Bridge

Project Presentation





FhG

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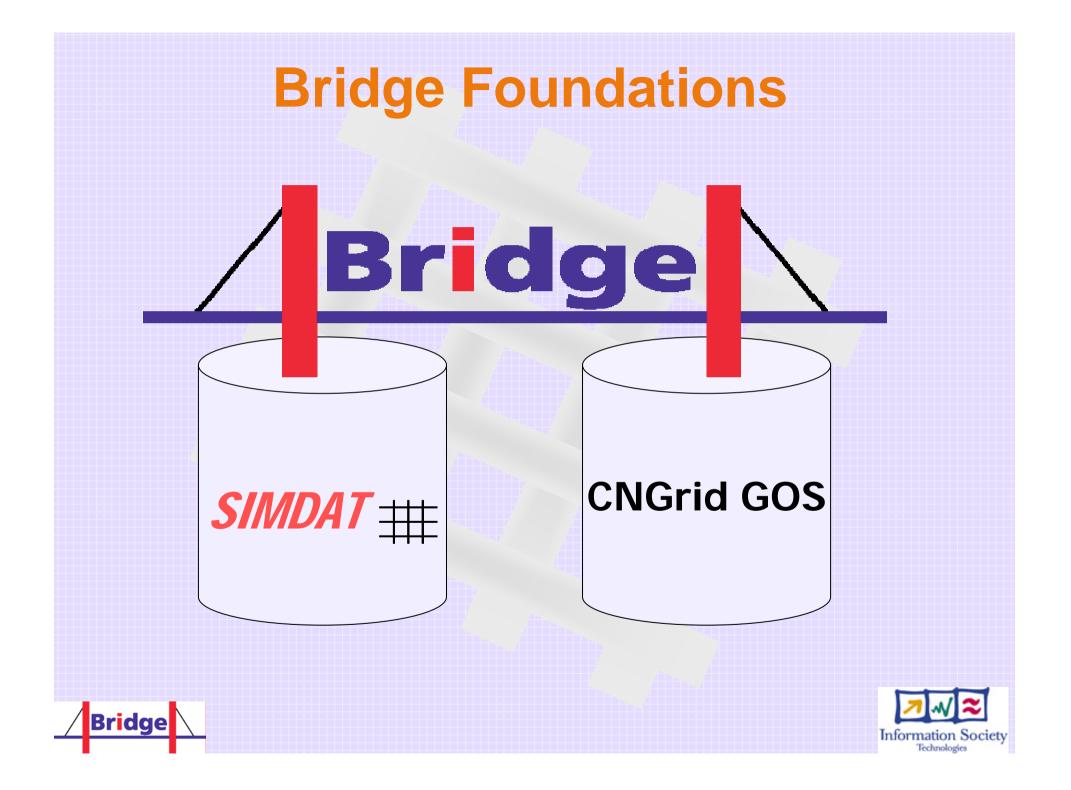
Third Grid@Asia Workshop 11 to 13 December 2006 Seoul –The WestinChosun

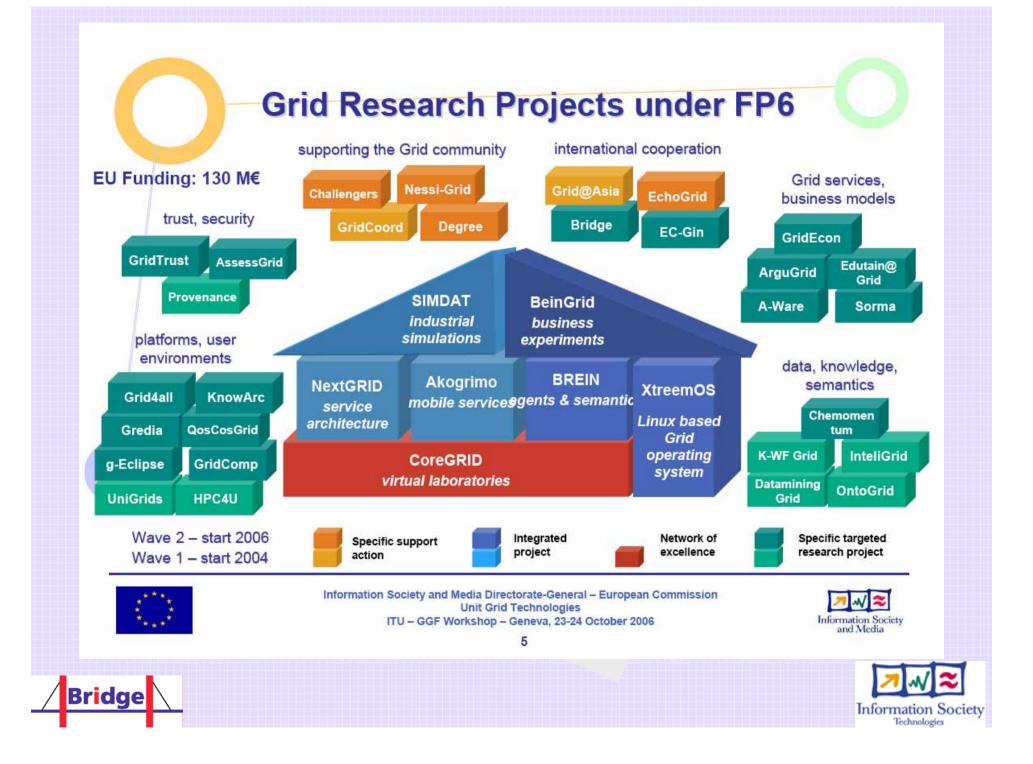




EU Funded Project - Start: January 1st, 2007 **Bilateral Research and** Industrial **Development enhancing and integrating** Grid **Enabled technologies** EADS Infor ense CECMWF FhG ٢ Information Soc

Technologies





Bridge Objectives Develop, enhance and interconnect European and Chinese Grid middleware technology

Set up integrated Grid test bed using European and Chinese middleware components for application demonstration

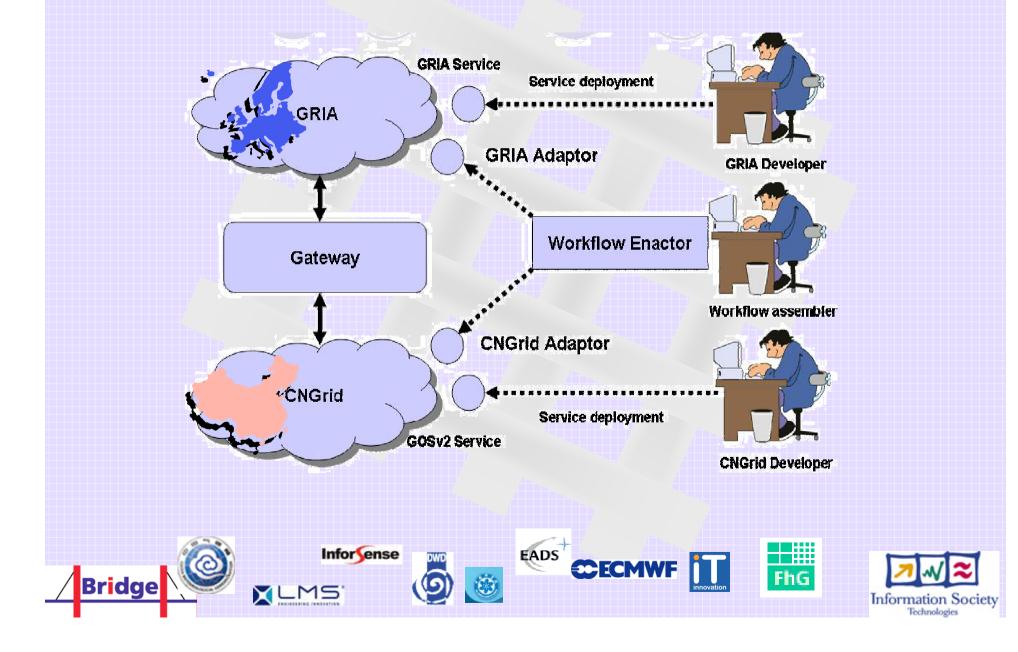
Set up joint application showcases using distributed workflow and data access technology

Disseminate the results of the project to industrial and academic communities

Demonstrate the benefits of Grid technology for international cooperation



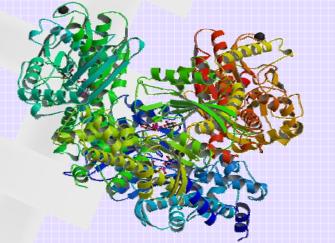




> Application showcases ⇒ Aerospace ⇒ Meteorology ⇒ Drug Design









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Meteo:

Seamless access to heterogeneous distribute data repositories

Aero:

Multidisciplinary collaborative configuration design

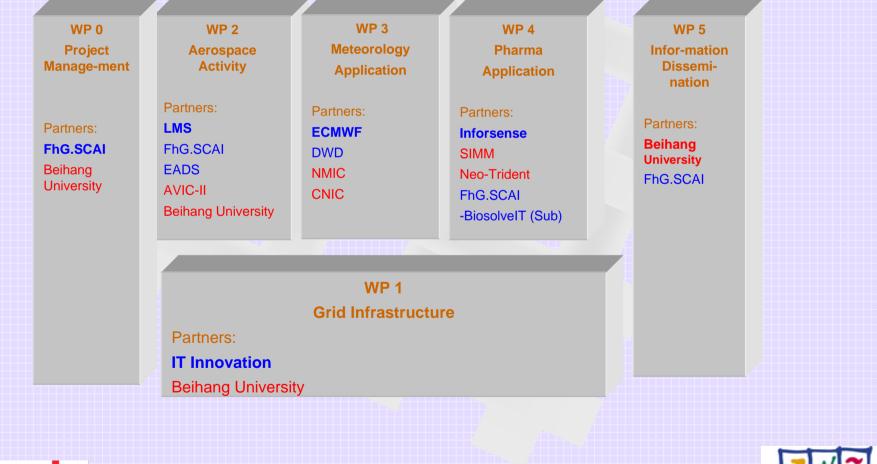
Pharma:

Algorithmic interoperability between different protein docking tools

Extended interoperability of Grid infrastructures



Work Packages: Approach & Structure

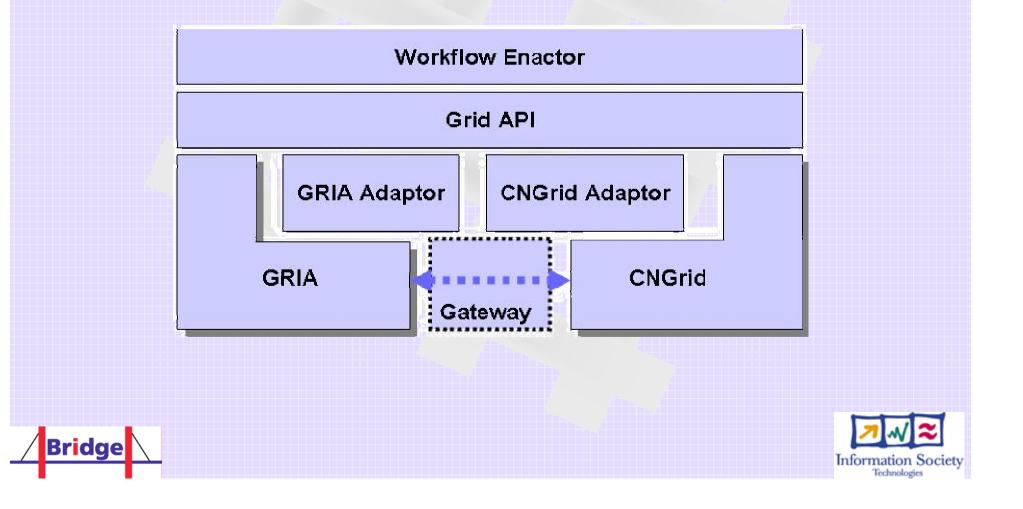


Bridge



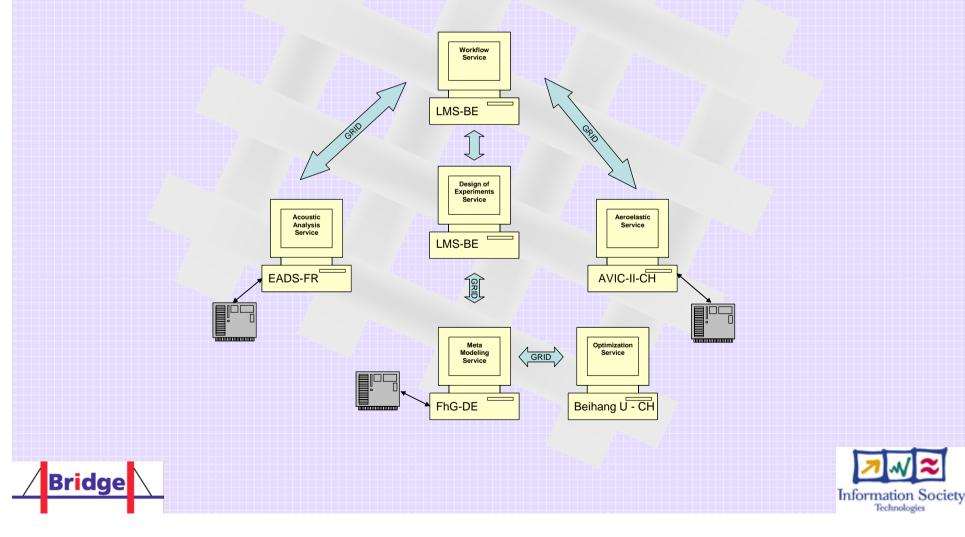
WP1: GRID Infrastructure

Key areas of interoperability



WP2: Aerospace Activity

Workflow, optimization, GRID



WP3: Meteo Activity

THORPEX Interactive Grand Global Ensemble (TIGGE):

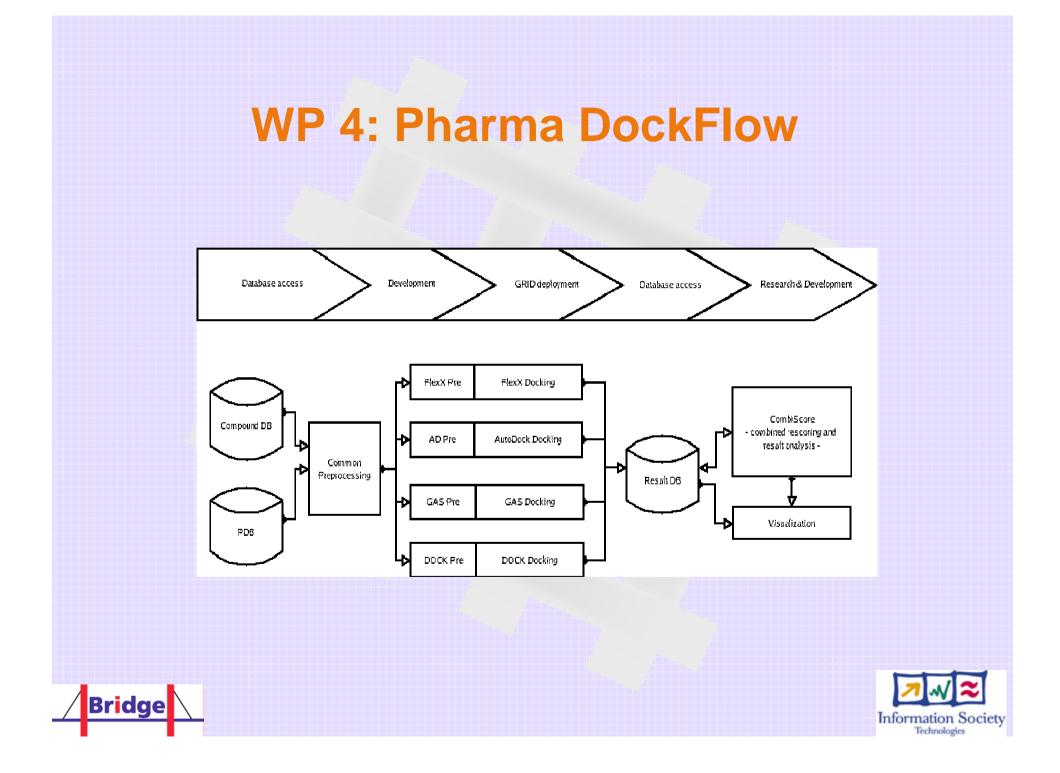
- WMO programme THORPEX will provide appropriate risk management tools for decision makers of all nations.
- First phase: building the TIGGE for daily output of global Ensemble Prediction System from around the world (~200GB per day)
- ECMWF and CMA will each host a copy of the database

Meteo activity in BRIDGE:

- Provide GRID enabled access to the TIGGE database, focussing on resource usage optimisation
- Provide multi-language cataloguing and data discovery
- Analysis Services: Risk Assessment Modules on regional disasters and planning







WP4: Pharma Activity - Dockflow

Grid-based Virtual Screening and Molecular Docking Application:

"Proof of concept" scientific experiment for identifying novel potential lead candidate drugs against Bird flu / Dengue fever / Malaria.

An integrated Virtual Screening Platform:

- Develop an integrated solution based on existing docking tools available to both the European and Chinese partners within a single platform.
- Development of an algorithmic approach towards interoperability of docking results is a real challenge and will be one of the main contributions of this task.
- Continued development of CombiScore to provide a unified score and visualization method to facilitate lead identification

Workflow Execution Models for Virtual Screening:

- Developing interoperability methods between Chinese and EU workflow tools
- Enable interactivity within workflow execution
- Production of reusable, validated "canned" virtual screening workflows authored by domain experts that can then be published for execution by a wider audience.





Bridge Partners

Project overall co-ordination response surface models, docking

LMS

FhG/SCAI

Integration and development of OPTIMUS software for the aerospace application

IT Innovation

Infrastructure, distributed data access, semantics, security and workflow

ECMWF

Co-ordination of meteorology application and database development

DWD

Implementation of a multi language thesaurus for the meteorology application





Bridge Partners

EADS	Aerospace activity, aero acoustics service
InforSense	Extension of grid-based workflow for protein docking applications and wf interoperability
CNIC, CAS1	Scientific data Grid, middleware for distributive data integration, risk analysis
Beihang University	Co-ordination of Chinese project part, Grid infrastructure and optimization services
AVICII	Aerospace activity, aeroelasticity service, provider of the aerospace model
Bridge	



Bridge Partners

NMIC

Meteorological activities, distributed data retrieval and sharing

IMM, CAS Pharmaceutical activities, wf processes for new drug discovery, docking service

NeoPharmaceutical activities, verification ofTridentresults and system integration





Research Challenges

To achieve interoperability between GRIA and CNGrid GOS

To implement <u>complex</u> and interactive workflows from different domains using European and Chinese resources, and interoperability between individual workflow representations

To achieve functionality of Grid services based on heterogeneous infrastructures, through the three application domains





Key technology advancements

Mechanism which achieves mapping between heterogeneous platforms

Cross-platform: Dynamic policy management Data processing and storage Monitoring and management Workflow management Quality of Service control





Key technology advancements

CNGrid<->GRIA Interoperability





Interconnection of CNGrid and European Grid Infrastructure

> Depei Qian Beihang University Feb. 20, 2006







What we need to do for interconnection

- Supporting Grid software interoperability study, deploy different software in the environment
- Deploying current applications and developing an deploying new applications on extended infrastructure
- Supporting harmonized security mechanism
- Supporting testing and training









