
Bridge: Bilateral Research and Industrial Development Enhancing and Integrating GRID Enabled Technologies

Gilbert Kalb

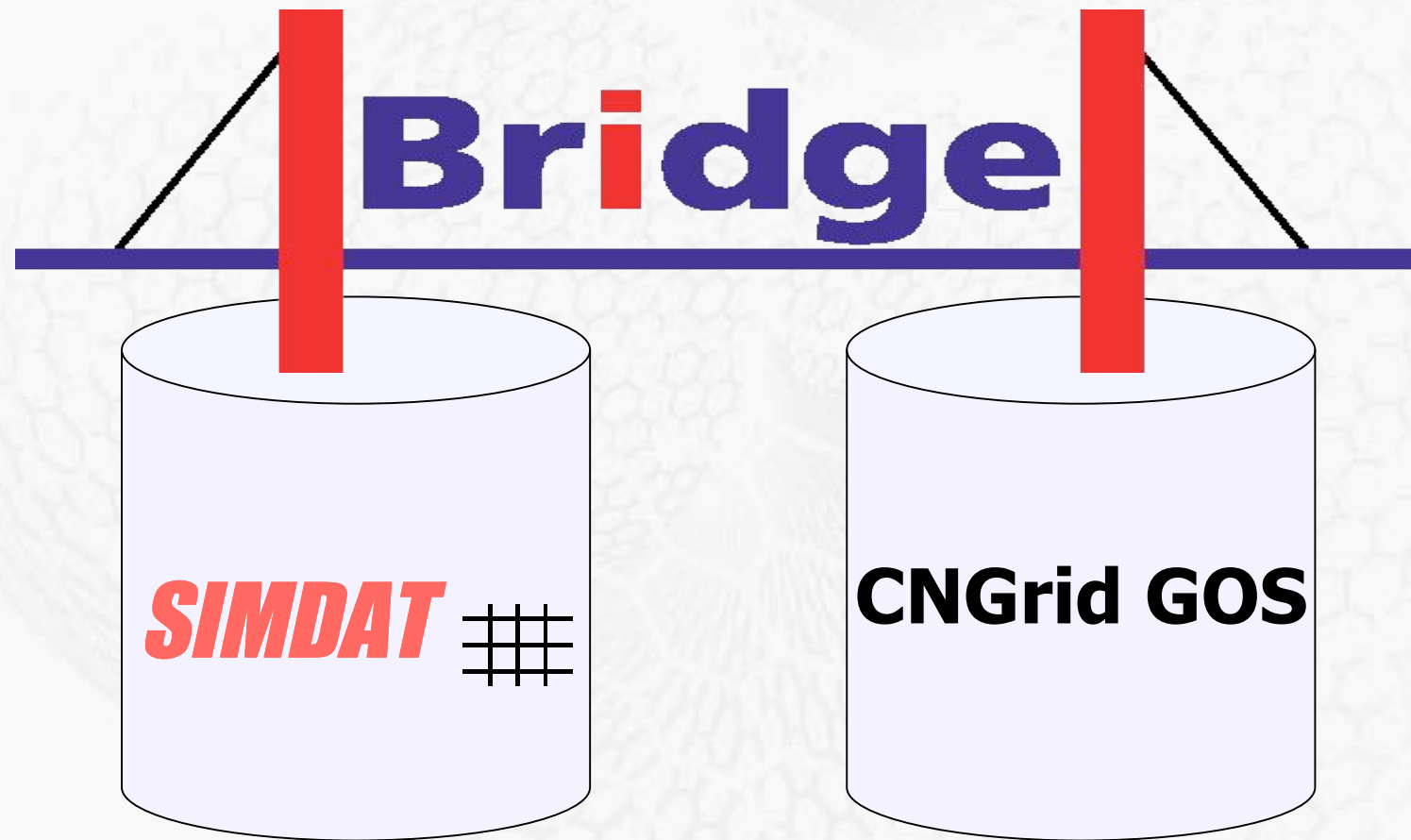
**EchoGRID Second Strategic Workshop
29-31 October 2007**



Joint meeting between EchoGrid, Bridge, GridComp and ETSI –



Bridge Foundations



Project Overview

- Runs from January 2007 to December 2008
- Supported by funding from EU 6th Framework Program (Information Society Technologies Project no. IST 045609)
- Consists of both European and Chinese partners:

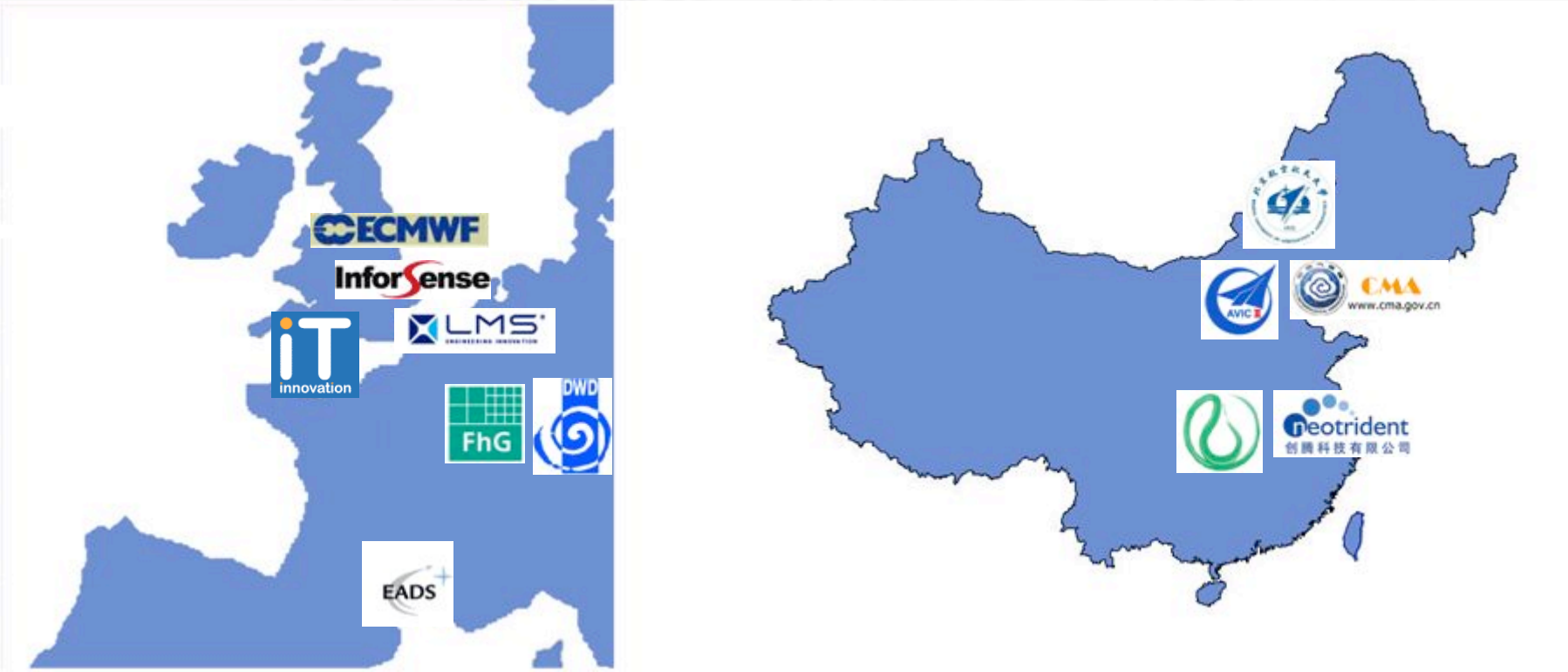
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Project Partners



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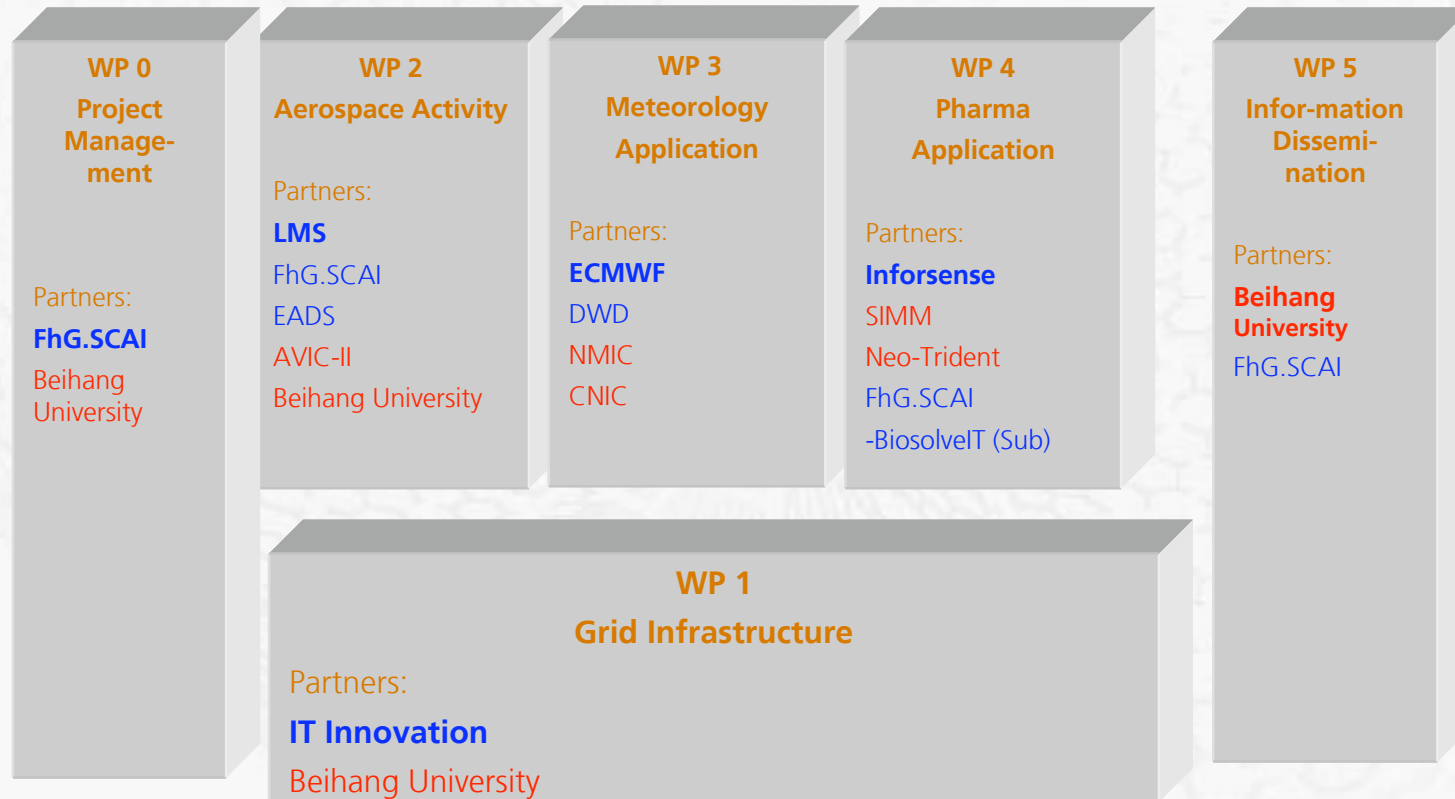


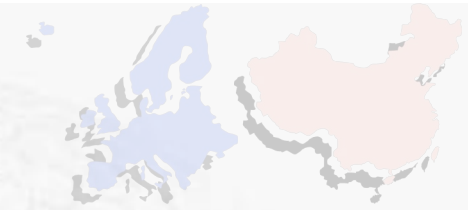
BRIDGE Objectives

1. To demonstrate the benefits of GRID technology for international cooperation
2. To develop, enhance and interconnect European and Chinese GRID middleware technology
3. To provide a software platform supporting distributed product and process developments, which respects and protects intellectual property rights
4. To set up integrated GRID test bed using European and Chinese middleware components for application demonstration
5. To set up joint application show cases using distributed workflow and data access technology
6. To disseminate the results of the project to industrial and academic communities



Work Packages: Approach & Structure





Meteo:

Seamless access to heterogeneous distributed data repositories

Aero:

Multi-disciplinary collaborative configuration design

Pharma:

Algorithmic interoperability between different protein docking tools

Extended interoperability of Grid infrastructures

Interoperability Requirements

Exchange of Information on the two infrastructure platforms, GRIA and CNGrid-GOS

Interoperability requirements

- Effective data management and large scale data transfer
- Automatic notification mechanism of long-lived job execution when job state changes
- Workflow support for cross-domain grid service interoperability
- Cross-domain security service
- Monitoring across different middleware
- Software licensing mechanisms



Application Interoperability Challenges

- Application partners have identified the following common interoperability challenges in BRIDGE:
 - Large-scale, transparent data transfer
 - Long-lived distributed data processing
 - Federated security in distributed workflows

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Achievements to Date

- Interoperability requirements capture from application partners
- Joint interoperability architecture designed by Chinese and European partners
- Successful progress meeting in early September 2007

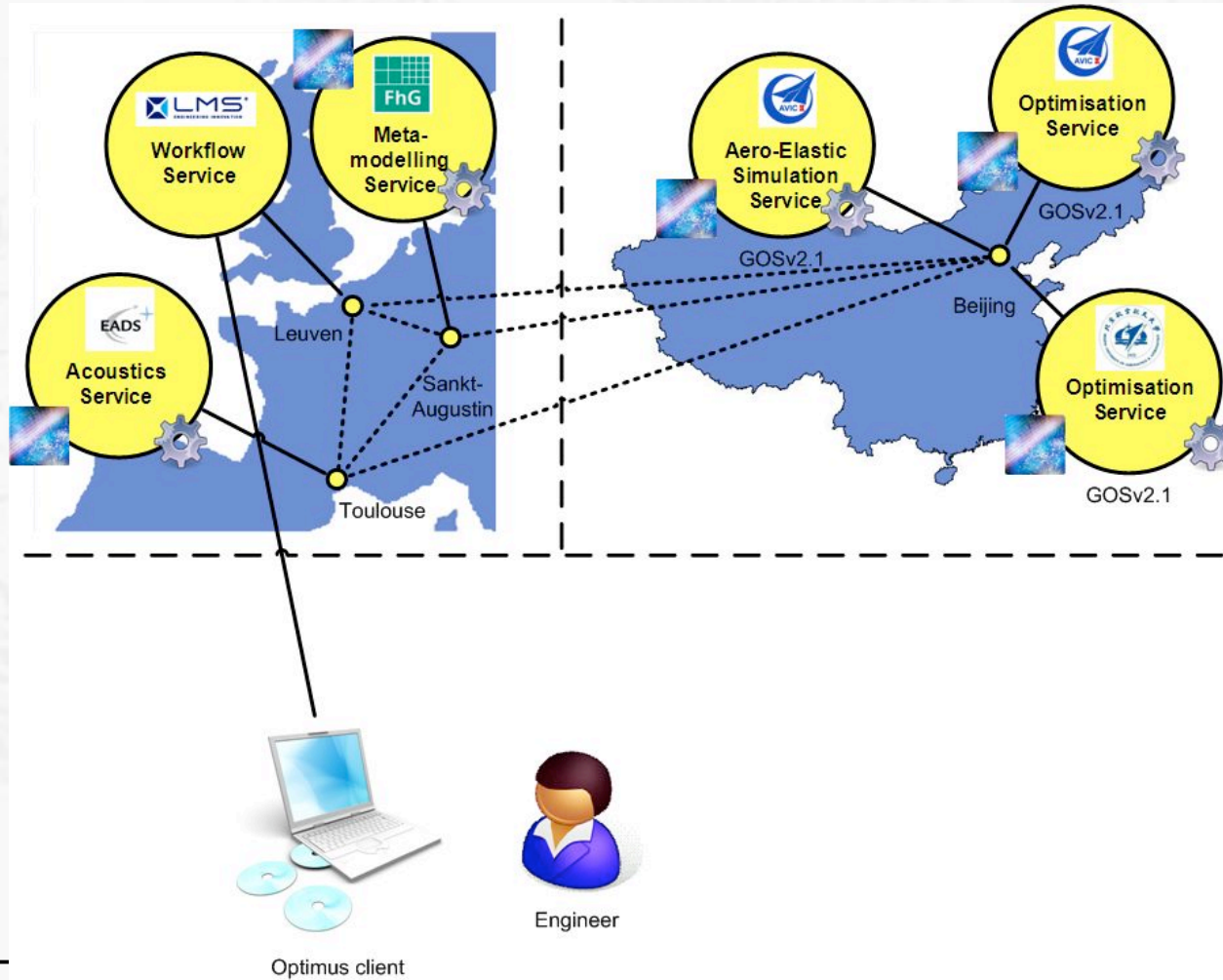
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Aerospace Workpackage Objectives

- Research, develop and implement a complete aerospace scenario that addresses an industrial application
- Capture and federate through Workflows the application scenario
- Utilize an integrated GRID test bed that is using European and Chinese provided Simulation Services for distributed computation and optimization of simulation based workflows
- Disseminate the results throughout the industry and academia
- Formulate and uptake as fit an exploitation plan for the commercial exploitation of the project results

Aerospace Scenario



BRIDGE Meteo scenario



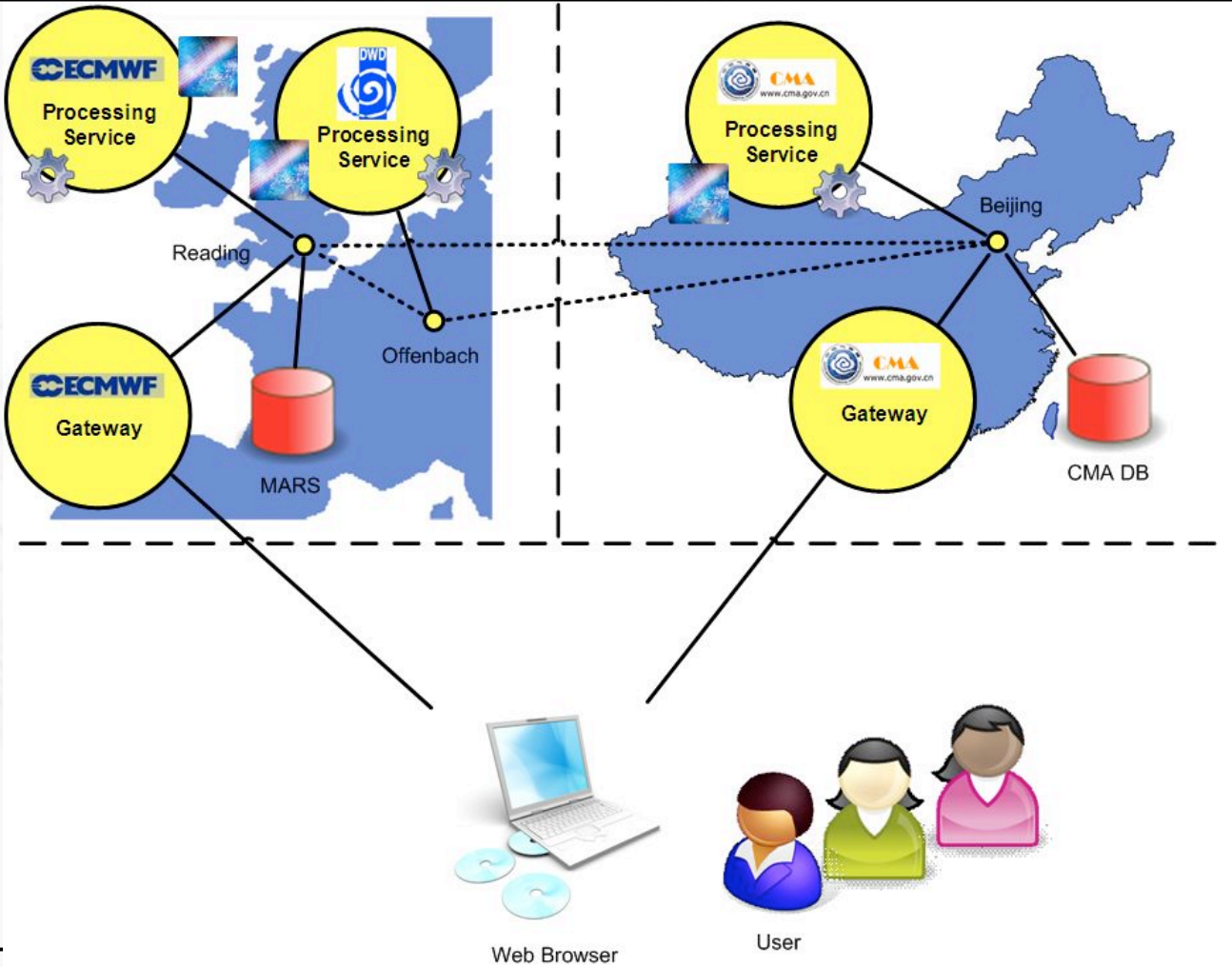
- Providing access to the TIGGE data
 - Creation of probabilistic weather forecasts products in a distributed fashion
 - Distributed processing on distributed data, across the two GRID middleware
 - Each site hosts only part of the data
 - Each site offers basic operations on the data (e.g. computing an average)
- Strategy: minimize data transfers (volumes involved are huge)
 - Run operations at data location when possible
 - Decompose operations in simpler ones
 - Most of the time intermediate results are much smaller



Background: TIGGE

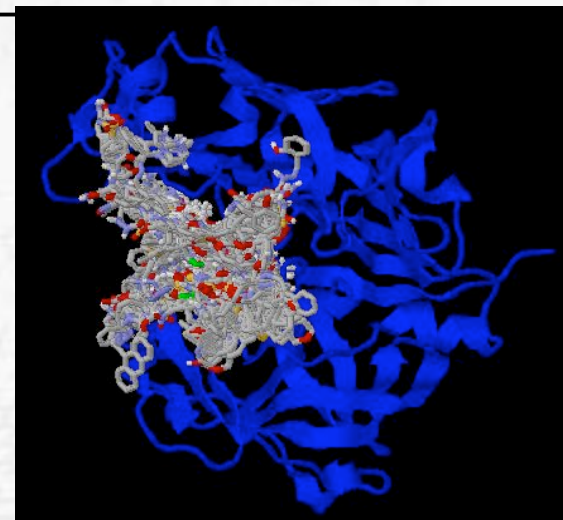
- Create a grand ensemble with forecasts from centres from around the world
 - 100s of forecast runs
- Outputs collected in near real time
- Archive data at **ECMWF** (Europe), **CMA** (China) and **NCAR** (USA)
- Provide access to the research community

Meteorology Scenario

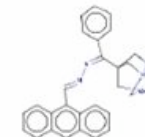
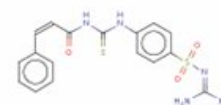
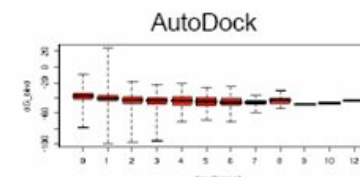
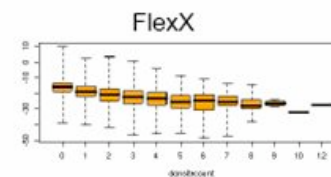


DockFlow Application Background and Challenges

- Positioning of small molecules (potential drugs) into the binding site of a target protein (associated with a specific disease)
- Various protein docking tools exist (FlexX, Dock, AutoDock, GasDock, ..) based on different principals
- Results vary based on tool/algorithm used
- How can all algorithms be compared and combined in a qualitative manner?



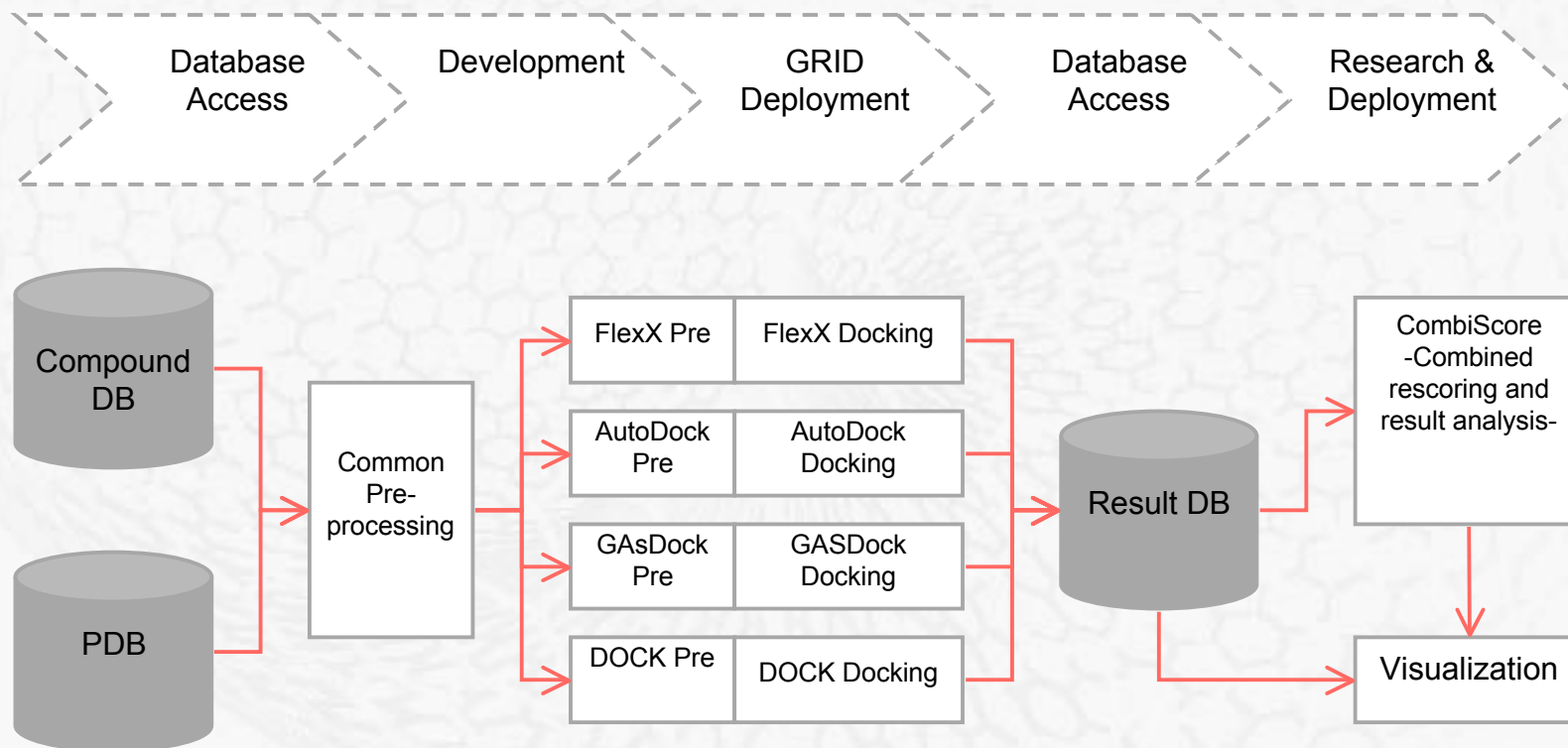
- Ligand descriptors:
 - Distinct differences in number of donors, number of rings and size of polar surface area



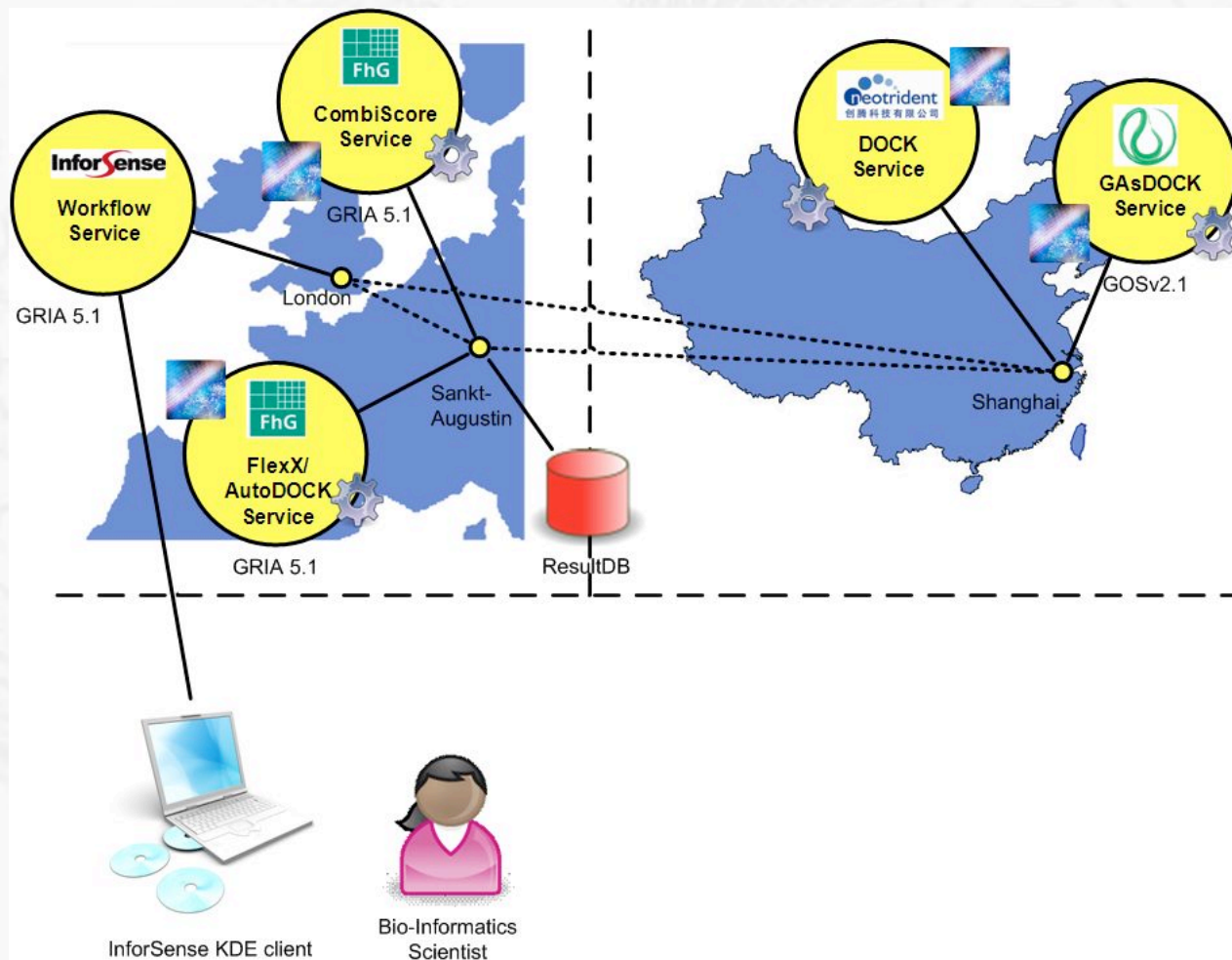
Directed and undirected hydrophobic interactions

Fraunhofer Institute Algorithms and Scientific Computing

Dockflow Overview: Grid-enabled Protein Docking



Pharmaceutical Scenario



Summary

Achievements to Date

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- Successful progress meeting in early September 2007

Ongoing Work

- First prototype (Nov 2007)
- Meeting in Beijing (Oct. 29th – Nov. 1st 2007)

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thank you

