NAREGI

The Japanese National Research Grid Project

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Project Overview

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

- ➤ A Japanese National <u>Grid R&D project</u>, 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)

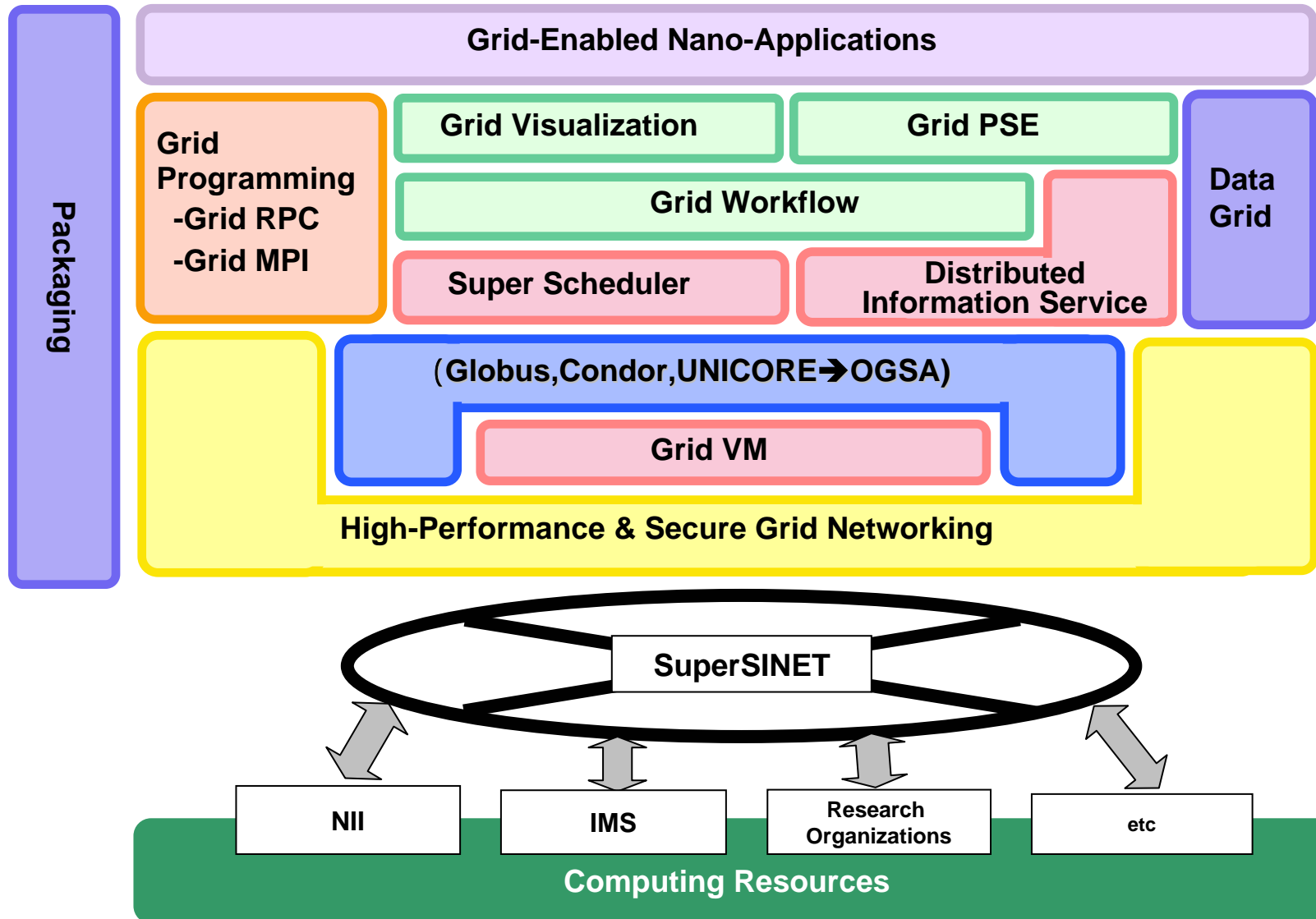➢ Consortium for Promotion of Grid Applications in industry

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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

Grid-Enabled Nano-Applications

Grid Programming
-Grid RPC
-Grid MPI

Grid Visualization

Grid PSE

Grid Workflow

Super Scheduler

Distributed Information Service

Data Grid

Packaging

Globus,Condor,UNICORE➔OGSA)

Grid VM

High-Performance & Secure Grid Networking

SuperSINET

NII

IMS

Research Organizations

etc

Computing Resources

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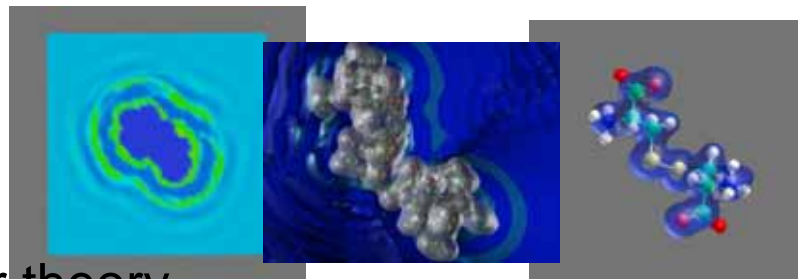
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Nano-Science: coupled simulations on the Grid as the sole future for true scalability

… between Continuum & Quanta.

Material physics
  (Infinite system)
Fluid dynamics
Statistical physics
Condensed matter theory
…

Molecular Science
  Quantum chemistry
  Molecular Orbital method
  Molecular Dynamics
…

10^{-6} 10^{-9} m

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
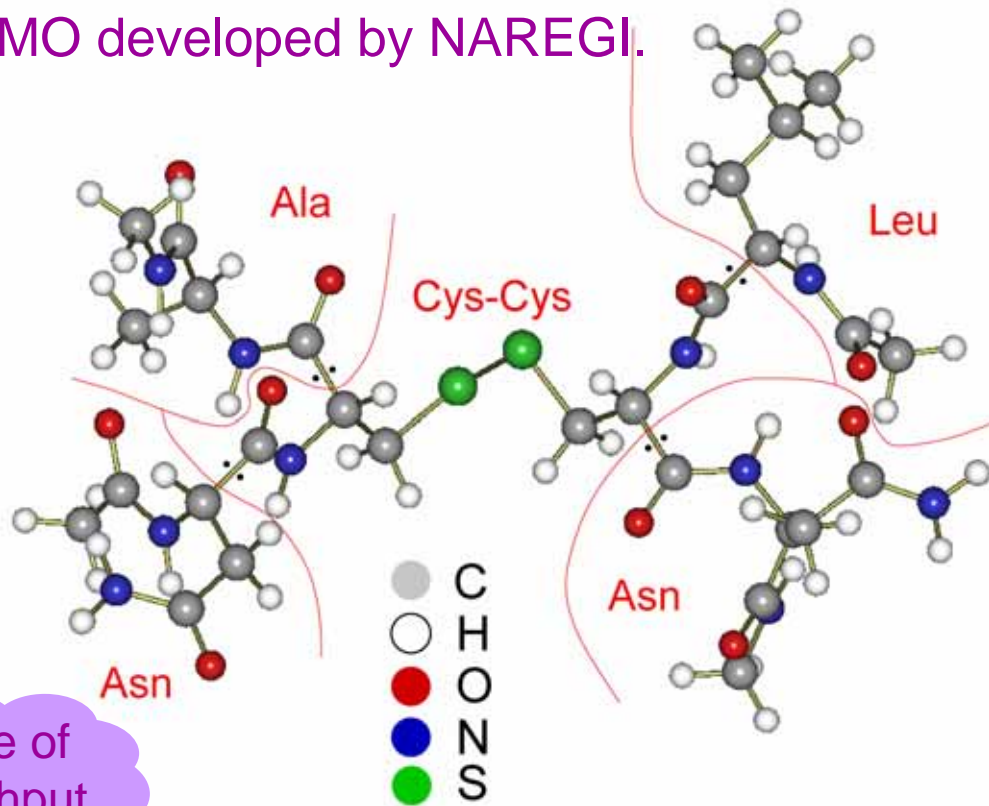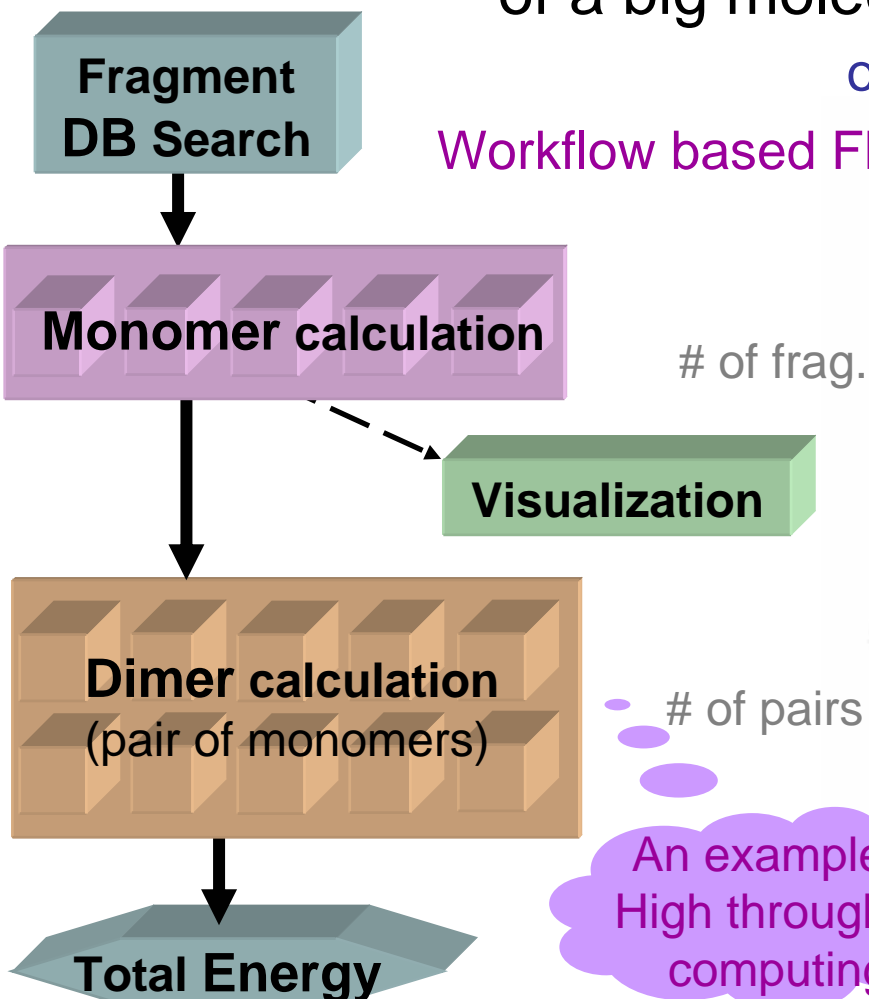w/ components and data from different groups
within VO composed in real-time

The only way to achieve true scalability!

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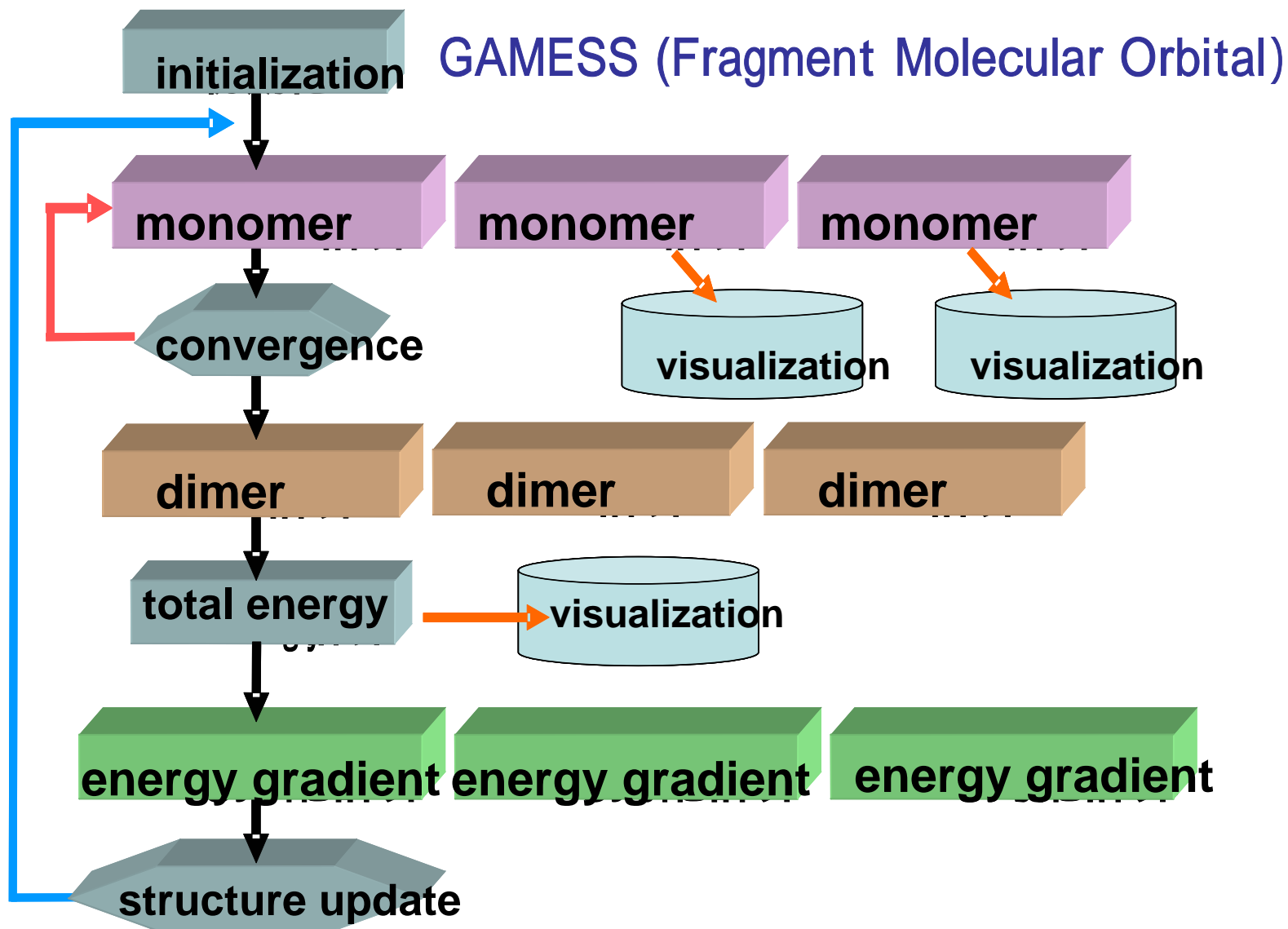# Use Case 1: Large and High Throughput MPI Job – Grid Enabled FMO

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.
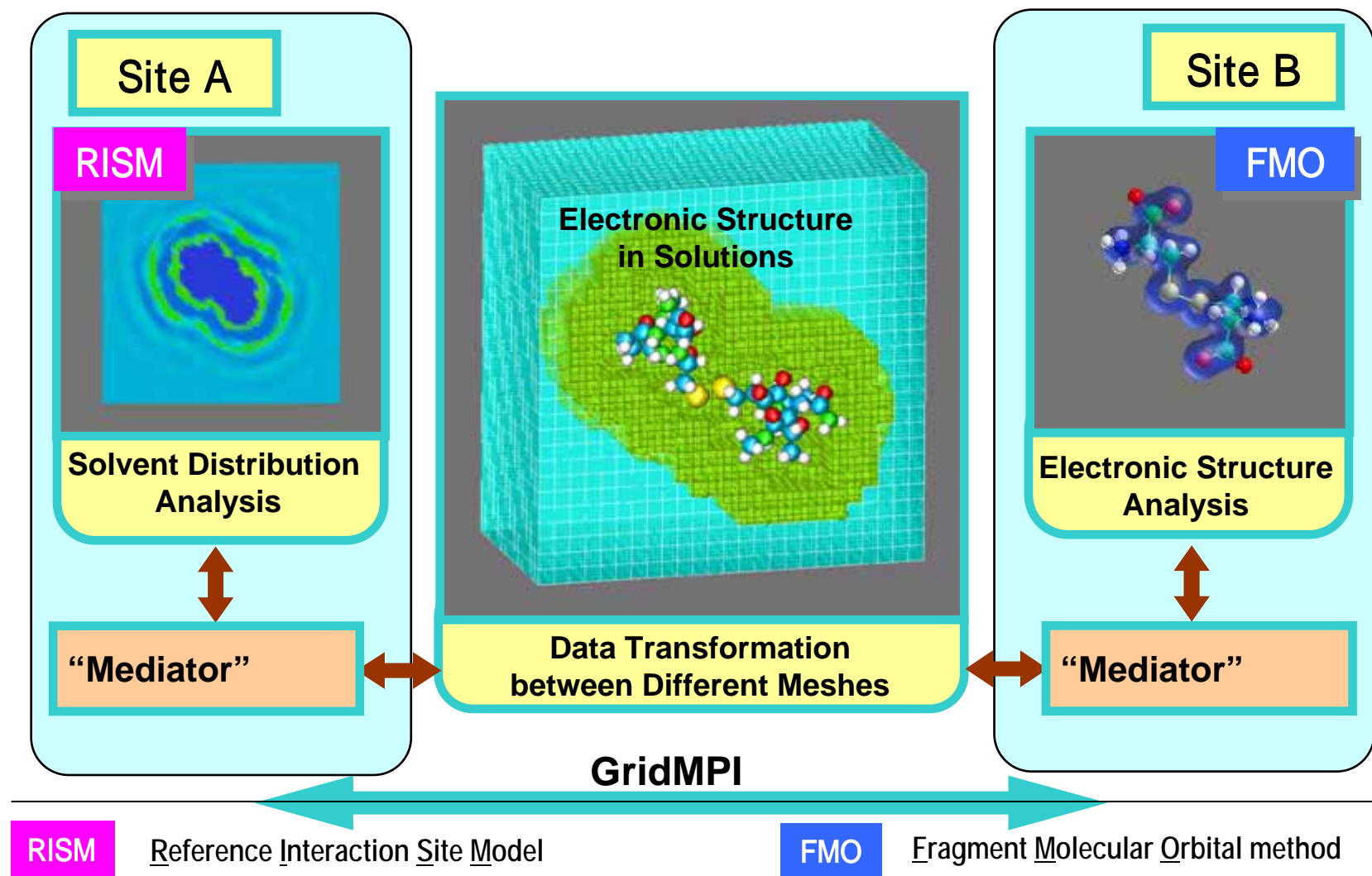
Workflow based FMO developed by NAREGI.

Fragment DB Search

↓

Monomer calculation

# of frag.

Visualization

Dimer calculation (pair of monomers)

# of pairs

An example of High throughput computing.

Total Energy

Ala

Cys-Cys

Leu

Asn

Asn

○ C
○ H
● O
● N
● S

Workflow of FMO

GAMESS (Fragment Molecular Orbital

Use Case 2: Complex MPI Job
RISM-FMO coupled simulation

Site A

RISM

Solvent Distribution Analysis

"Mediator"

Electronic Structure in Solutions

Data Transformation between Different Meshes

Site B

FMO

Electronic Structure Analysis

"Mediator"

GridMPI

RISM Reference Interaction Site Model

FMO Fragment Molecular Orbital method

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Scenario for Multi-sites MPI Job Execution
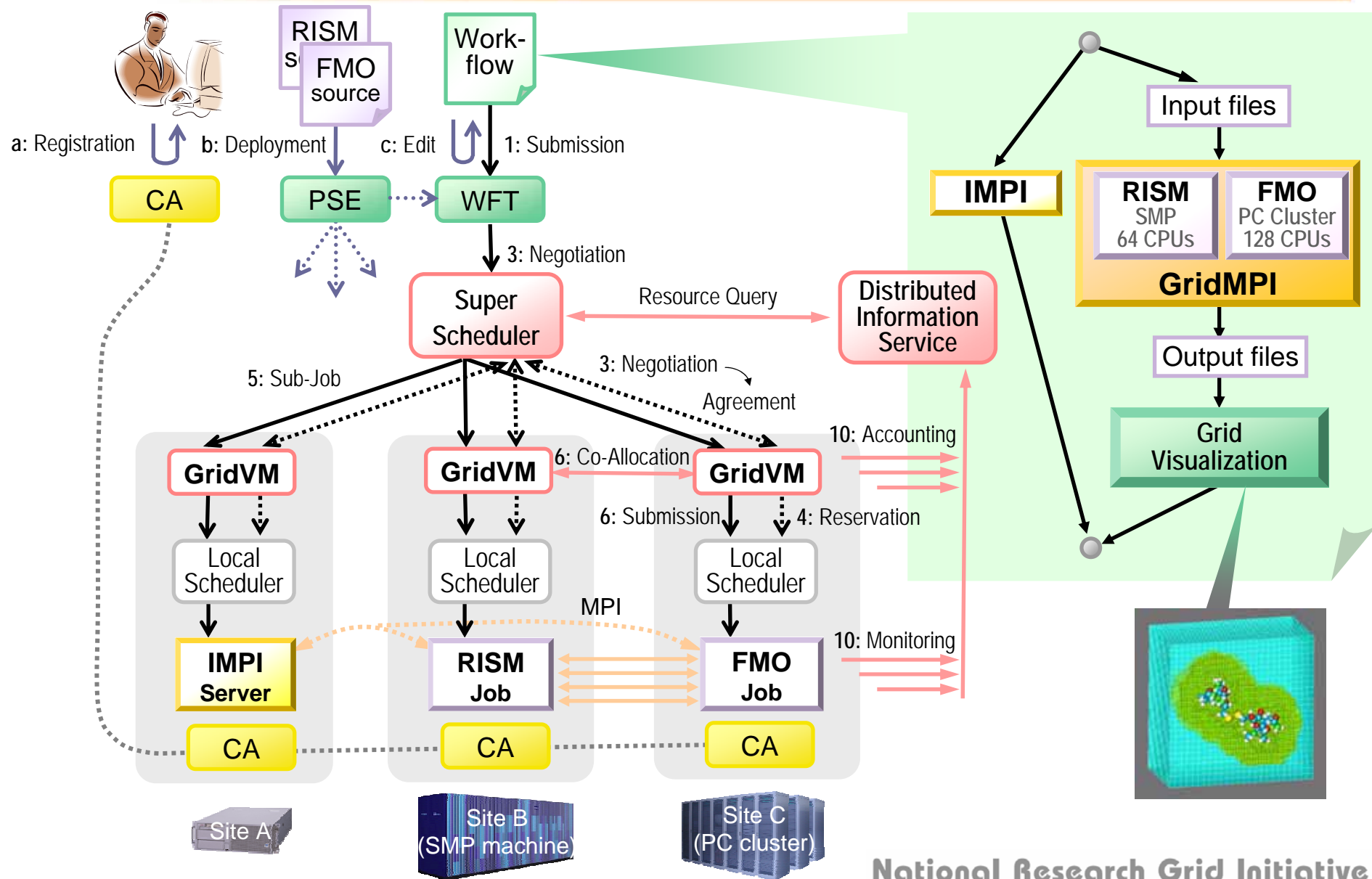
Examples of Nano-Applications Research (1)

Functional Nano-Molecules

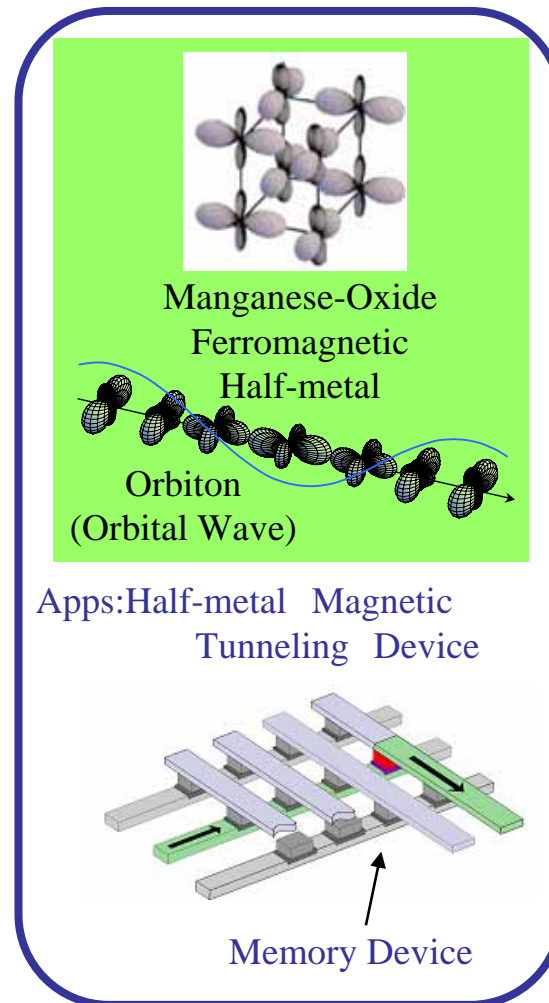Molecular Isomerizaton
by Low Energy Integration
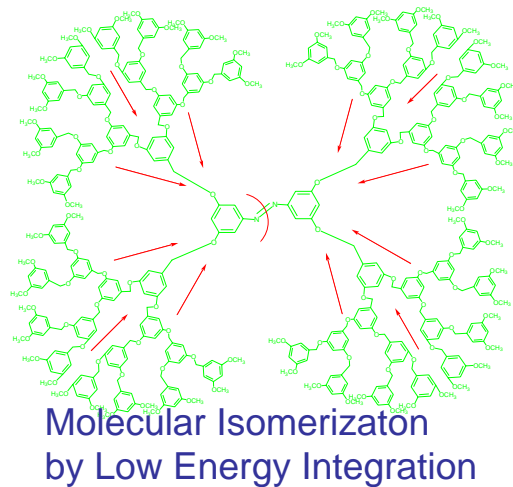
Nano-Molecular Assembly

Protein Folding
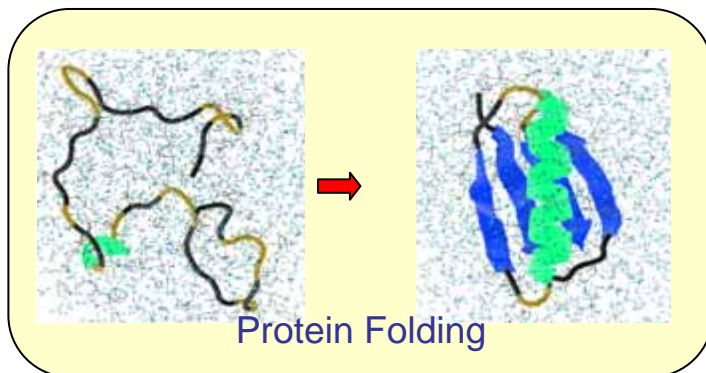
Nano-Electronic System

Manganese-Oxide
Ferromagnetic
Half-metal

Orbiton
(Orbital Wave)

Apps:Half-metal Magnetic
Tunneling Device

Memory Device
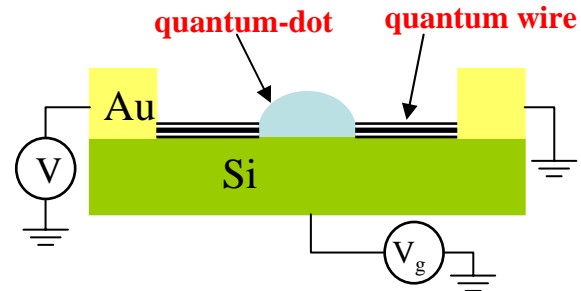
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Examples of Nano-Applications Research (2)

Nano-Magnetism

Magnetic Nano-dots
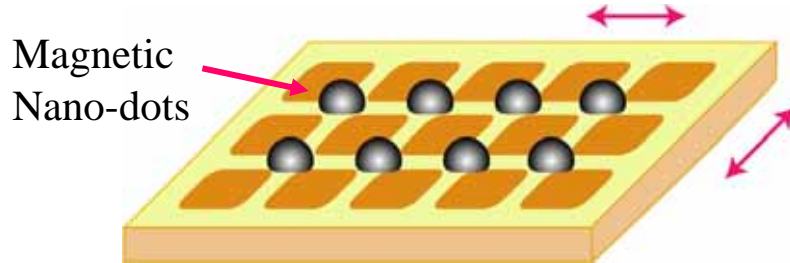
Controling Arrangement of
Nano-dots by Self Organization

Nano-system Design

quantum-dot   quantum wire

Au

V

Si

V_g

Metal,organic Molecules

Nano-device, Quantum Transport

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Thank you

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