

Applications Interoperability: some case studies within EU-IndiaGrid project

Stefano Cozzini

CNR/INFN National Simulation Center
DEMOCRITOS

EU-IndiaGrid Technical Director

www.euindiagrid.eu



Scope of this talk

- Discuss the need of the applications' need toward interoperability
- Discuss / present some case studies
- Identify propose solutions (in place / to come)

Interoperability at Application level

- Why the same computational experiments across multiple grids ?
 - Users need to grab as many as possible resources (no matter the kind)
 - size of the experiments
 - Users need different kind of resources
 - Types of experiment
 - Some VO can spawn different grids
 - Type/Size of the User-Community

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What do we need as users ?

- Same grid services in different environments =>
 - Transparency should be provided for both low level and high level services
- Correct/detailed information about the differences among grids =>
 - To perform right choices for the computational experiments.

Selected case studies in EU-indiaGrid

- Size of the experiment:
 - BEMUSE tool for biosimulations
- Kind of the experiment:
 - Quantum Simulations in material science
- High level services to provide:
 - Finance (new area within the project)

Ex # 1: BEMUSE

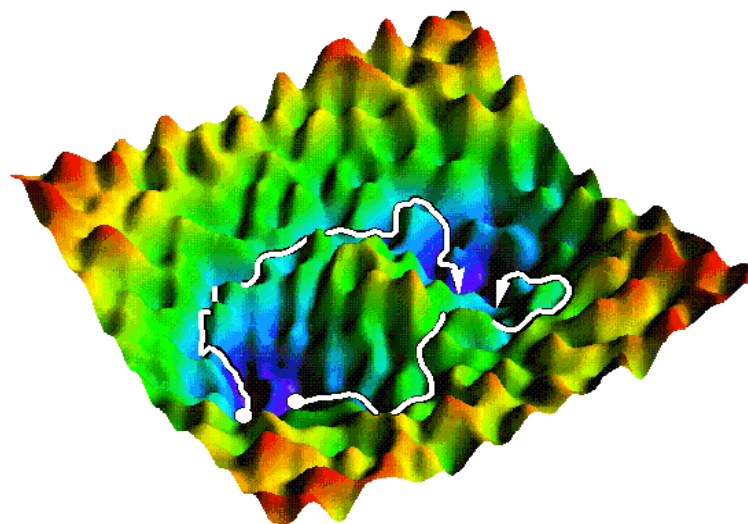
- Biased Exchange Metadynamics Submission Environment
- developed by EU-IndiaGrid Team at ICTP in strict collaboration with SISSA / Democritos people
- It allows to easily manage complex BES computational experiments on EU-Indiagrid infrastructure

BES in a nutshell

- An enhanced sampling technique capable of predicting **rare events** in biological systems with an unforeseen accuracy.

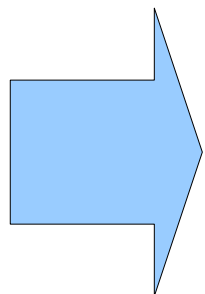
[S. Piana and A. Laio, J. Phys Chem B 111 4553 (2007)]

**SCIENTIFIC PROBLEM:
PROTEIN FOLDING OF
SMALL PROTEIN**



BES & the GRID

- BES algorithm:
 - loosely coupled
 - CPU intensive
 - not I/O bounded



FITS PERFECTLY the
GRID COMPUTING
ENVIRONMENT ala
EGEE/gLITE

FULLY DEVELOPED AND IMPLEMENTED
WITHIN EU-INDIAGRID INFRASTRUCTURE

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Do we need interoperability ?

- Experiments on large proteins can involve hundreds of CPUs
- Based on client/server architecture: simulation can run in an asynchronous way.
- CPU can be recruited **anytime** and **everywhere**

Work on interoperability within BEMUSE

- Bemuse already allows to recruit computational resource among different computational environments
 - EU-IndiaGrid
 - Desktop PC's and local batch-systems
- On-going Collaboration with CDAC Bangalore (dr. Janaki) to allow Recruiting CPU's on GARUDA Grid
- Future development: Replace job submission procedure within BEMUSE with a standard OGSA-BES approach

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Ex 2: Quantum Simulations

- Case study discussed among EU-Indiagrid project and OMII-Europe project
- Several on-going discussions with the aim to run quantum simulation on three different grids: DEISA / EU-IndiaGrid / Garuda
- Reference: “Fact-Sheet EU-IndiaGrid Interoperability Scenario”

Quantum Simulations

- Quantum atomistic simulations that are very demanding in terms of CPU and memory requirements.
- Idea: Use the seamless access of the different Grid infrastructures GARUDA, EGEE and DEISA for **different kinds of scalable calculations** in terms of dimension of the simulations

Tools for Quantum Simulations

- Standard packages like Quantum / Espresso VASP and WIEN2K are widely use
- All the tools already ported on different Grid environments
- They are extremely demanding in RAM and they do have tightly coupled MPI parallel implementation
- Serial runs are therefore limited to small system (# of atoms / size of input parameter)

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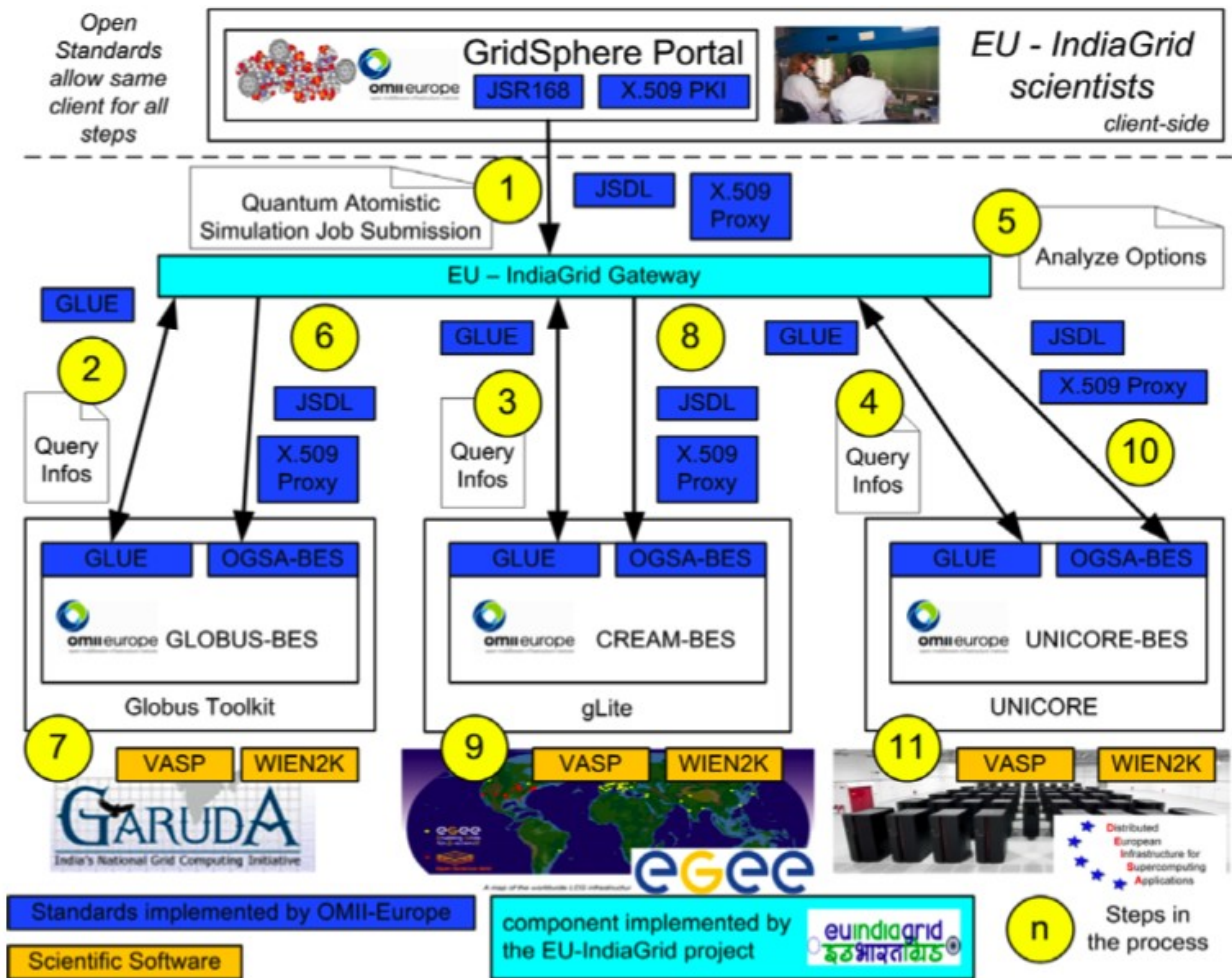
Possible Scenario

- Serial version of the packages are suitable to run in GARUDA and EGEE. But those serial versions are limited to study very small systems (e.g. in the order of few atoms).
- Small SMP versions (e.g. using 2-16 CPUs in parallel) are suitable to run in EGEE or DEISA and allow for simulation of larger systems (e.g. order of few tens of atoms)
- Large parallel versions to go beyond the previous mentioned sizes of systems for atomistic simulations are only suitable for DEISA HPC platforms (e.g. hundreds of atoms)

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The approach under discussion



Example # 3: Finance application

- Developed within EU-IndiaGrid jointly by ICTP and Business University of Athens (EUINDIA and SEEGRID Virtual Organization)
- Statistical analysis of 700 securities that include stocks, bonds, options, etc.
- For each security there is several years of data (order of 10 GB).
- Each security can be separately processed in a different node.
- Fits perfectly on the Grid

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Security requirements

- The data used by the researchers is bought from Stock Exchanges and/ or data providers.
- Such data comes with strict disclosure policies.
- The price charged for it depends on how well the researchers can prove that only them will be able to access it.
- The less well data can be confined, the higher the charge.

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EU-IndiaGrid solution

- High level service: based on an integration of:
- STORM Server:
 - first GRID service to allow physical ACLs to be set up on files in GRID storage, for members of the same VO
- Hydra server
 - CERN's key encryption server to crypt files on the Storage elements

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Interoperability issues

- The high level security service should be made available across different grids
- At the moment we are studying the issue among Garuda (SRB based) and EGEE (StoRM+Hydra)
- Open points:
 - Is SRB ACL enabled ?
 - Is encryption supported ?

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Conclusions

- Interoperability among grids is really needed by applications and scientists within EU-IndiaGrid.
- EU-IndiaGrid scientists are collaborating in defining their needs and they requirements.
- Interoperability among grids can only be successfully accomplished if users' need are taken into accounts.

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