

NAREGI

The Japanese National Research Grid Project

Kazushige Saga

National Institute of Informatics

Project Overview

Name: **National Research Grid Initiative (NAREGI)**

- A Japanese National Grid R&D project, funded by MEXT
~**\$(US)17M** FY'03 (similar until FY'07) (**\$125million** total planned)
- One of two major Japanese Govt. Grid Projects
- Collaboration of **National Labs. Universities** and **Major Computing and Nano-technology Industries**
- 17 Teraflops Dedicated Testbed (FY2003)
Aiming for 100TF Grid and beyond (FY2007)

MEXT: Ministry of Education, Culture, Sports, Science and Technology

Project Goals

1. To **develop a Grid Software** System (R&D in Grid Middleware and Upper Layer) as the prototype of future Grid Infrastructure in **scientific research** in Japan
2. To **provide a Testbed** to prove that the High-end Grid Computing Environment (100+Tflop/s expected by 2007) can be practically utilized in the [Nano-science Simulations](#) over the Super SINET.
3. To Participate in **International Collaboration** (U.S., Europe, Asian Pacific)
4. To Contribute to **Standardization** Activities, e.g., GGF

Participating Organizations

- National Institute of Informatics (NII)
(Center for Grid Research & Development)
- Institute for Molecular Science (IMS)
(Computational Nano science Center)
- Universities and National Laboratories (Joint R&D)
(AIST, Titech, Osaka-u, Kyushu-u, Kyushu Inst. Tech.,
Utsunomiya-u, etc.)
- Research Collaboration
(ITBL Project, National Supercomputing Centers etc.)
- Participating Vendors (IT and Chemicals/Materials)
- Consortium for Promotion of Grid Applications in industry

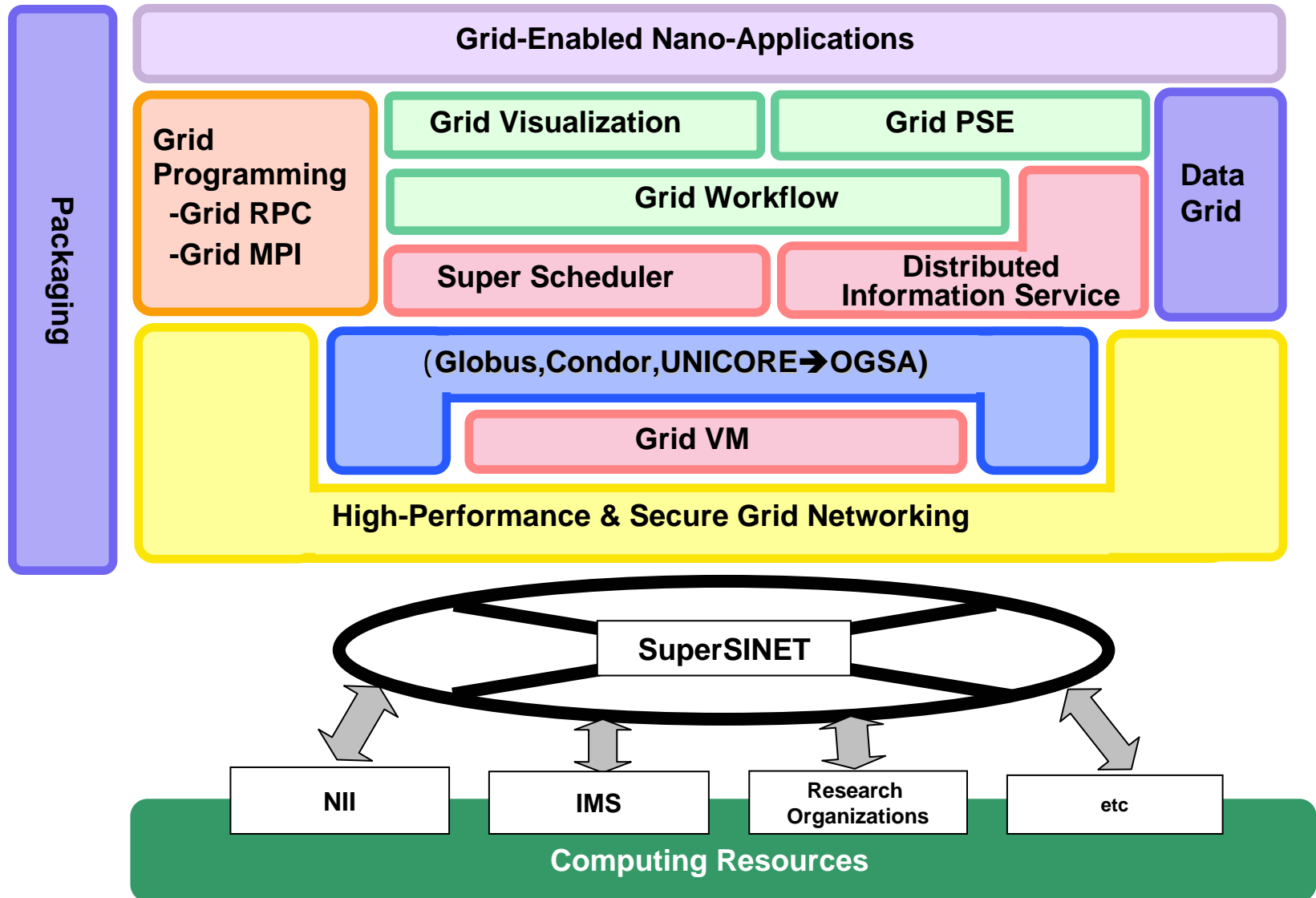
Target Applications

Focus on Nano Science and Technology Applications

- Functional nano-molecules (CNT, Fullerene etc.)
- Nano-molecule Assembly (Bio-molecules etc.)
- Magnetic Properties
- Electronic Structure
- Molecular System Design
- Nano-simulation Software Integration System

and more ...

NAREGI Software Stack



Requirement schemas, Requirement/Use case DB

- Requirements schemas, representations
 - NAREGI doesn't have any requirement schemas. However, we think, requirement schemas are useful to share requirements between grid projects.
- Requirements databases
 - Currently, NAREGI doesn't have any permanent databases for requirements. We are managing our requirements in documents. However, we think that when the NAREGI moves into software deployment phase (soon), public requirement DB, such as EGEE's requirement DB, is necessary to understand what users want.
 - Public requirement databases will help to make multiple grids project interoperable.
- Use case repositories
 - Use cases are very important items in standardization. However each WG is using its own use cases. It may make miss match between specifications which were standardized in each WG.

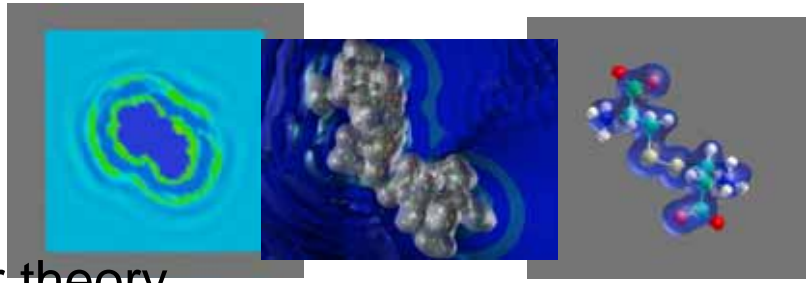
We think, if GGF develops above schemas and DBs, they will accelerate and improve standardization.

Nano-Science: coupled simulations on the Grid as the sole future for true scalability

... between Continuum & Quanta.

Material physics
(Infinite system)

- Fluid dynamics
- Statistical physics
- Condensed matter theory



Molecular Science

- Quantum chemistry
- Molecular Orbital method
- Molecular Dynamics



Limit of Idealization

Multi-Physics

Limit of Computing Capability

Old HPC environment:

- decoupled resources,
- limited users,
- special software, ...

Coordinates decoupled resources;
Meta-computing,
High throughput computing,
Multi-Physics simulation
w/ components and data from different groups
within VO composed in real-time

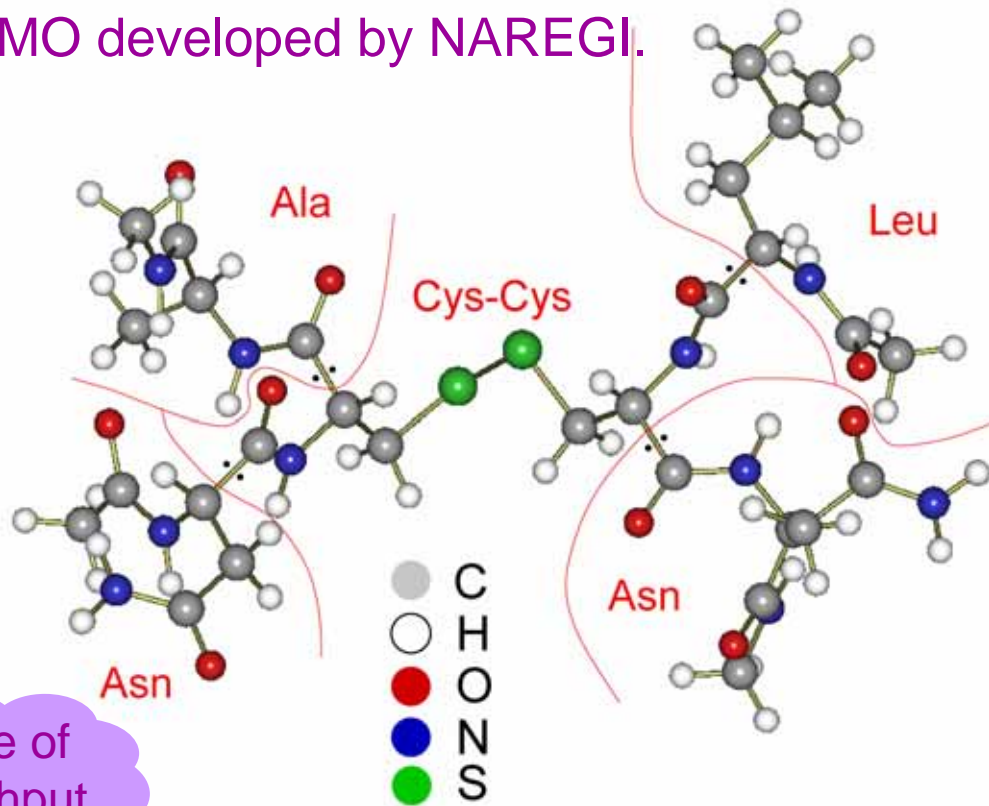
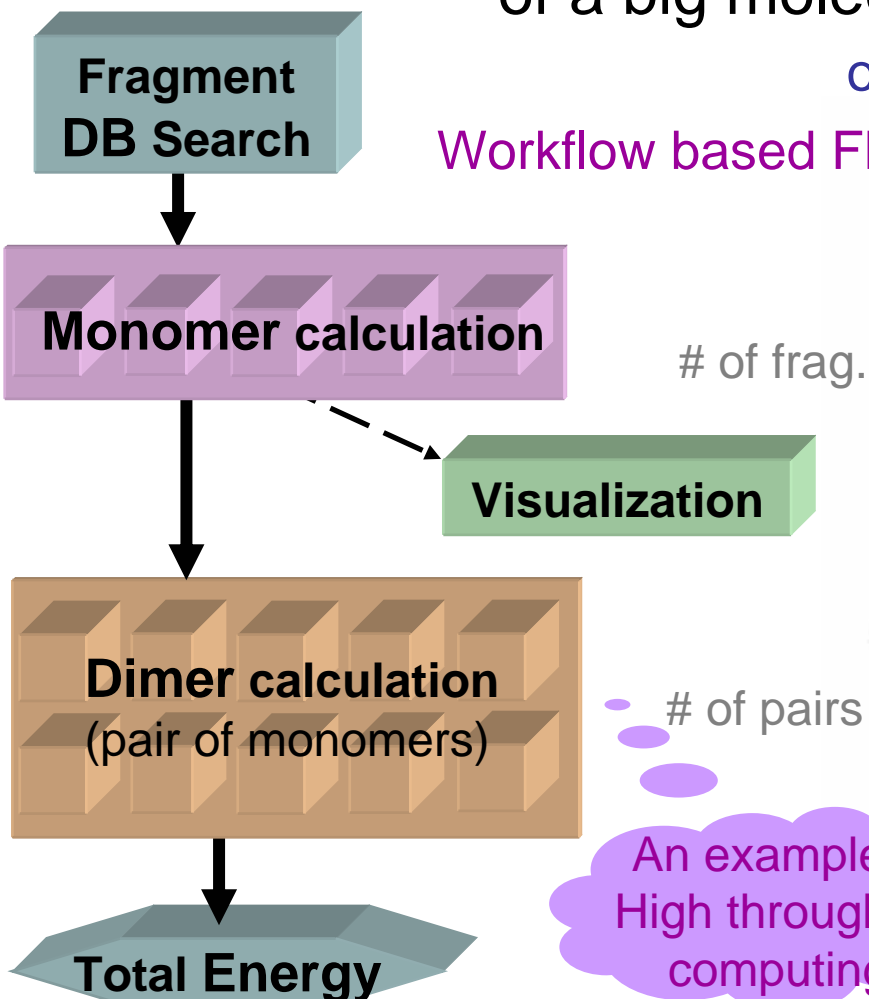


The only way to achieve true scalability!

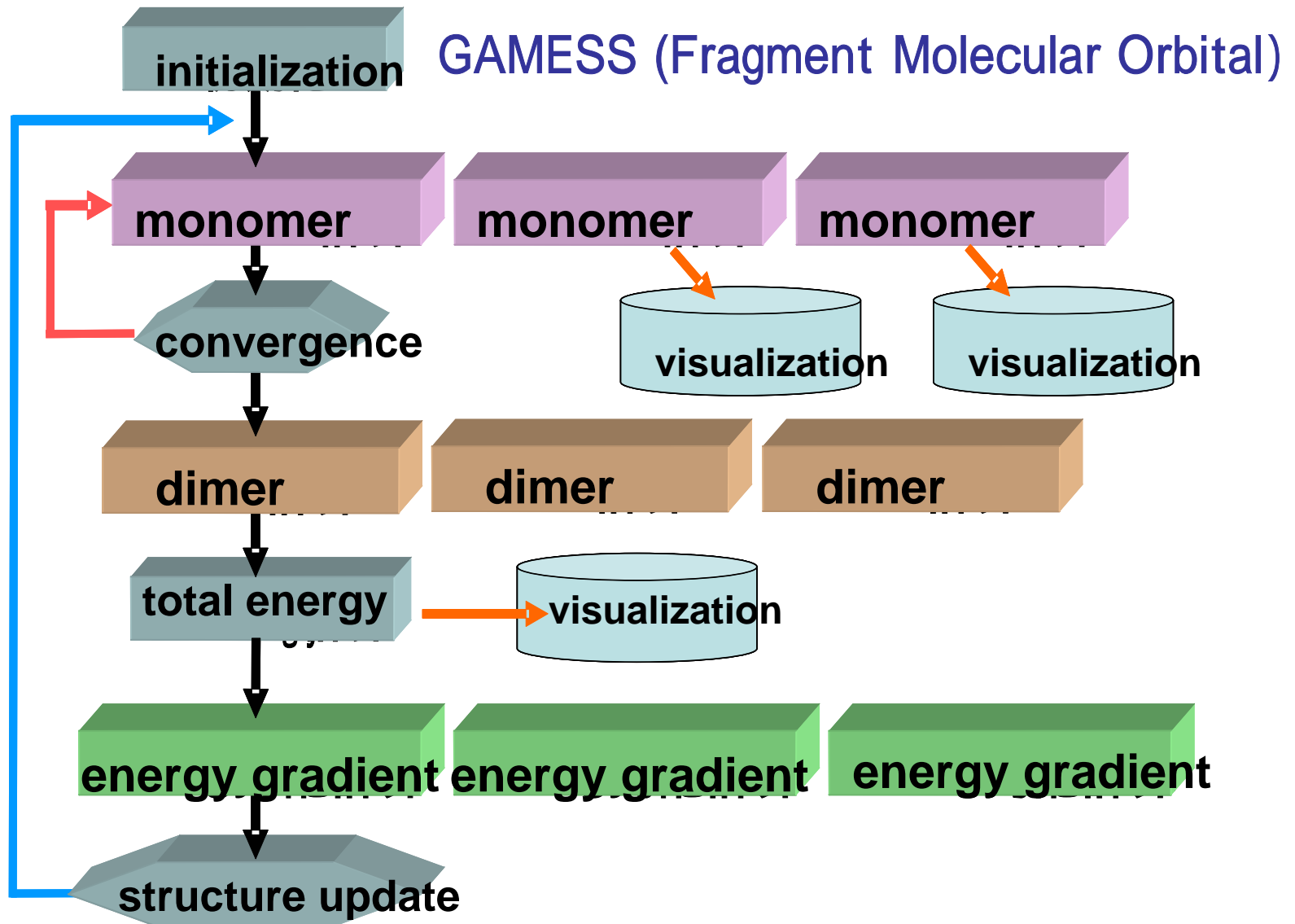
Use Case 1: Large and High Throughput MPI Job – **Grid Enabled FMO**

Grid enabled FMO (Fragment Molecular Orbital method)
 : a method of calculating electron density and energy of a big molecule, divided to small fragments, originally developed by Dr. Kitaura, AIST.

Workflow based FMO developed by NAREGI.

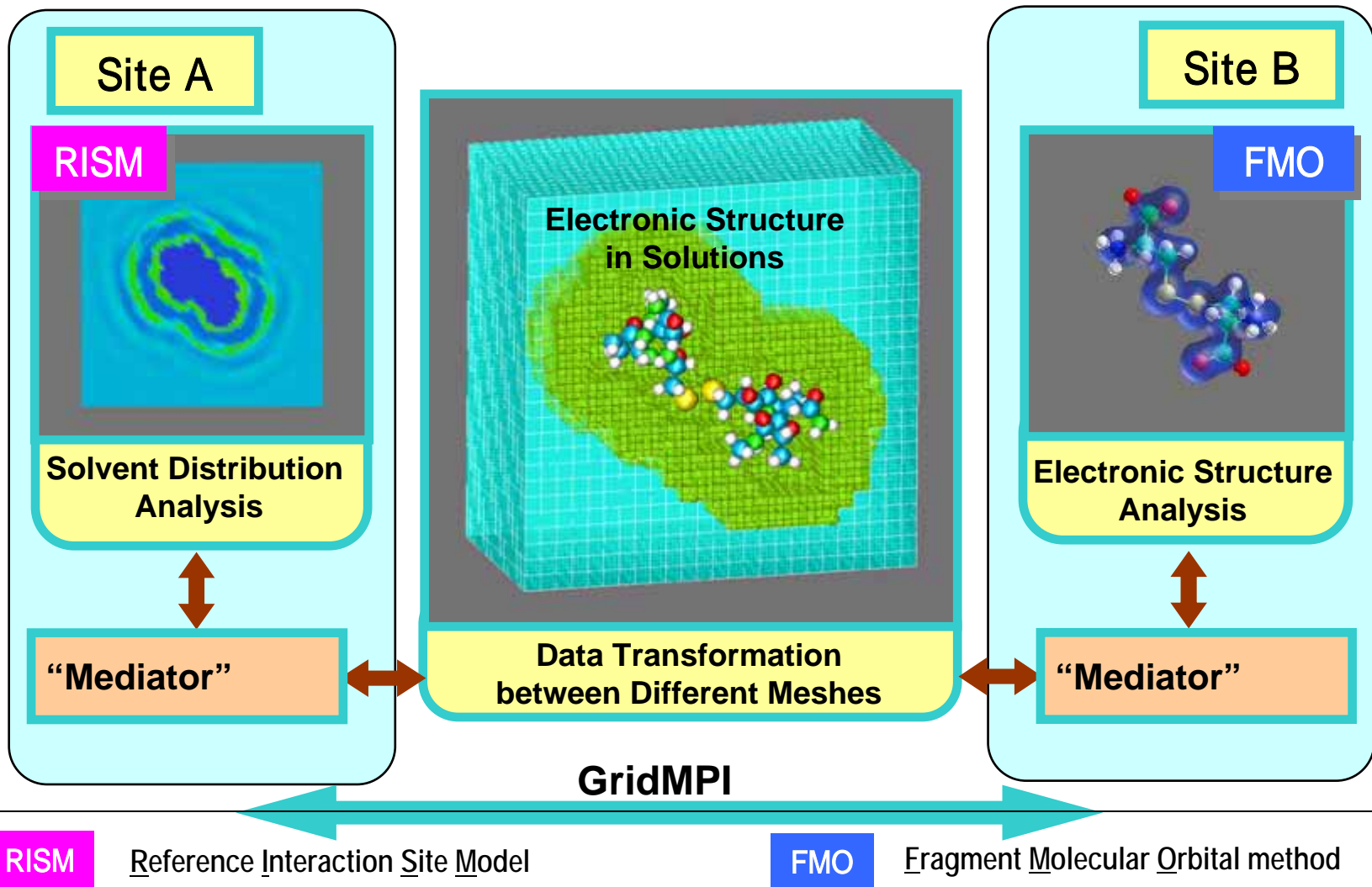


Workflow of FMO

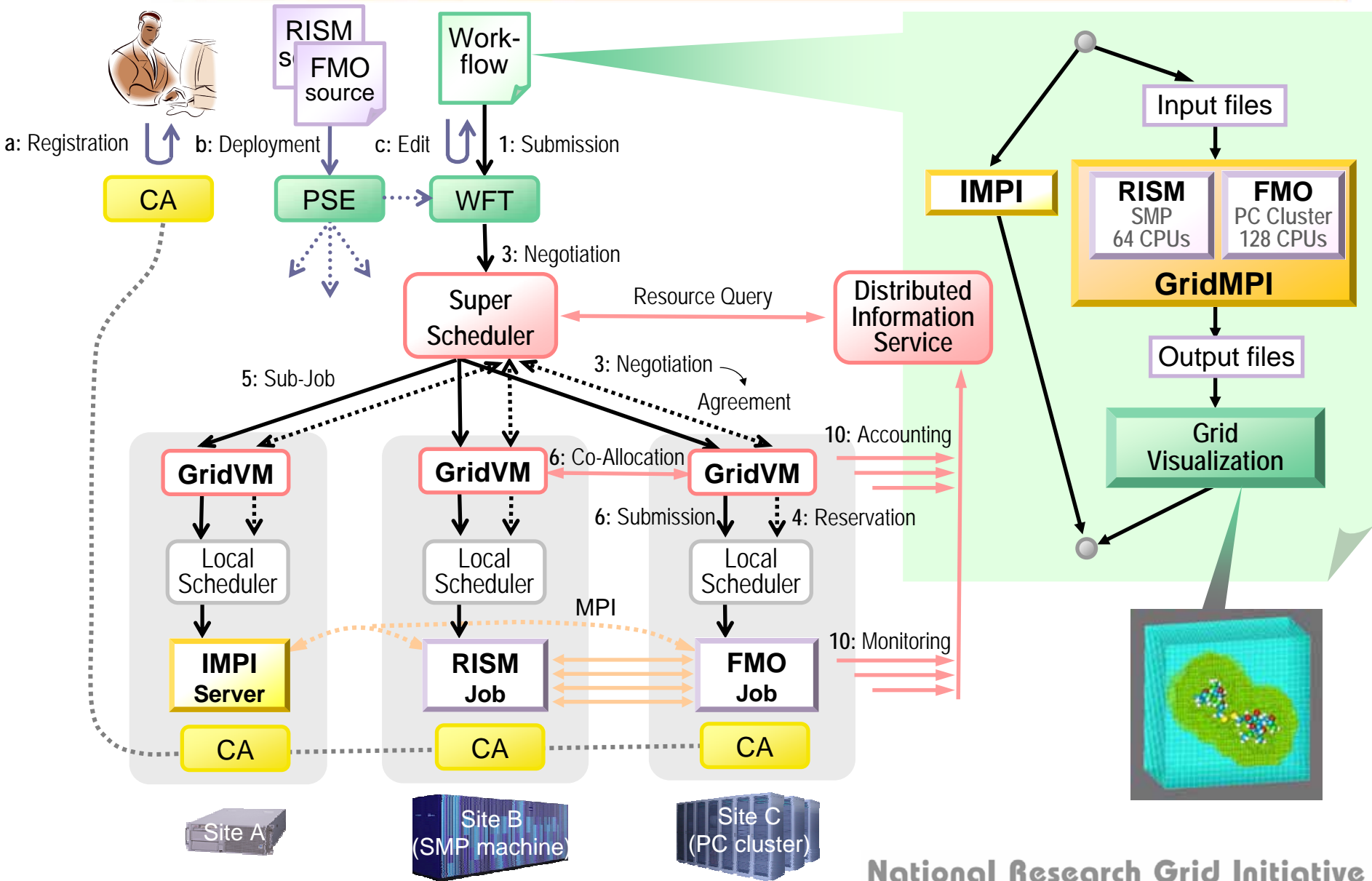


Use Case 2: Complex MPI Job

RISM-FMO coupled simulation

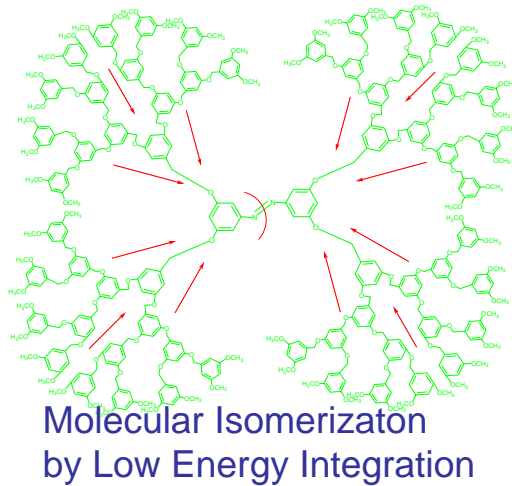


Scenario for Multi-sites MPI Job Execution

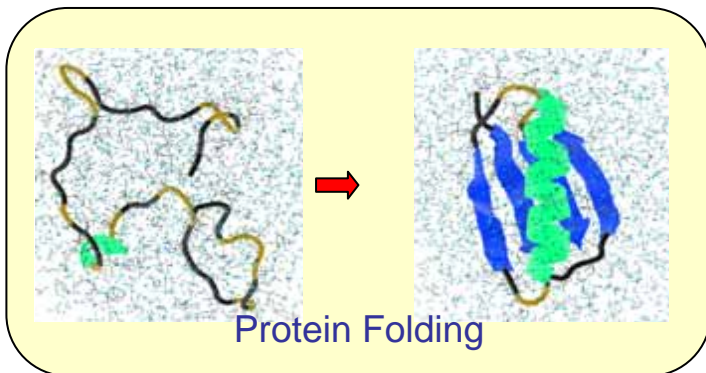


Examples of Nano-Applications Research (1)

Functional Nano-Molecules



Nano-Molecular Assembly



Nano-Electronic System

Manganese-Oxide
Ferromagnetic
Half-metal

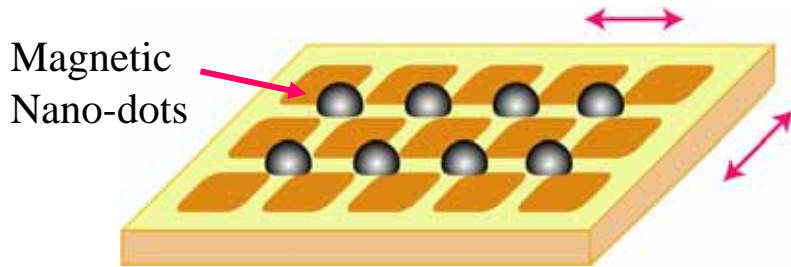
Orbiton
(Orbital Wave)

Apps: Half-metal Magnetic
Tunneling Device

Memory Device

Examples of Nano-Applications Research (2)

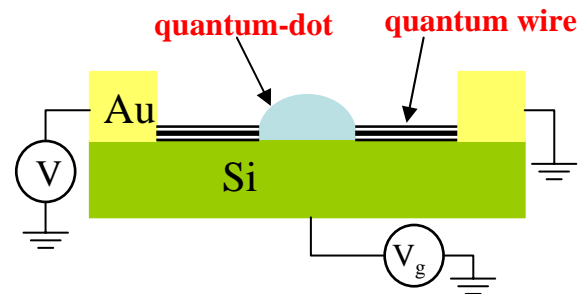
Nano-Magnetism



Magnetic Nano-dots

Controlling Arrangement of Nano-dots by Self Organization

Nano-system Design



(Metal,organic Molecules)

Nano-device, Quantum Transport

Thank you