



NAREGI Overview

NAREGI Project Goals

Establishment of a research grid infrastructure

Revitalization of the IT industry through commercialization of grid middleware and strengthened international competitiveness

Dissemination of grid environments throughout industry (through cooperation with The Computational Nano science Center)

Leadership in the standardization of grid technology

Cultivation of human resources specializing in IT technology for grids

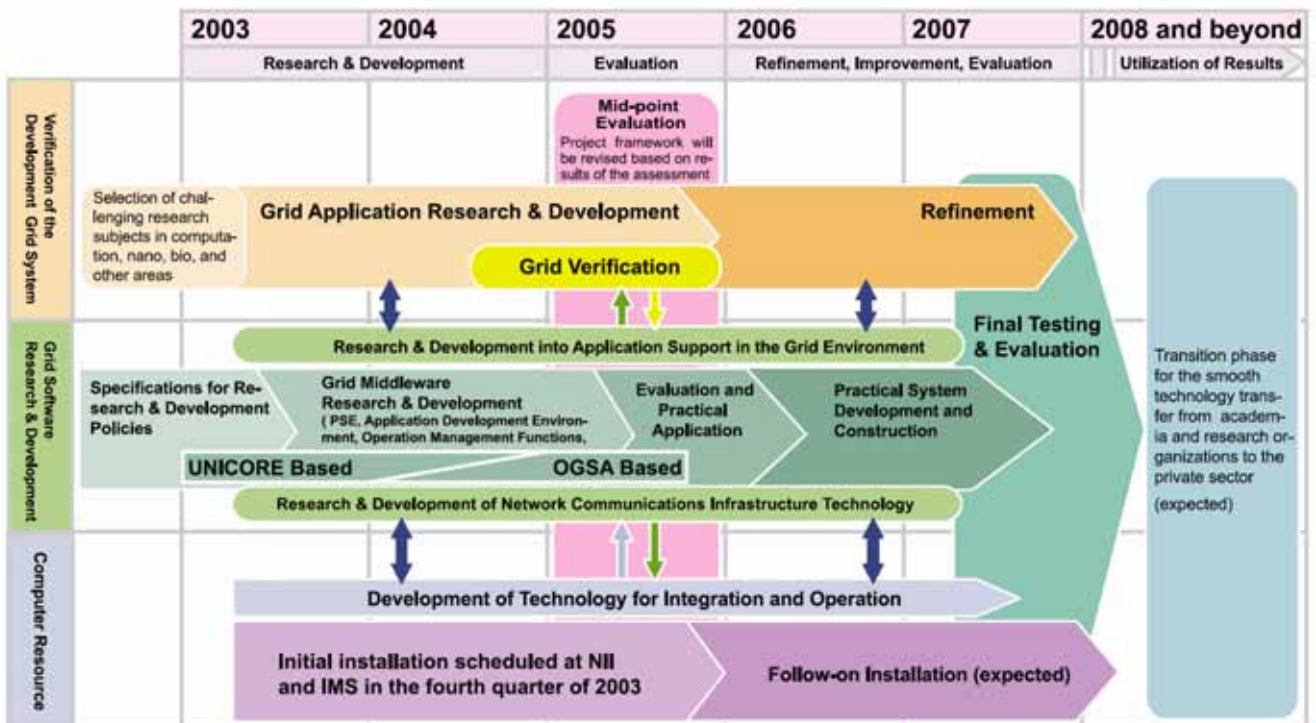
NAREGI is a collaborative research project between industry, academia, and government organizations. Our goal is to develop a new science grid that will be able to perform large- scale simulations for next-generation R&D.

The Center for Grid Research and Development and the Computational Nano-science Center serve as the bases of project activities.

The Center for Grid Research and Development develops grid infrastructure software and network technology.

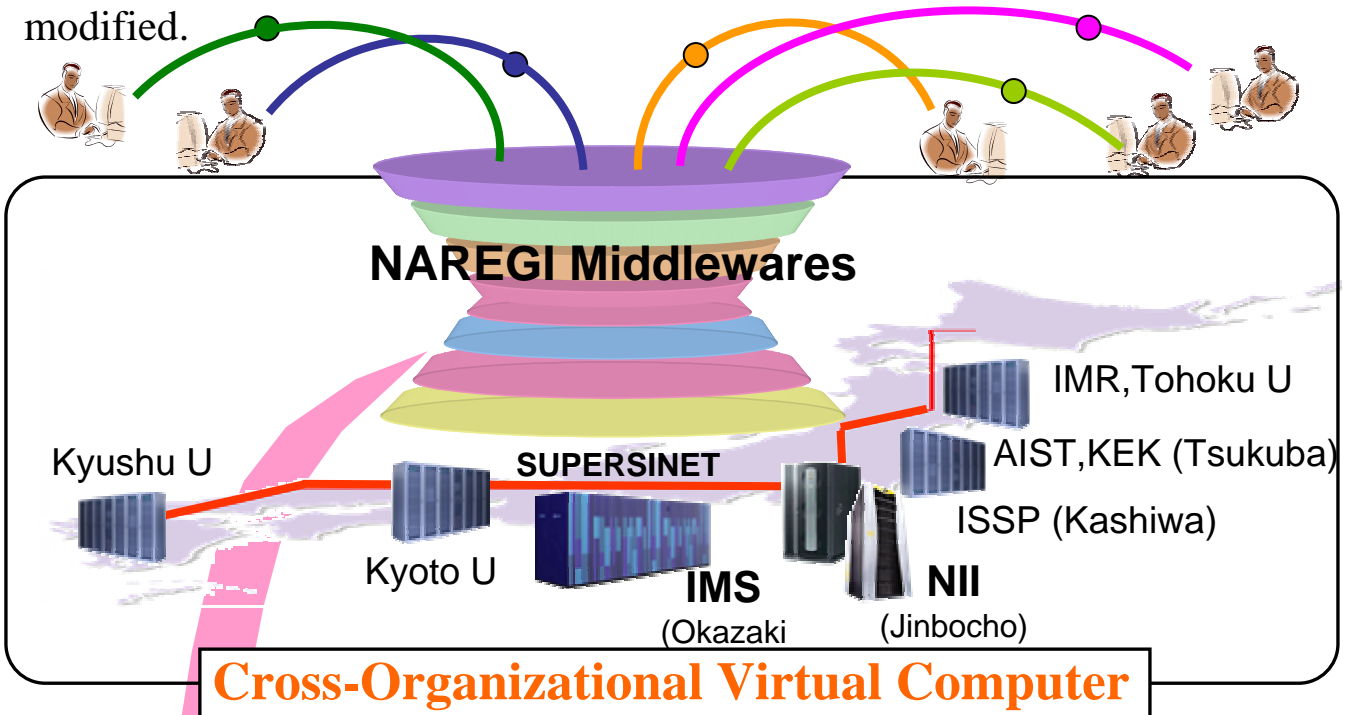
The Computational Nanoscience Center evaluates the new grid system using application software and advanced nano-science simulation technology.

NAREGI Five-year Plan



NAREGI/ Server Grid Resource Framework

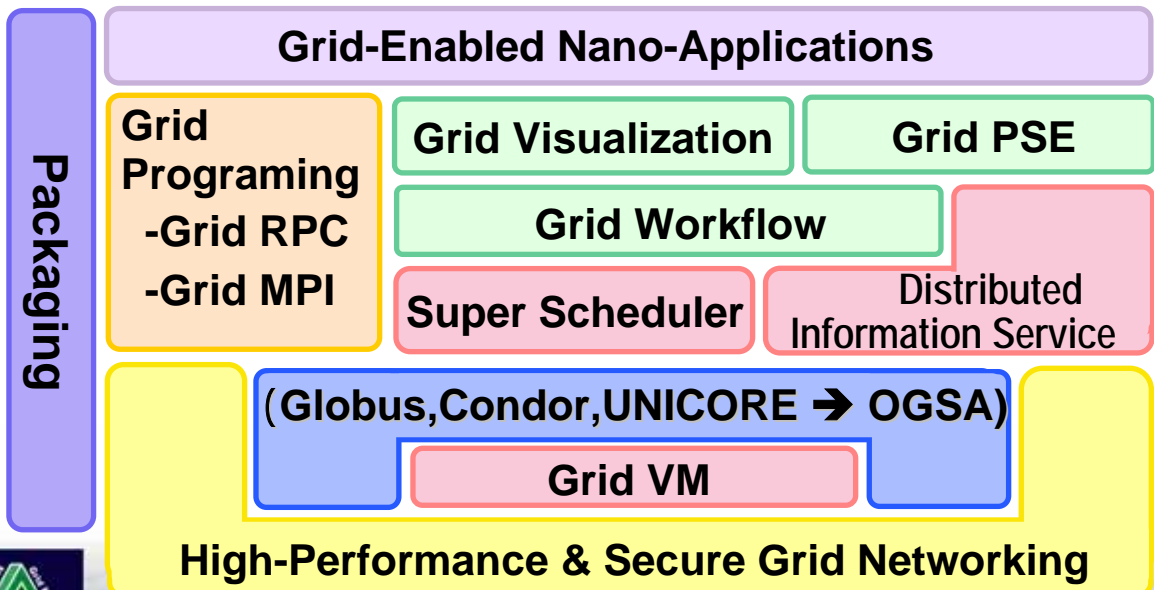
Resource allocation on Server Grid, Automatic scheduling of executing jobs, where users can run their HPC application programs as it is or slightly modified.



Seamless resource coordination across many different research organizations.

- Higher Utilization
- Higher Reliability
- Tight collaboration of VOs
- Ultra-Scaling of Resources

NAREGI Middlewares



Scenario for Inter-site MPI Job Execution

Users can execute huge MPI jobs such as coupled simulations in nano-science, without being conscious of actual complicated configuration of the grid resources.

Preliminaries

- A user has MPI programs for **RISM-FMO** coupled simulation. Before its execution,
- The user receives his/her own user certificate issued by the **CA** after user registration.
 - The user transfers and compiles his/her programs on the grid resources by using **PSE**.
 - The user describes the way of execution and the requirements of resources for the MPI job in a workflow by using **WFT**.

Reservation

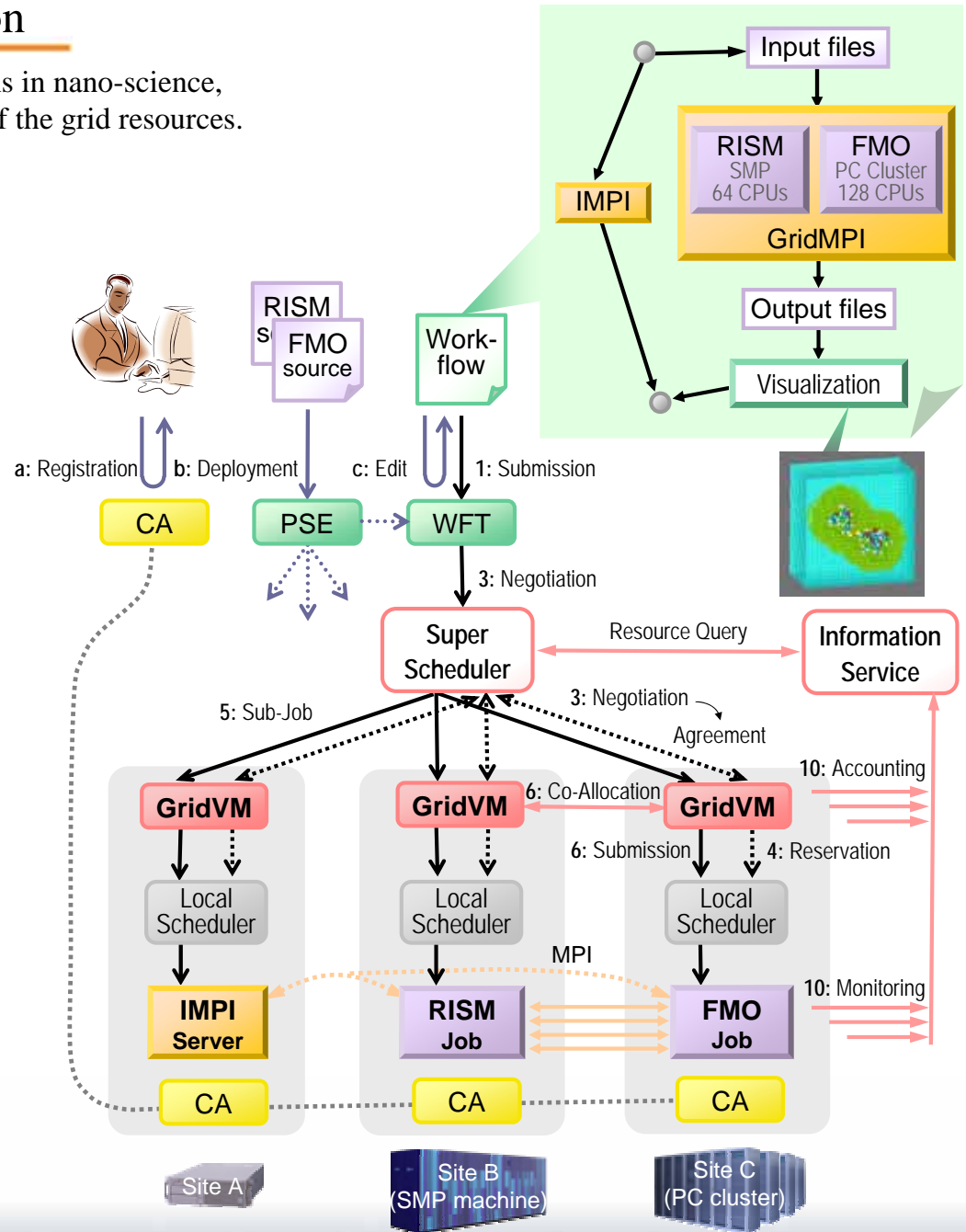
- The workflow is submitted to the **Super Scheduler** through **WFT**.
- The **Super Scheduler** asks the **Information Service** to find adequate **GridVMs** for the MPI job described in the workflow.
- The **Super Scheduler** negotiates with these **GridVMs** to reserve resources for job execution.
- If these **GridVMs** agrees with the **Super Scheduler**, they reserve resources under the **local schedulers**.

Execution

- When the reservation time comes, an **IMPI** (Interoperable MPI) server is started.
- After that, **GridVMs** co-allocate job queues with 64 CPUs on an SMP machine and with 128 CPUs on the PC cluster.
- RISM** is started on the SMP machine and **FMO** is started on the PC cluster.
- IMPI** server initiates and manages MPI communication.

Monitoring

- The results of the MPI job can be visualized under and/or after the job execution by using **GVS**.
- After the job ends, her resource usage is recorded in **Information Service**.

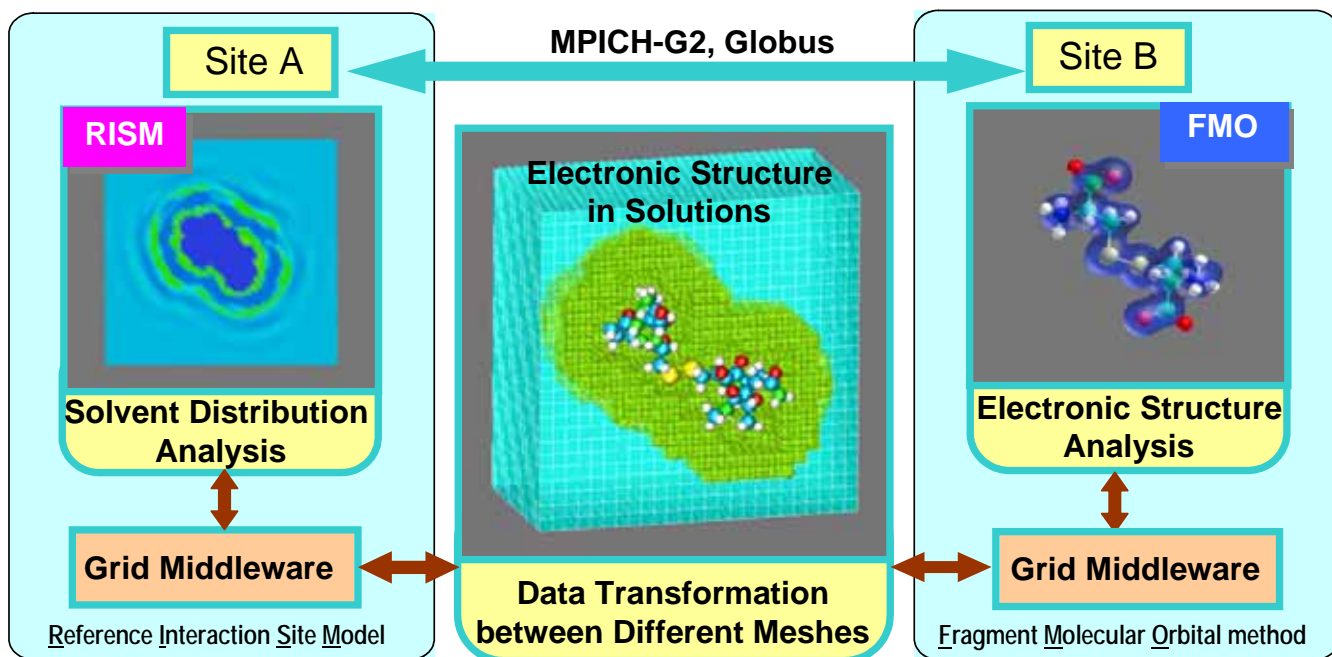




RISM-FMO Coupled Simulation

Mediator-based grid middleware allows coupled simulations of nano applications to calculate the electronic structure of nano-scale molecule in solution.

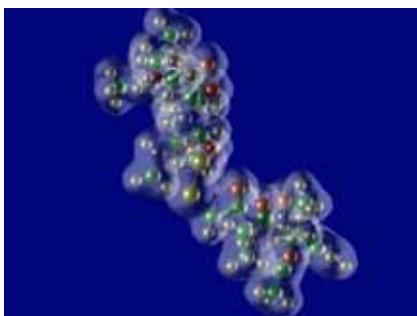
1. RISM-FMO Coupled Simulation in Grid Environment



2. Simulation Result for Oligopeptide

Statistical high density in O molecular orientation of H_2O to the solute decreases electronic charge on H atom.

Electronic density of solute
in FMO (in vacum)



Solute in H_2O Solvent

