
  - Input to the OGSA - BES GGF working group
- Refactoring of UAS when OGSA-BES is revised

Grid Programming Environment (GPE) Clients

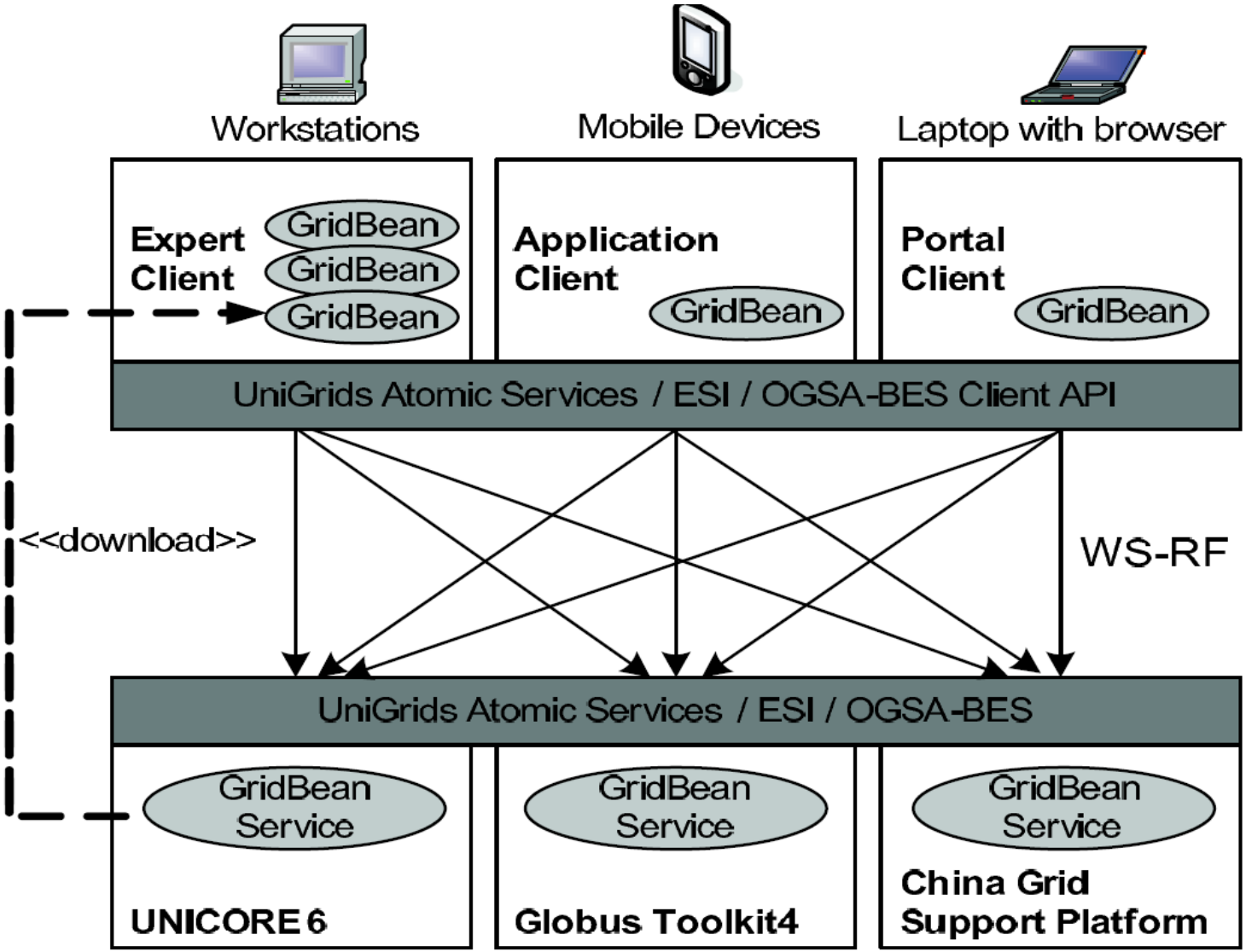
- GPE consists of a set of Grid tools
- e.g. GPE Client Framework for UNICORE 6
  - Client-side for UNICORE 6 and other Grid systems
  - Three different clients for three different usages
  - GridBeans as scientific-area specific Plugins





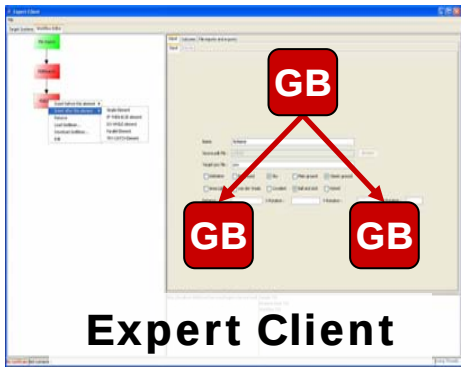


GPE Clients and GridBean Deployments



Portable Clients and GridBeans

GB GridBean

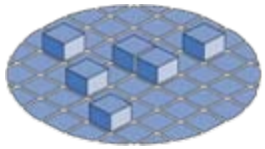


- GPE Clients work on top of Unicore/GS, GTK4 or ChinaGrid
  - Only requirement: Atomic Service interfaces
- GridBeans are portable without modifications
  - Client API hides underlying infrastructure details

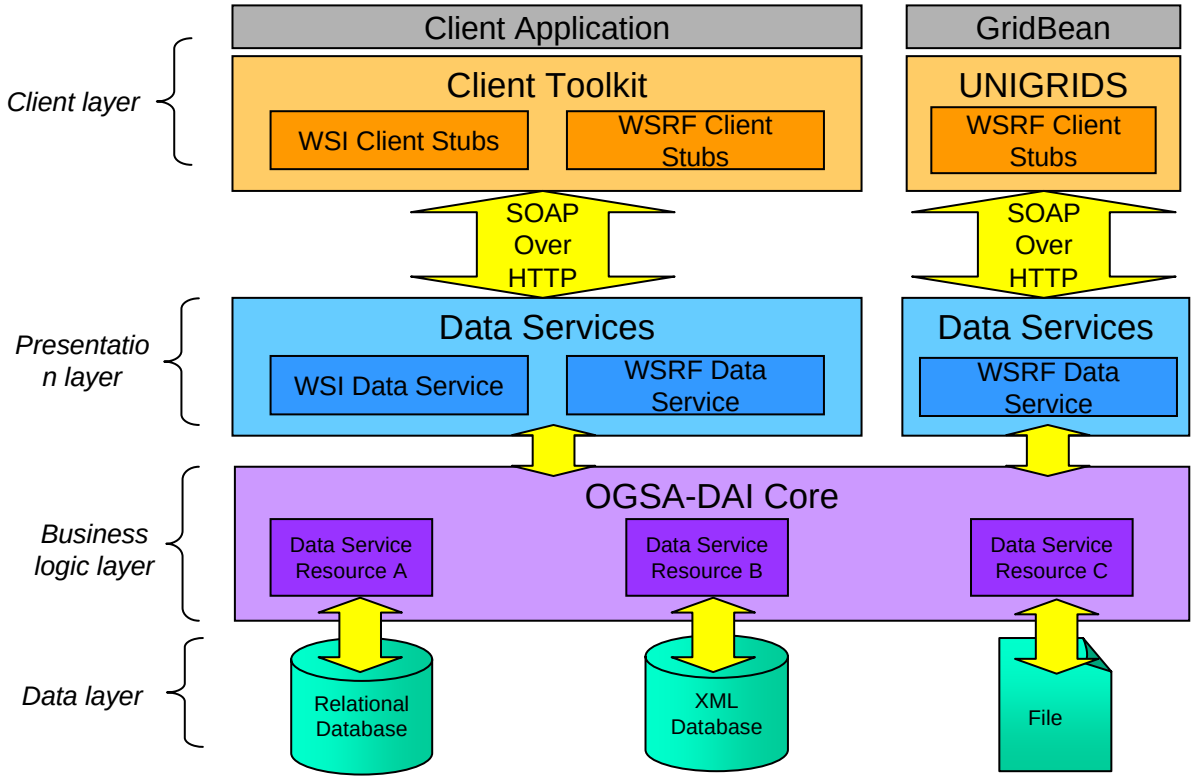
UNICORE

Database Access: OGSA - DAI

- OGSA – Database Access and Integration Services
  - Initially implemented within UniGrids

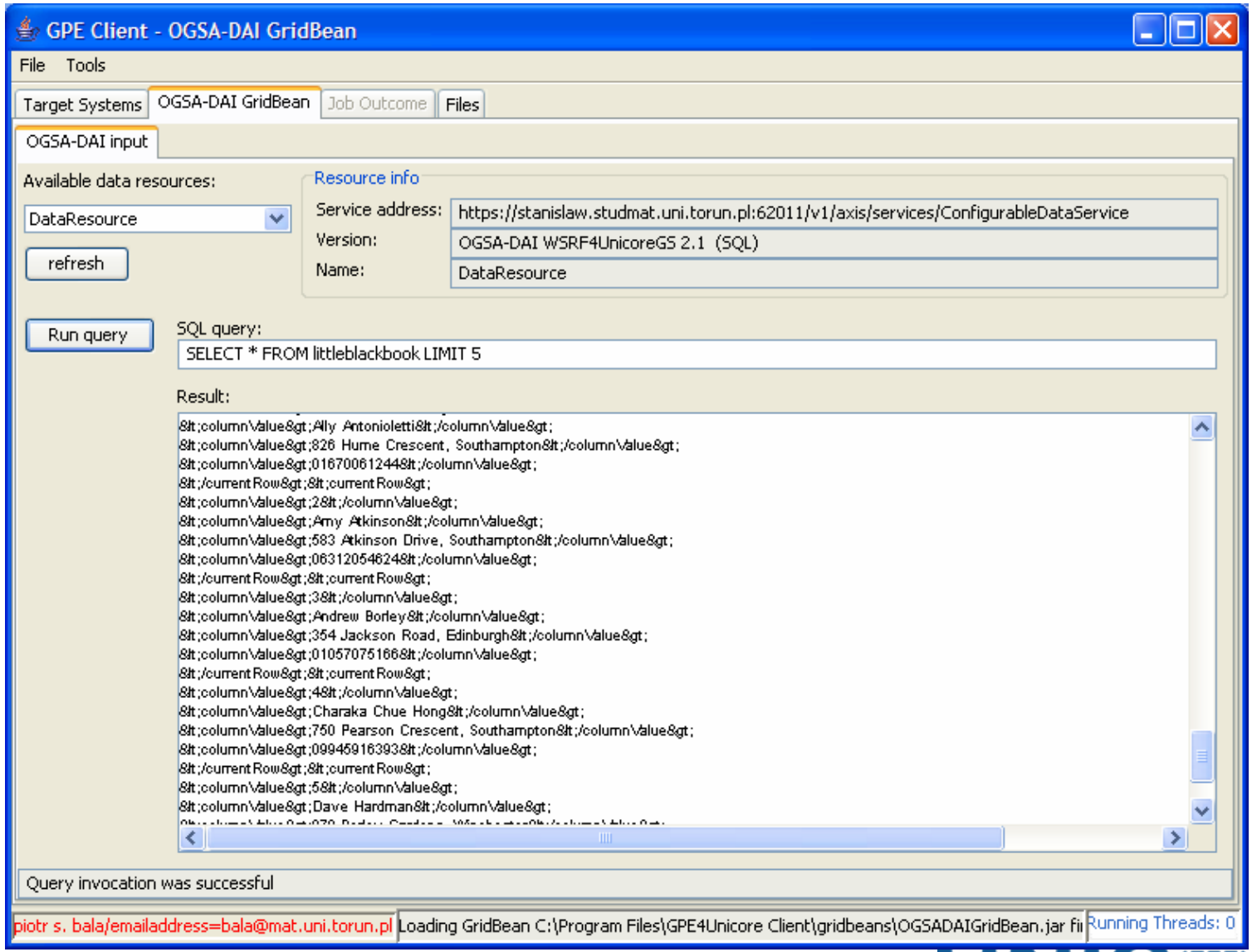


  - Re-engineering of OGSA-DAI alpha implementation within EU Project OMII - Europe



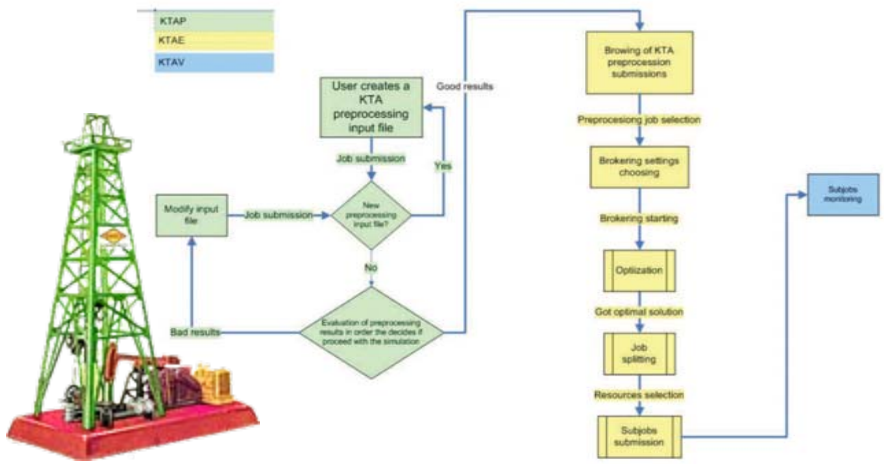
- OGSA – DAI services hosted in UNICORE 6

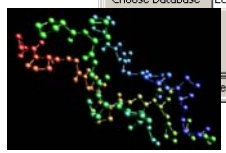
Database Access: OGSA-DAI GridBean

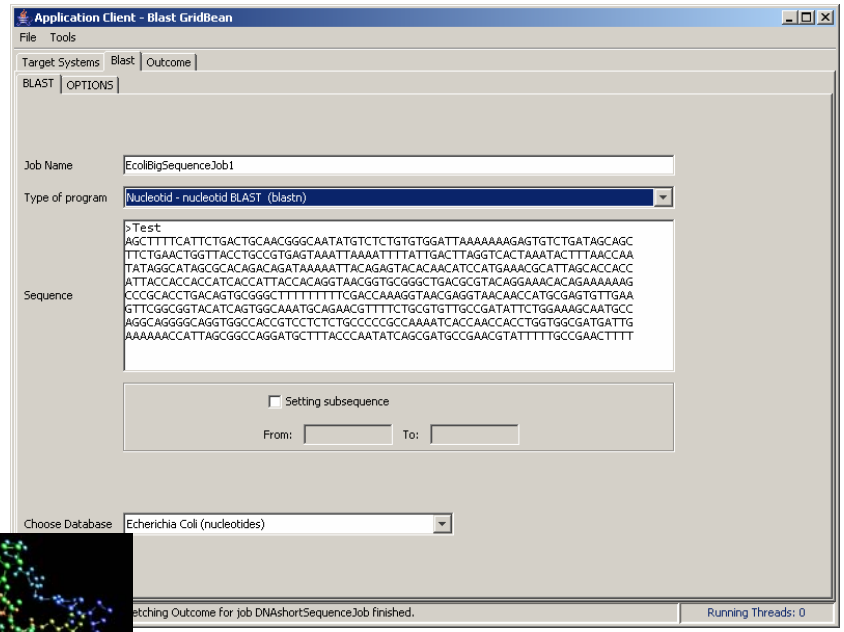


Other Grid Beans for Applications

- BLAST GridBean used by molecular biology scientists to determine the structure and sequence of DNA
- KTA GridBeans provide solutions for an industrial application
  - Application named as the PreStack Depth Migration (PSDM)
  - Application belongs to the Kirkhoff True Amplitude (KTA) methods class for seismic signal processing
  - Runs on machines with MPI



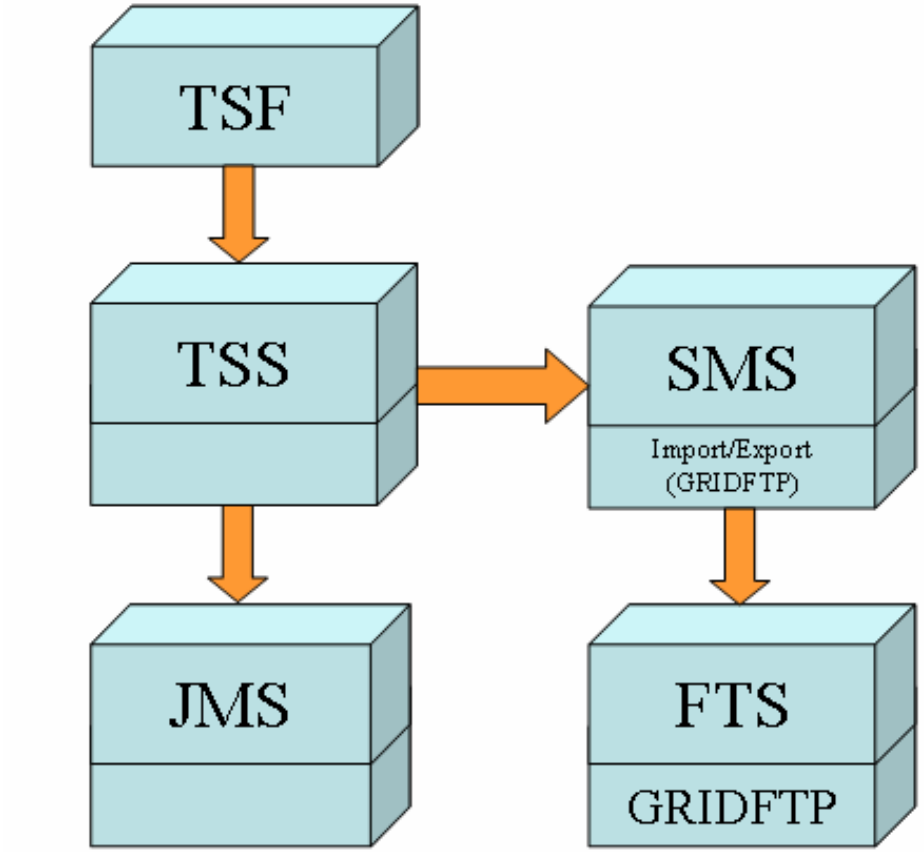




UNICORE

GridFTP File Transfer Service Architecture

- Client – Server transfers
- Server – Server transfers
  - Including SRB
- GFTS GridBean available for clients



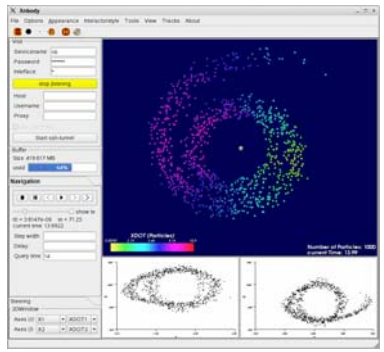
Data Transfer of huge files via GridFTP

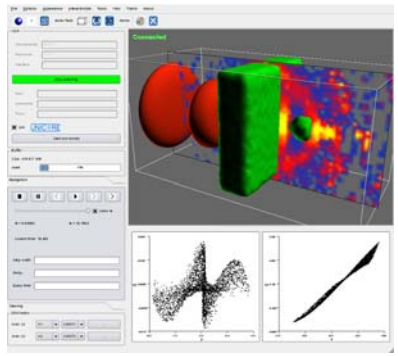
UNICORE

Collaborative Visualization & Steering (1)

- **VISualization Interface Toolkit (VISIT)**
  - Light-weight library that supports bi-directional data exchange between visualizations and parallel applications
  - Visualisation application acts as a server:
    All operations have to be initiated by the simulation
  - SSH Tunnel for using the VISIT protocol for secure communications with short latency (UGSF optionally)

- **VISIT / GS Family**
  - A higher level service family for collaborative visualizations
  - Hosted within the Unicore/GS WS-RF hosting environment
  - Parallel to the atomic services





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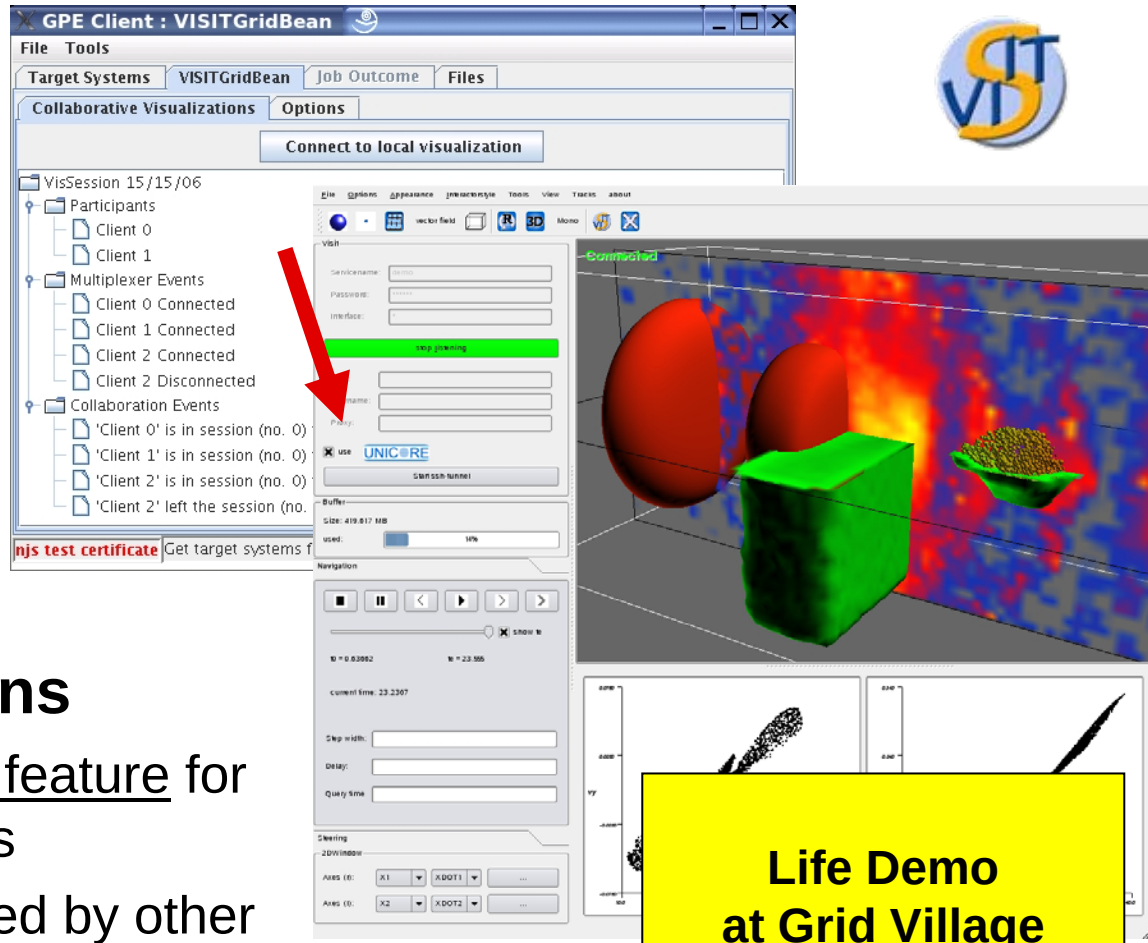
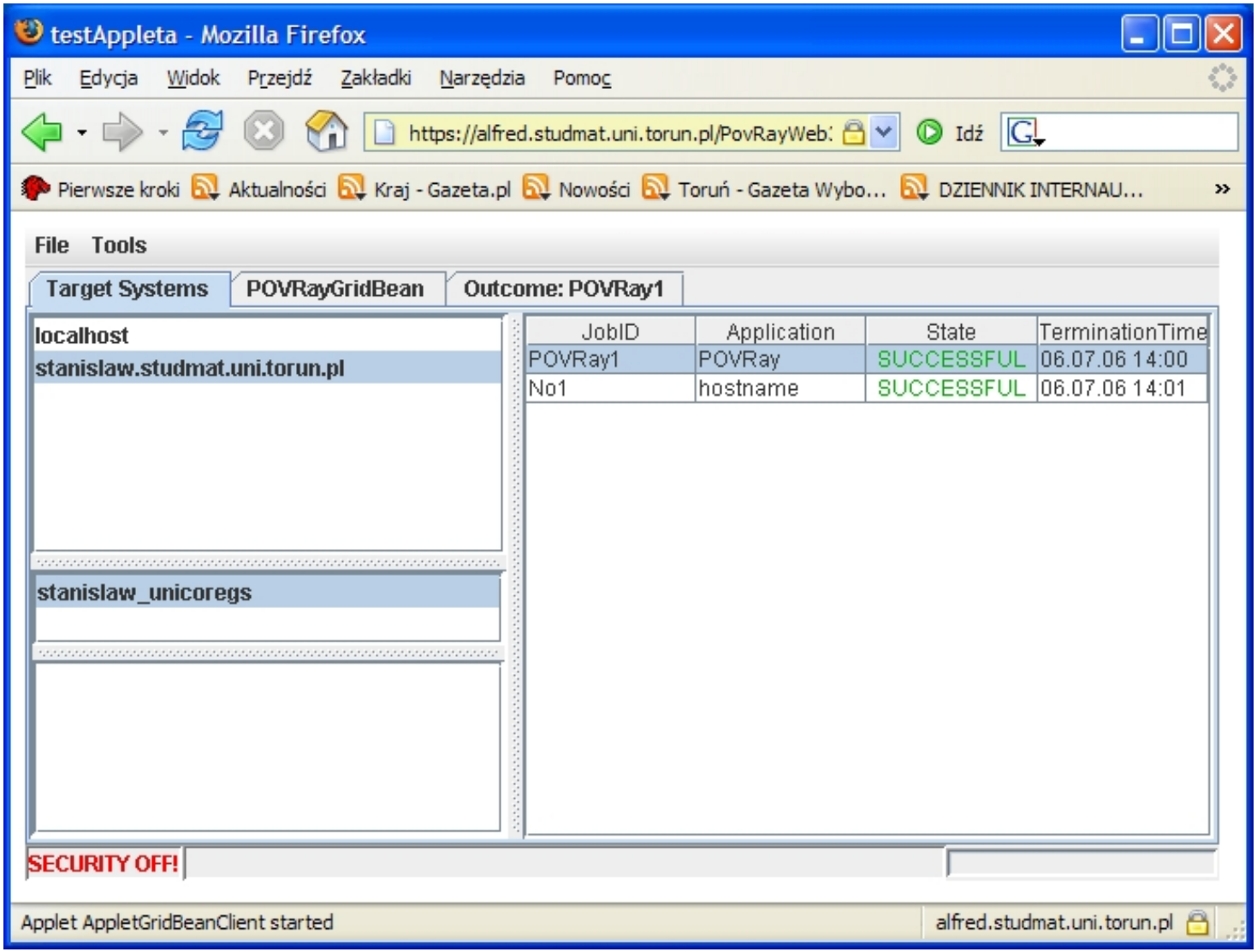
Collaborative Visualization & Steering (2)

- **VISIT GridBean**
  - Manage participants of visualization sessions via VISIT / GS family
- **Framework works with all VISIT - enabled applications**
  - Unique Unicore/GS feature for interactive scenarios
  - Not naturally provided by other Grid middleware, e.g. Globus, gLite
  - Used in Astrophysics (nBody), Laser-Plasma Physics (PEPC),…

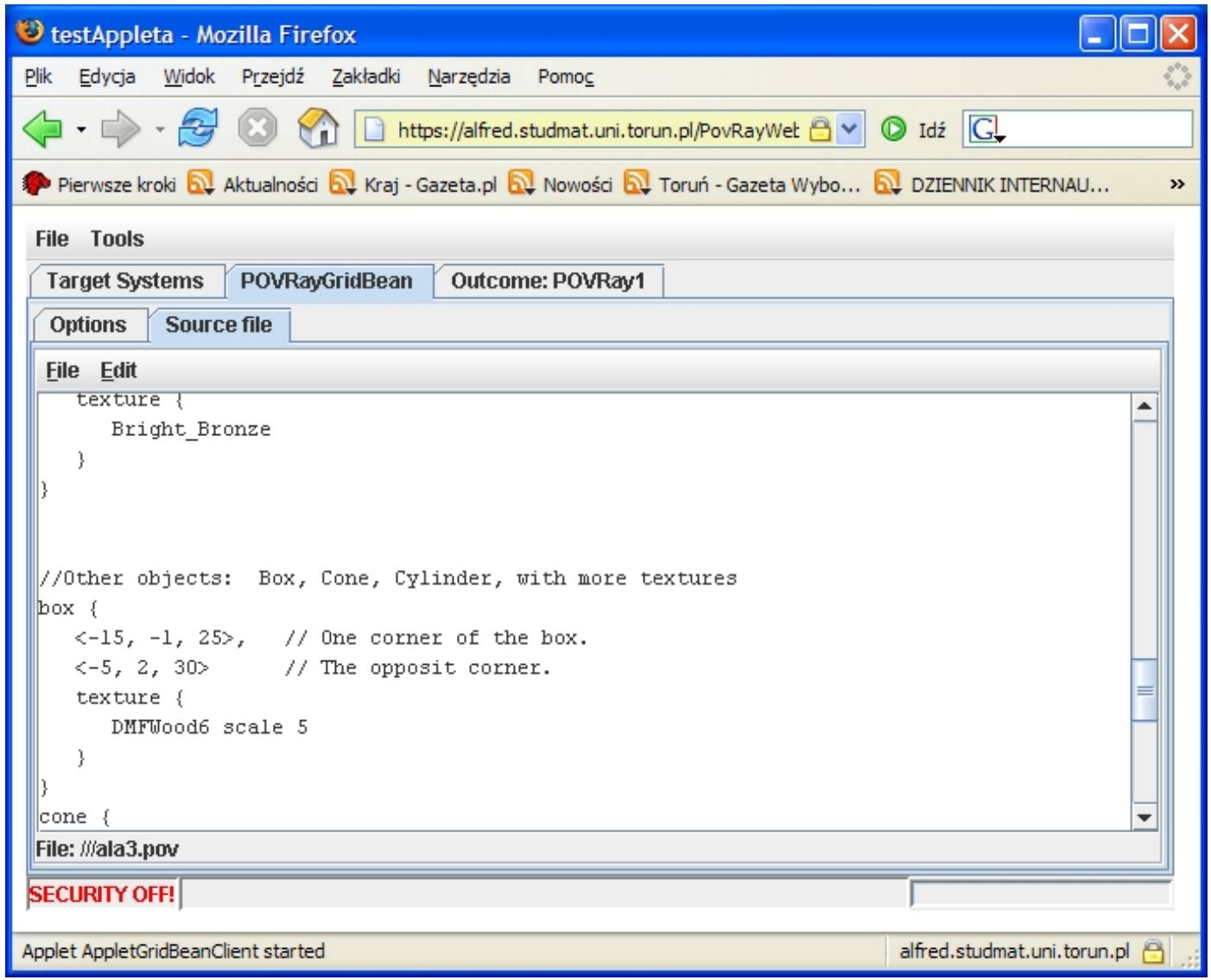


Life Demo at Grid Village

Initial Portal Clients & Services (1)



Initial Portal Clients & Services (2)



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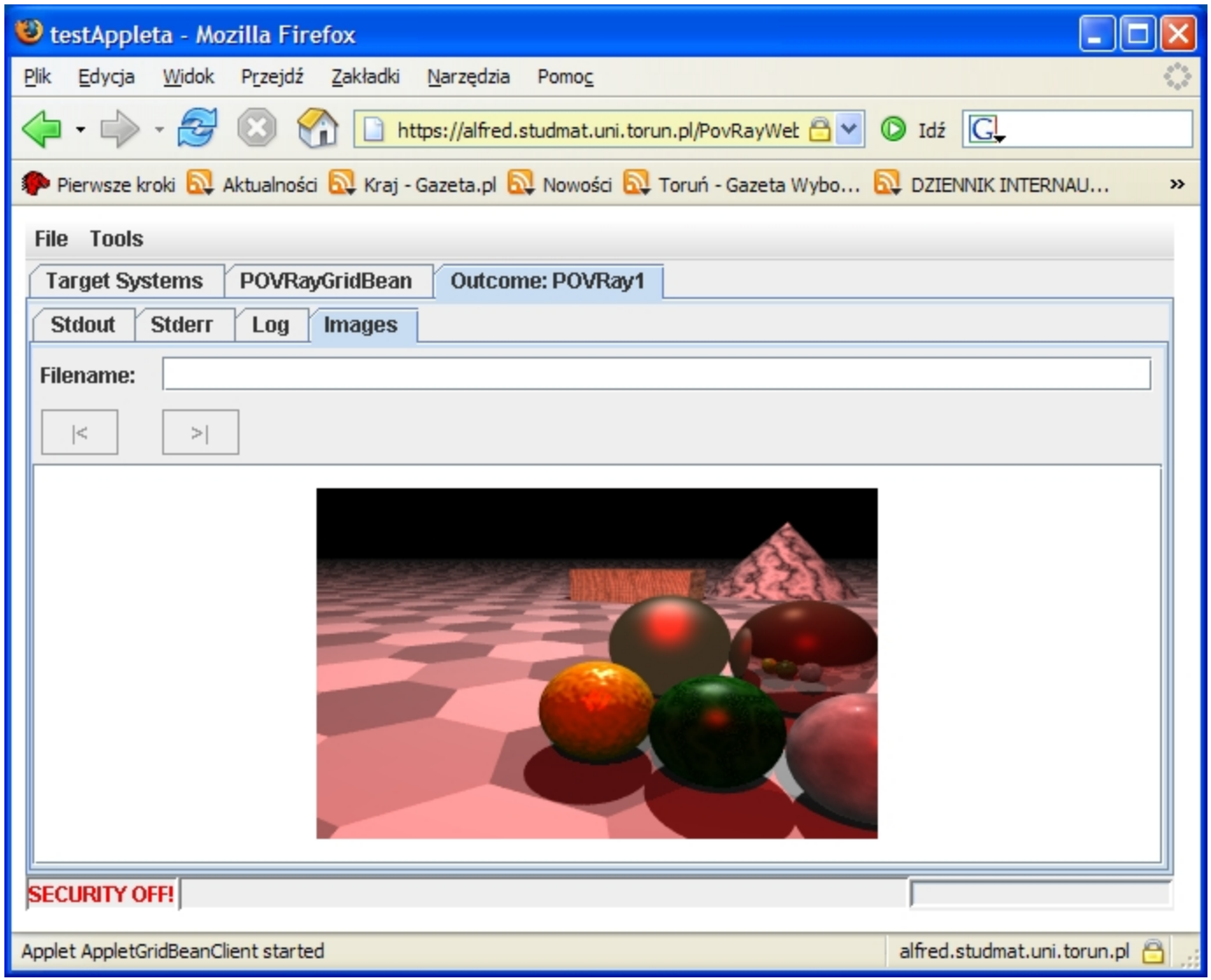
Initial Portal Clients & Services (3)



UNICORE

Roadmap to UNICORE 6 Production Quality

- New infrastructure based on Web services
  - OGSA-based and WS-RF-compliant
  - Heavily committed to Open Standards from GGF & OASIS
  - Various useful and modern higher level services (e.g.streaming)
- Alpha was released at the end of July 2006
  - **http://unicore.sourceforge.net**
  - TBD: Name des Bundles!
- Beta in July 2007
- Final in End 2007 (production quality)

Some Future Developments

- Improving the knowledge oriented scientific/industrial workflow capabilities & usability

- Improving the maturity of atomic and higher level services
  - Job Submission → OGSA - BI
  - Data Access → OGSA – DAI
  - Accounting → RUS and UR
  - VO Management → VOMS
  - Portals → GridSphere

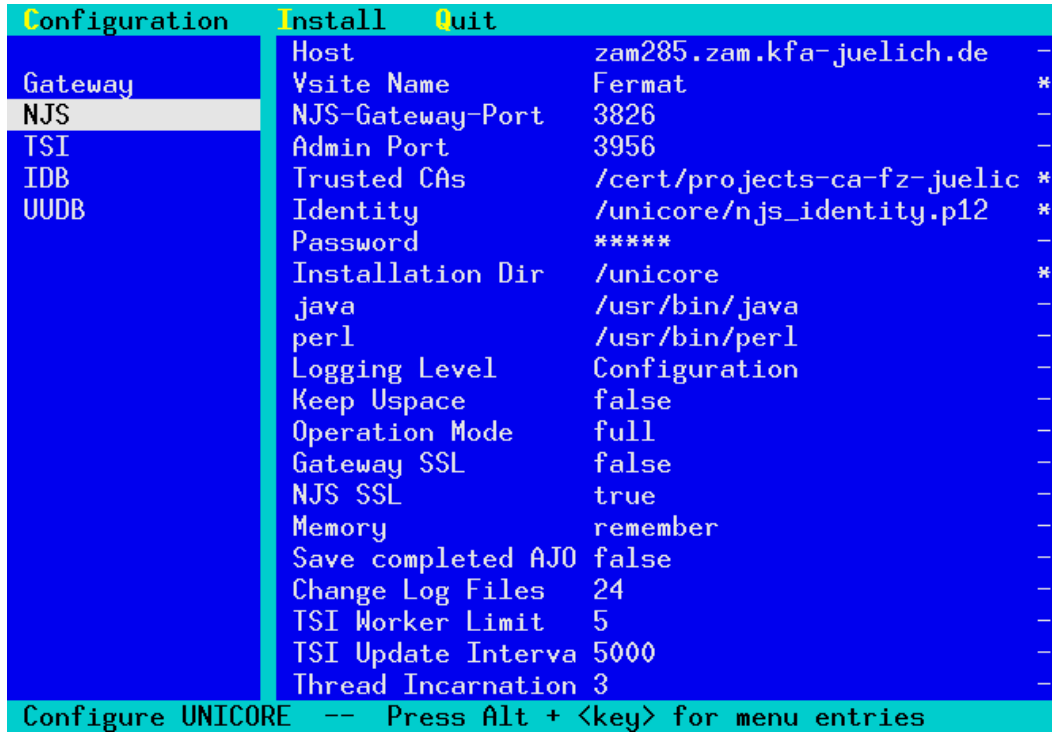
- Improving Interoperability & Interoperation with other Grid systems

UNICORE

UNICORE OPEN SOURCE

- http://unicore.sourceforge.net

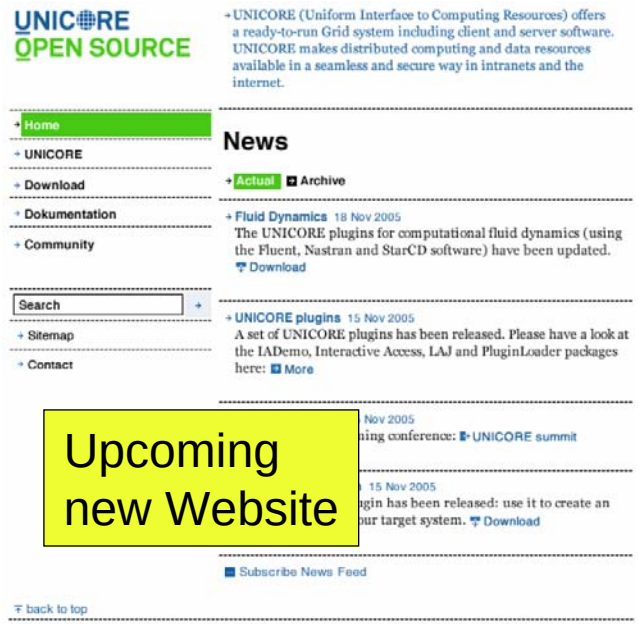
- Open Source under BSD license
- Ready-to-use for research and industry
- Strong security
- Easy installation & configuration



UNICORE OPEN SOURCE

- http://unicore.sourceforge.net

- Academic support by FZJ
  - Integration of own results and from other projects
  - Release management
  - Problem tracking, assistance
  - CVS, Subversion, mailing lists, docs



- Viable basis for many other projects

Chemomentum
eGee
D-GRID
omii europe
open middleware infrastructure institute
A-WARE
An easy Way to Access grid REsources
Distributed European Infrastructure for Supercomputing Applications
UNICORE

UNICORE FORUM

- Founded by developers, leading EU HPC centres, and supporting hardware vendors as a non-profit association
- Foster the distribution and use of UNICORE, organize workshops, support presentations at conferences, publish and maintain the specifications, coordinate further developm certify implementations and extensions

UNICORE

Summary

- UNICORE is a Grid System from Europe, is open-source and is used in production worldwide (e.g. DEISA)
- UNICORE 6 base upon OGSA concepts
- Emerging standards such as WS-RF implement OGSA
- UNICORE 6 is compliant with the WS-RF OASIS Standard
- UniGrids Atomic Service as basic set for job management
- UniGrids Atomic Service contribute to ESI & OGSA-BES
- UNICORE 6 massively commits to emerging Grid standards
  - OASIS WS-RF&WSN, GGF JSDL, W3C WS-Addressing
- UNICORE OPEN SOURCE … under BSD license
- UNICORE FORUM … supports activities after projects
- UNICORE SUMMIT … to meet the UNICORE community

UNICORE SUMMIT

VISIT THE GRID VILLAGE UNICORE BOOTH

- http://summit.unicore.org/2006/index.html
- http://summit.unicore.org/2005/index.html

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