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Outline of the “Next Generation Supercomputer System Project” in Japan

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And

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Next Generation Supercomputer R&D Center

RIKEN



Outline

**1. Next Generation Supercomputer
Development Project**

2. National Research Grid Initiative (NAREGI)

3. Cyber Science Infrastructure (CSI)

Background

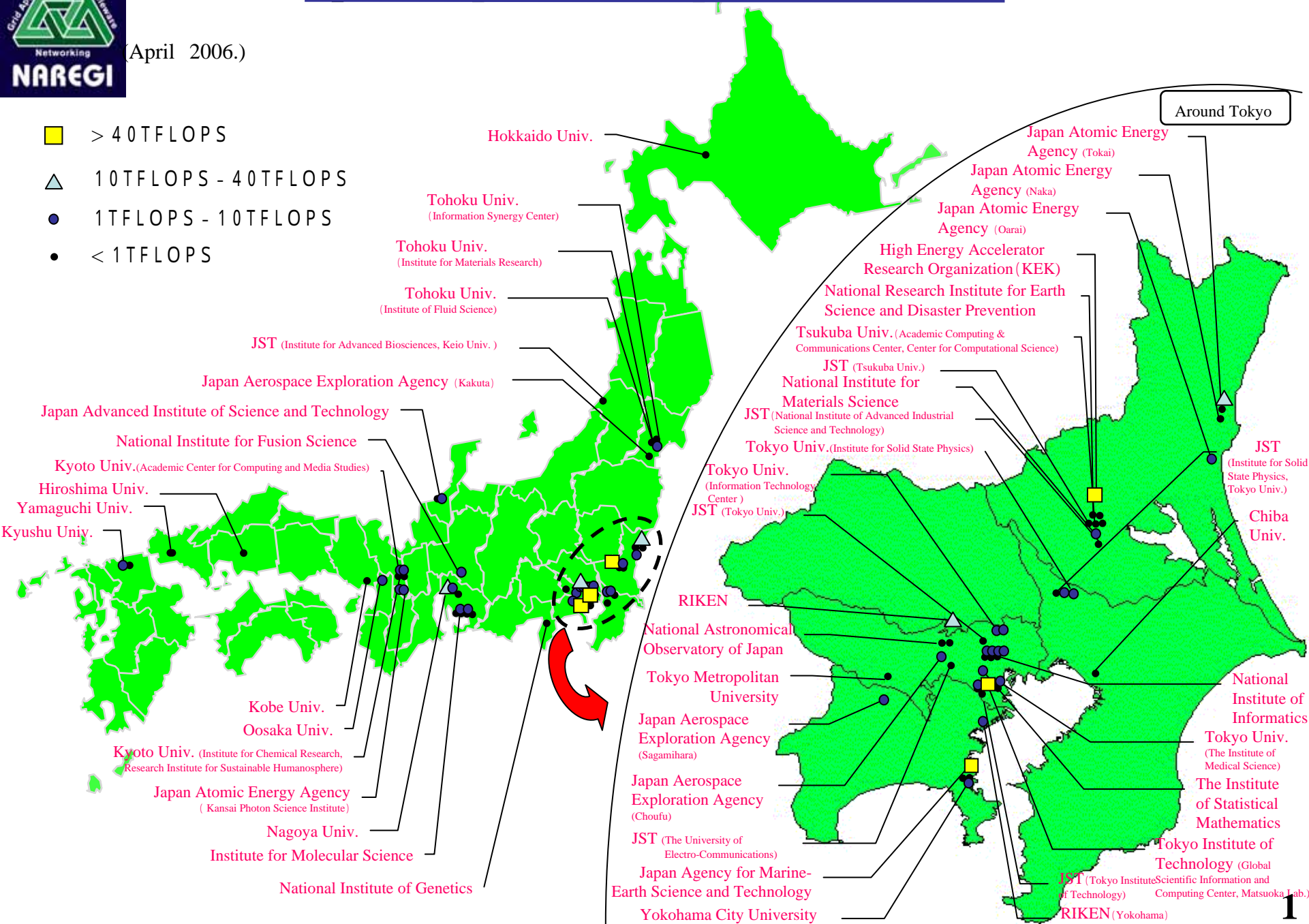
- Supercomputing Technology has been selected as one of the “Nation’s Key Technologies”
- To enhance the competitiveness of Japanese science, technology and industry.
- To maintain capability of development of a supercomputer within the country, and to enable continuous development.



Supercomputers in Japan under MEXT

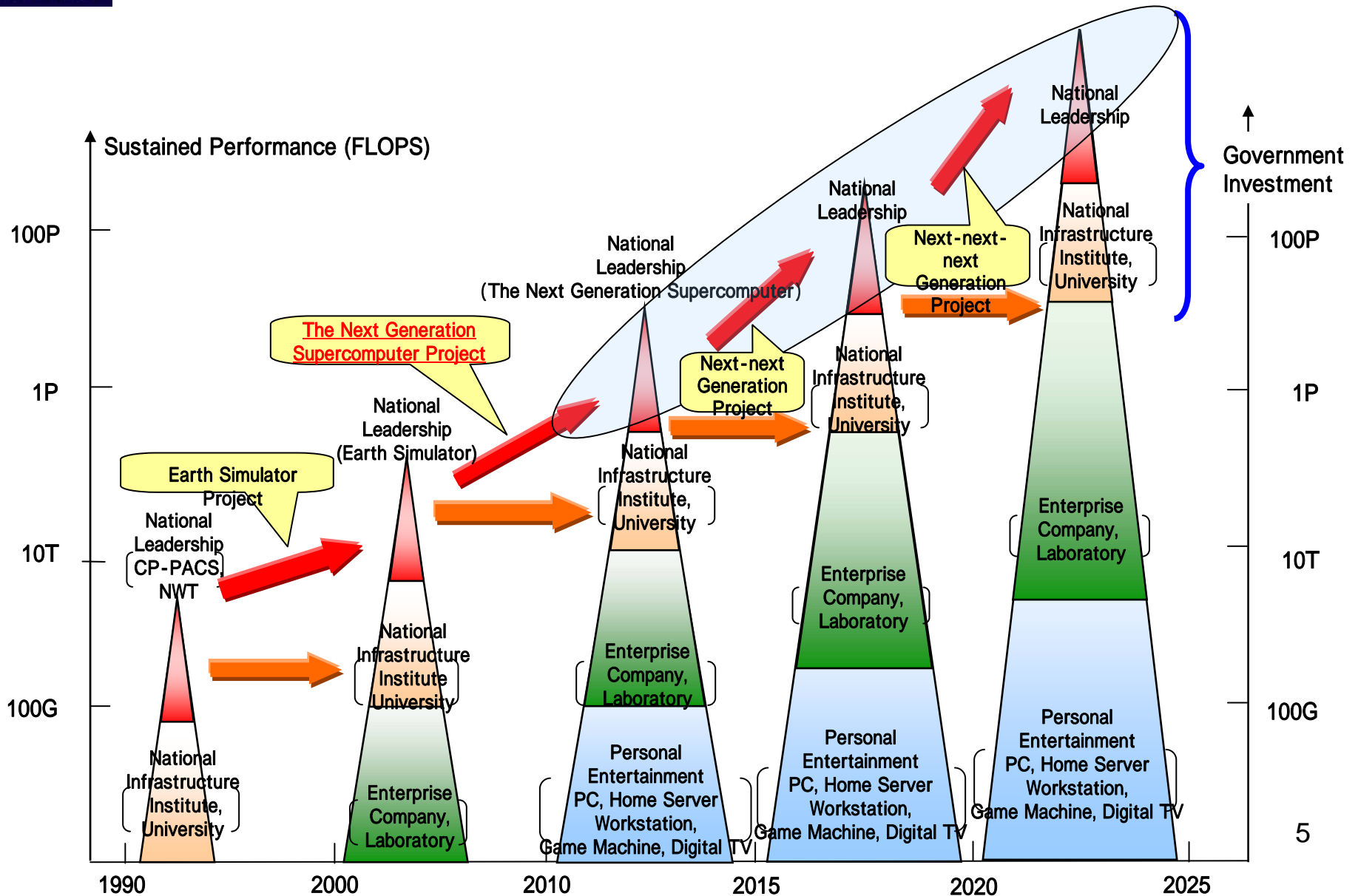
(April 2006.)

- > 40TFLOPS
- △ 10TFLOPS - 40TFLOPS
- 1TFLOPS - 10TFLOPS
- < 1TFLOPS





MEXT's Vision for Continuous Development of Supercomputers





Development & Applications of Advanced High-performance Supercomputer Project

FY2006 3,547Million yen (New)

FY2006-FY2012 (total national budget) ~110 billion yen

1 . Purpose

Development, installation, and applications of advanced high-performance supercomputer system

2 . Effect

Together with theory and experiment, simulation has been recognized as the third methodology for science and technology today.

In order to lead the world for the future and progress of science, technology and industries,

- (1) Development and deployment of the system and application software for utilizing supercomputer system**
- (2) Development and installation of the advanced high-performance supercomputer system**
- (3) Establishment and Operation of “Advanced Computational Science and Technology Center (tentative)”, where the developed supercomputer system is the core computational resource.**

With the above (1),(2) and (3), creative talented people who can improve the level of research in Japan and lead the world, will be fostered.

3 . Framework for use and administration

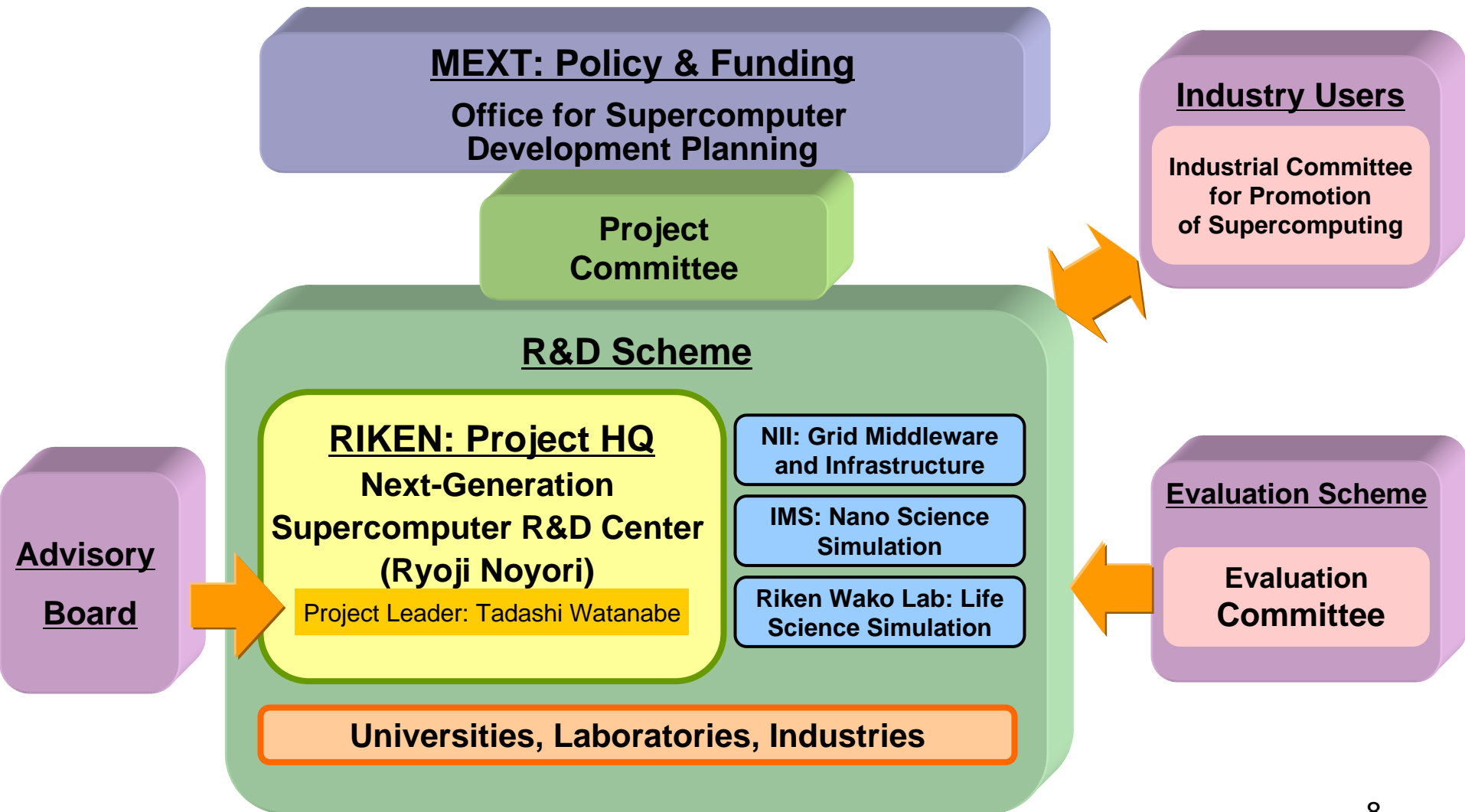
- MEXT is responsible for installation, use, and administration of the facilities comprehensively.**
- The new law will be enacted for the framework of usage and administration.**
- The facilities for fundamental research and industrial applications will be open to universities, research institutes and industries.**



Development & Application of the Next-Generation Supercomputer

- Objective of the project:
 - To develop and implement the world's most advanced and high-performance Next-Generation Supercomputer,
 - To develop and disseminate its usage technologies.
- Targets
 - Achieve the world's fastest computing speed
 - effective (application) performance first
 - Keep low-cost in order to encourage widely use
 - expect other sites adopt the same kind of supercomputers
 - Development of a hardware technology which is something new and will spread widely.
 - e.g., low-power CPU, efficient cooling, interconnect, etc.

Project Organization



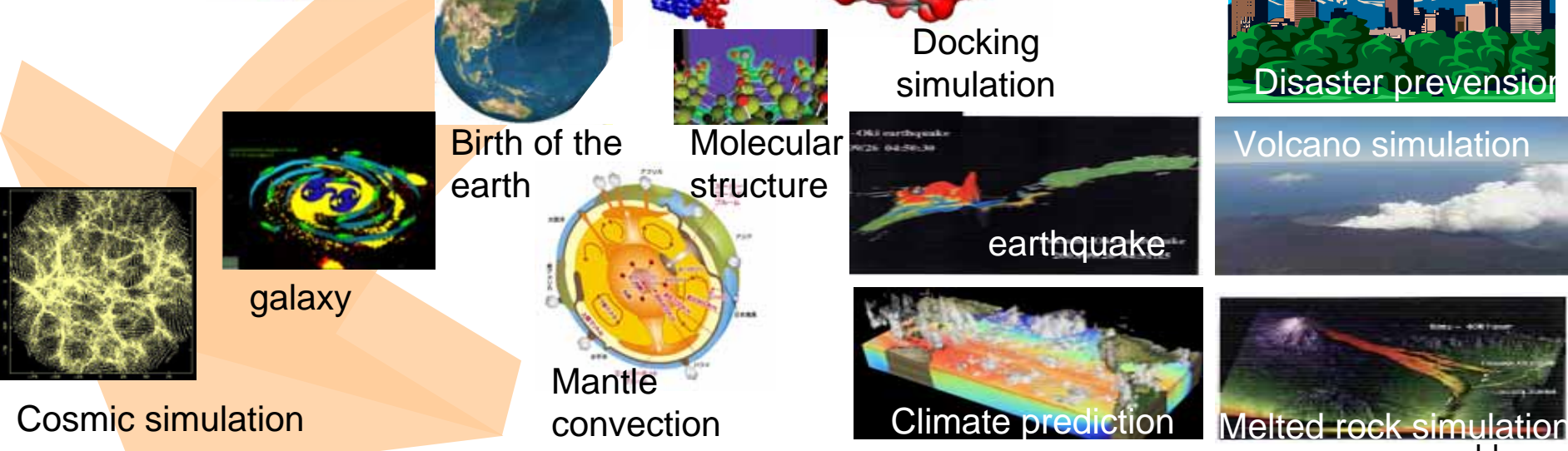
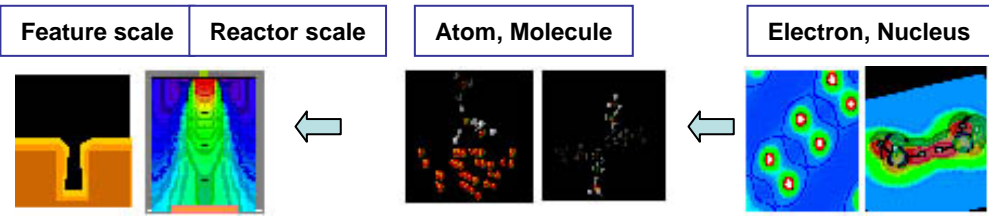
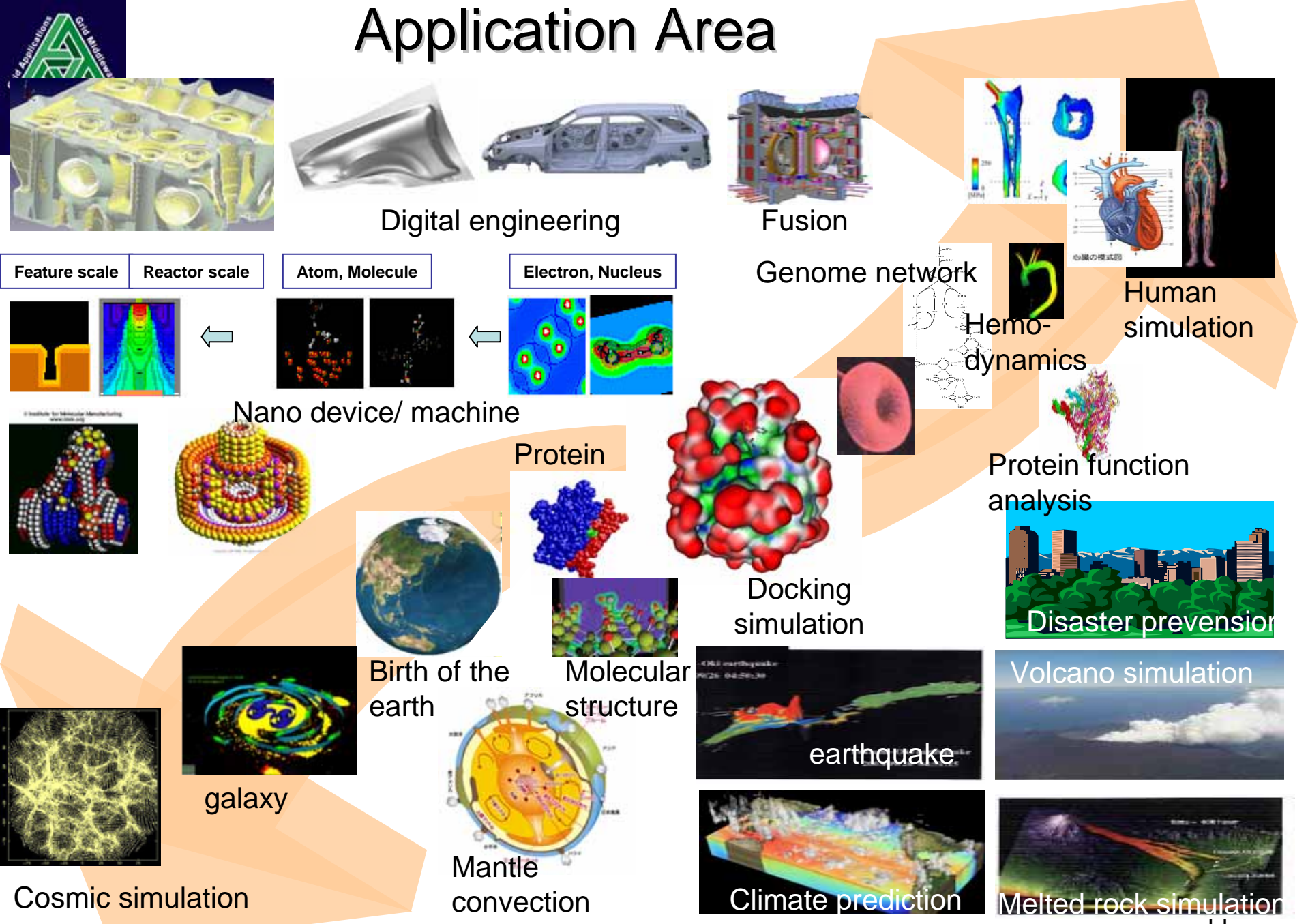
Current Schedule

FY		2006	2007	2008	2009	2010	2011	2012
Operation						Start Operation	Full Operation	
	R&D							
Software	System Software	OS/Tools/GRID middleware Design & Production			Evaluation			
	Grand Challenge Application Software	Next Generation Nano-Science Simulation, Design & Production			Evaluation			
		Next Generation Life Science Simulation, Design & Production					Evaluation	
Hardware	Basic Design	Detail Design		Production		Enhancement		
File Systems and others			Design	Production		Enhancement		
Geographical investigation, Construction	Investigation	Design	Construction					

Key points of the project

- The **first step** of continuous development of supercomputers in the next few decades.
- Not limited to a particular research field
 - This supercomputer will be **a public facility**.
 - “A law regarding promotion of common use” has made.
- RIKEN is in charge of development.
 - Operation and management by other organization
- Aiming to establish **CoE (Center of Excellence)** for supercomputing research
 - Including human resource development and education
- Use of **Highspeed Network Infrastructure/GRID Technology**
 - One of computational resources over **Cyber Science Infrastructure**

Application Area



Multi-scale Multi-physic simulation

Grand Challenge Applications

- **Nano Science:**
 - Institute for Molecular Science
- **Life Science:**
 - “Total Simulation of Living Matter”
 - from “Molecular”, “Cell” to “Organ/Whole Body” scale
 - Wako Institute, RIKEN

Application Analysis for Architecture Evaluation

So far, 21 application programs have been identified as candidates to be used for architecture evaluation

- **Nanoscience (6)**

e.g., MD, Fragment MO, First Principle MD (physical space formulation), RISM, OCTA

- **Life Science (6)**

e.g., MD(Protein), DF(Protein), Folding, Blood Flow, Gene network

- **Climate/Geoscience (3)**

Earth Quake Wave Propagation, Hi-res. Atmospheric GCM, Hi-res. Ocean GCM

- **Physical Science (2)**

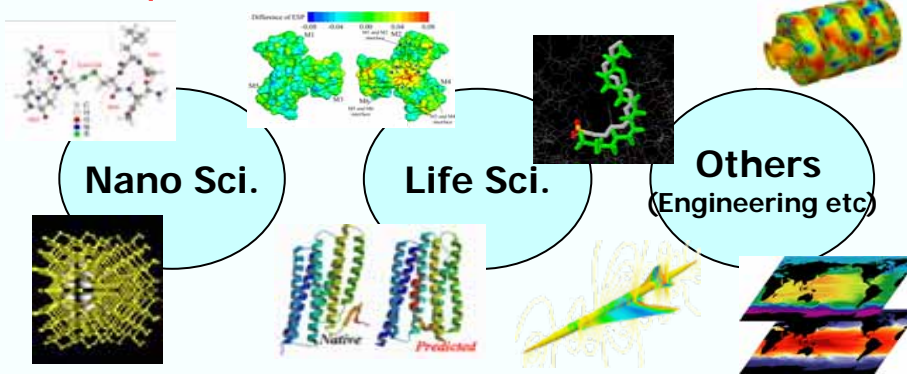
Galaxy Formation (hydro + gravitational N-body), QCD

- **Engineering (4)**

e.g., Structural Analysis by FEM, Non-steady Flow by FDM, Compressive Flow, Large Eddy Simulation

Optimization of System Design

Requirement from Grand Challenges

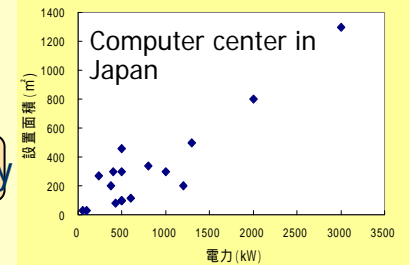


Requirements from Computer Centers

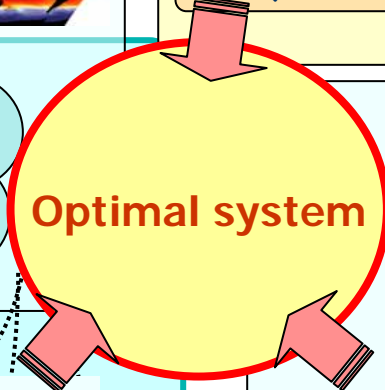
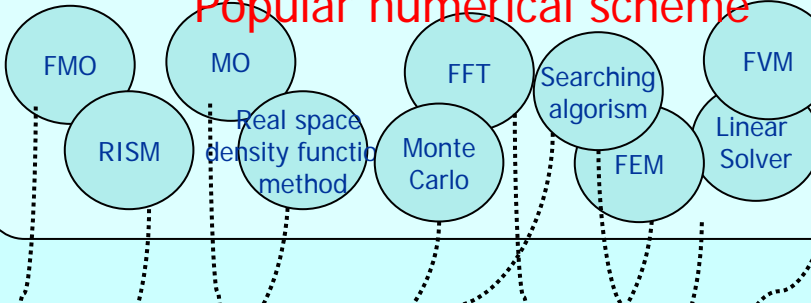
Power, Space

Reliability, operability

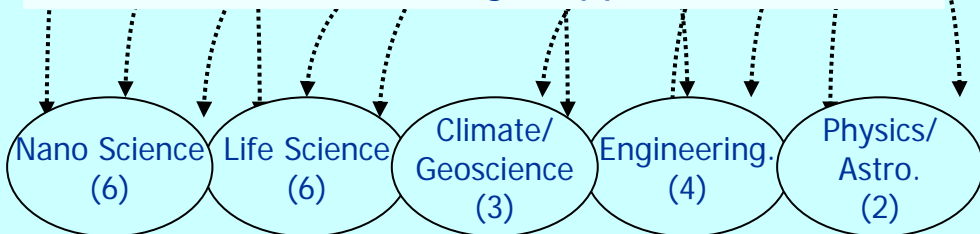
Cost (development, manufacturing, maintenance)



Popular numerical scheme



21 Selected Target applications

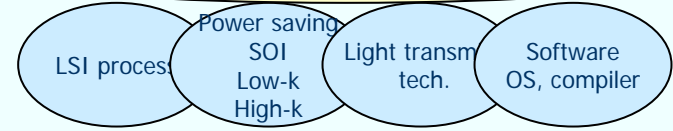


Other Project Watch

Technology Survey

Operation & Utilization

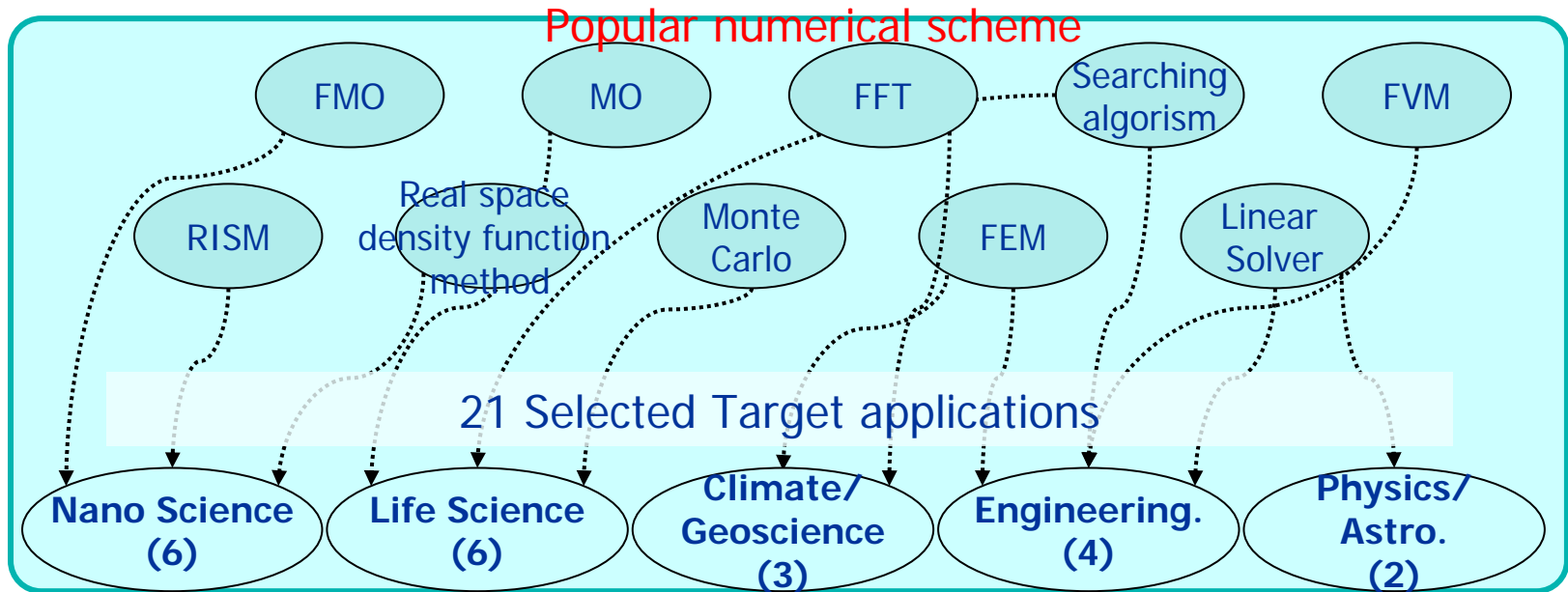
Essential Element technologies



Spin off to the consumer electronics

Technology Limit

Target applications for system performance estimation



- 21 application programs have been identified as candidates to be used for **system performance estimation** by the application committee.
- Modified to be a benchmark test suite
 - **benchmarking on the desk** on each proposed system



The Next Generation Supercomputer System Project

- Total National Budget requested: 110 Billion Yen in 7 years (including, system software, applications, hardware, facility etc.)

< System >

- Performance Target:

10 petaflop/s class machine

Over 1 petaflop/s (Application-dependent)

- High Priority Applications:

- Nanoscience/Nanotechnology
- Life/Bio

- System Architecture Candidates proposed: Summer 2006

➔ Evaluation FY2006

- System Completion: end FY2010(initial) -
end FY2011 (final)



Outline

1. Cyber Science Infrastructure (CSI)
- 2. National Research Grid Initiative (NAREGI)**
3. Next Generation Supercomputer Development Project



National Research Grid Initiative (NAREGI) Project: Overview

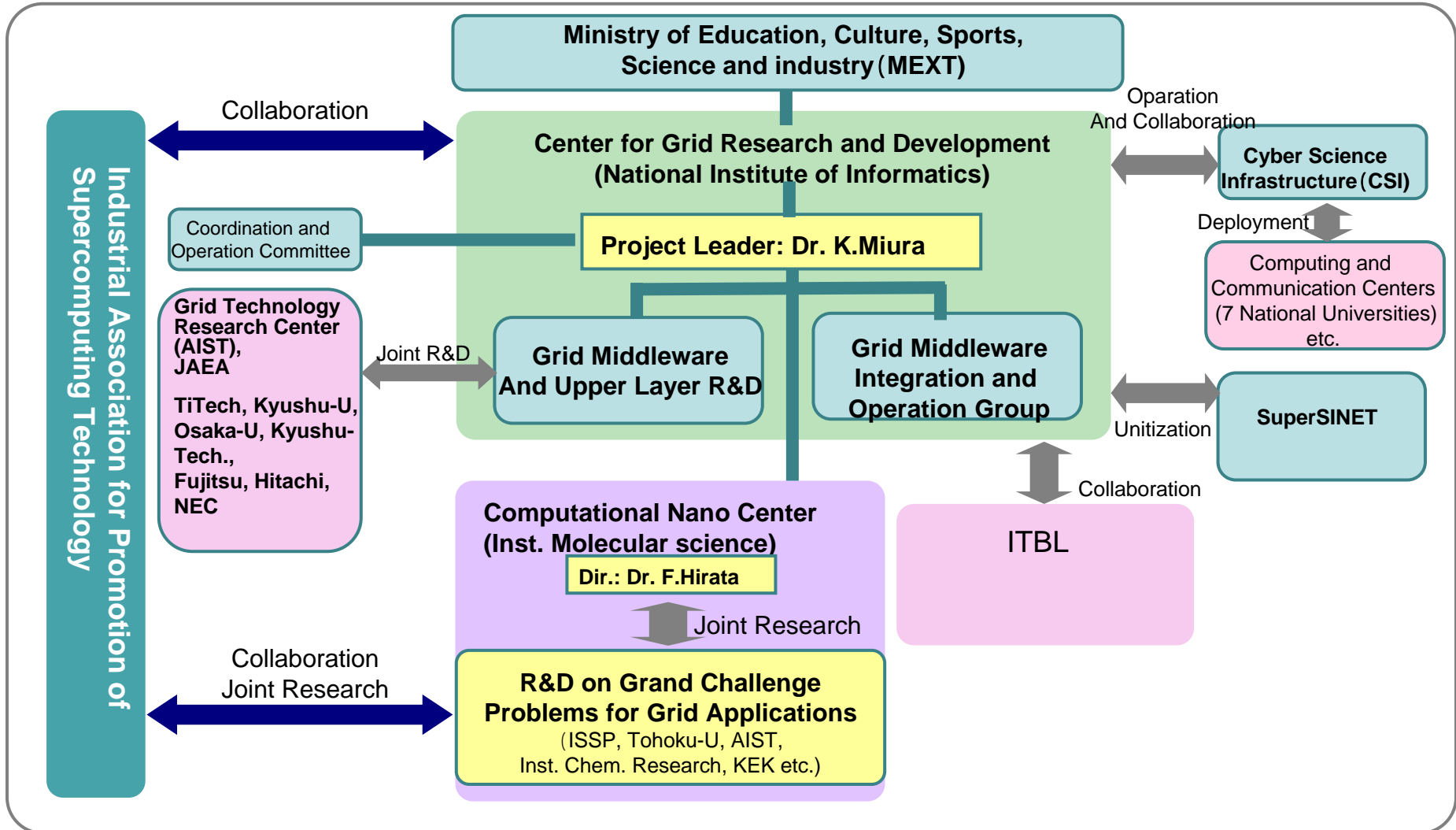
- Originally started as an R&D project funded by MEXT (FY2003-FY2007)
2 B Yen (~17M\$) budget in FY2003
- Collaboration of National Labs. Universities and Industry in the R&D activities (IT and Nano-science Apps.)
- Project redirected as a part of the Next Generation Supercomputer Development Project



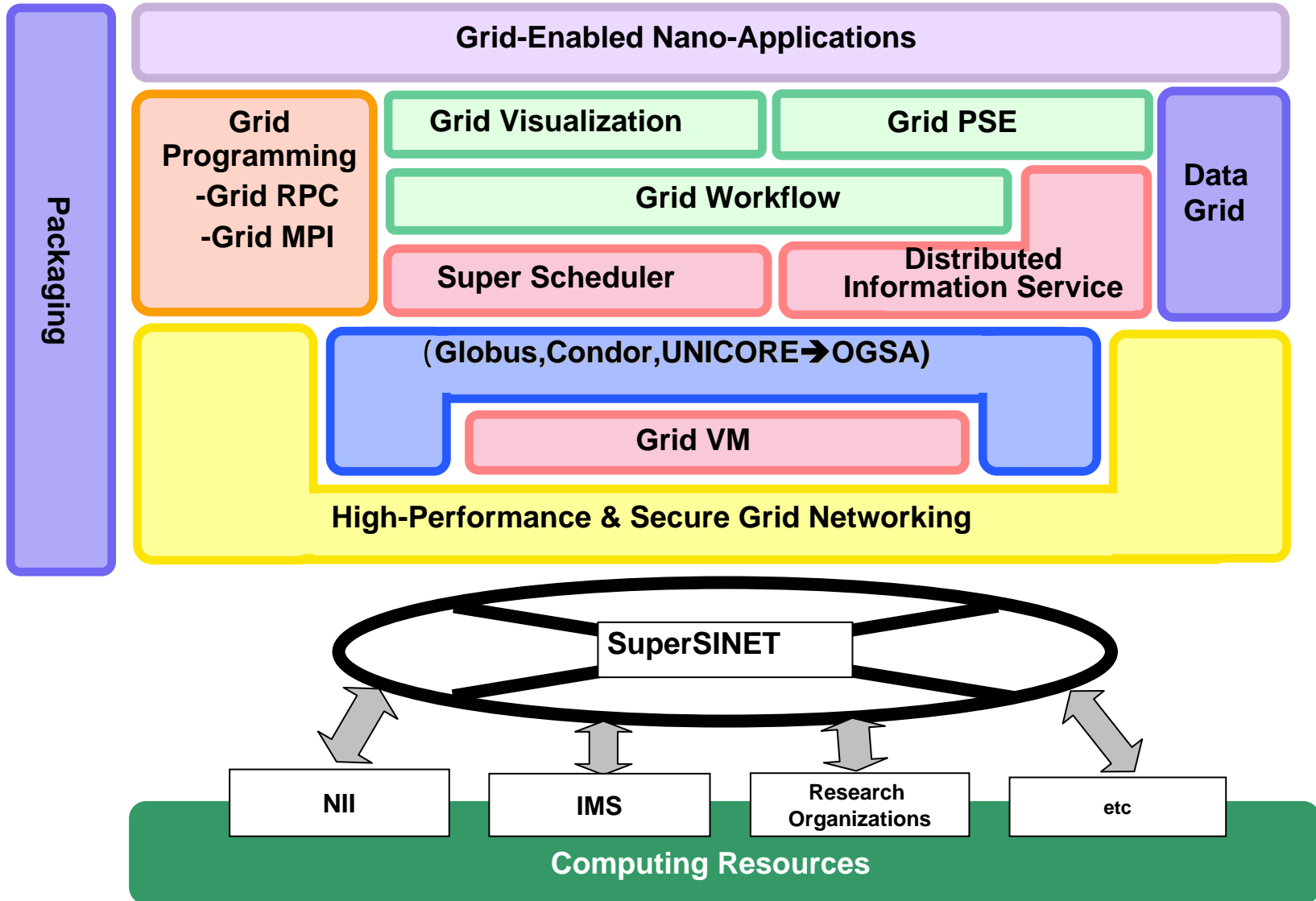
National Research Grid Initiative (NAREGI) Project:Goals

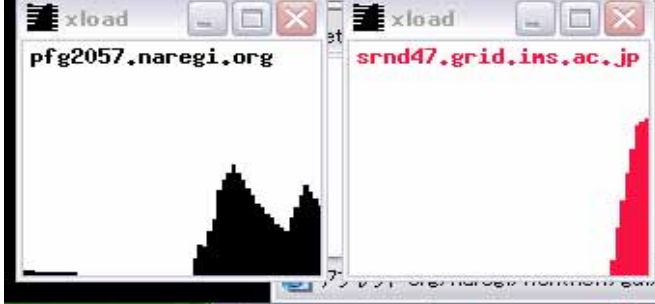
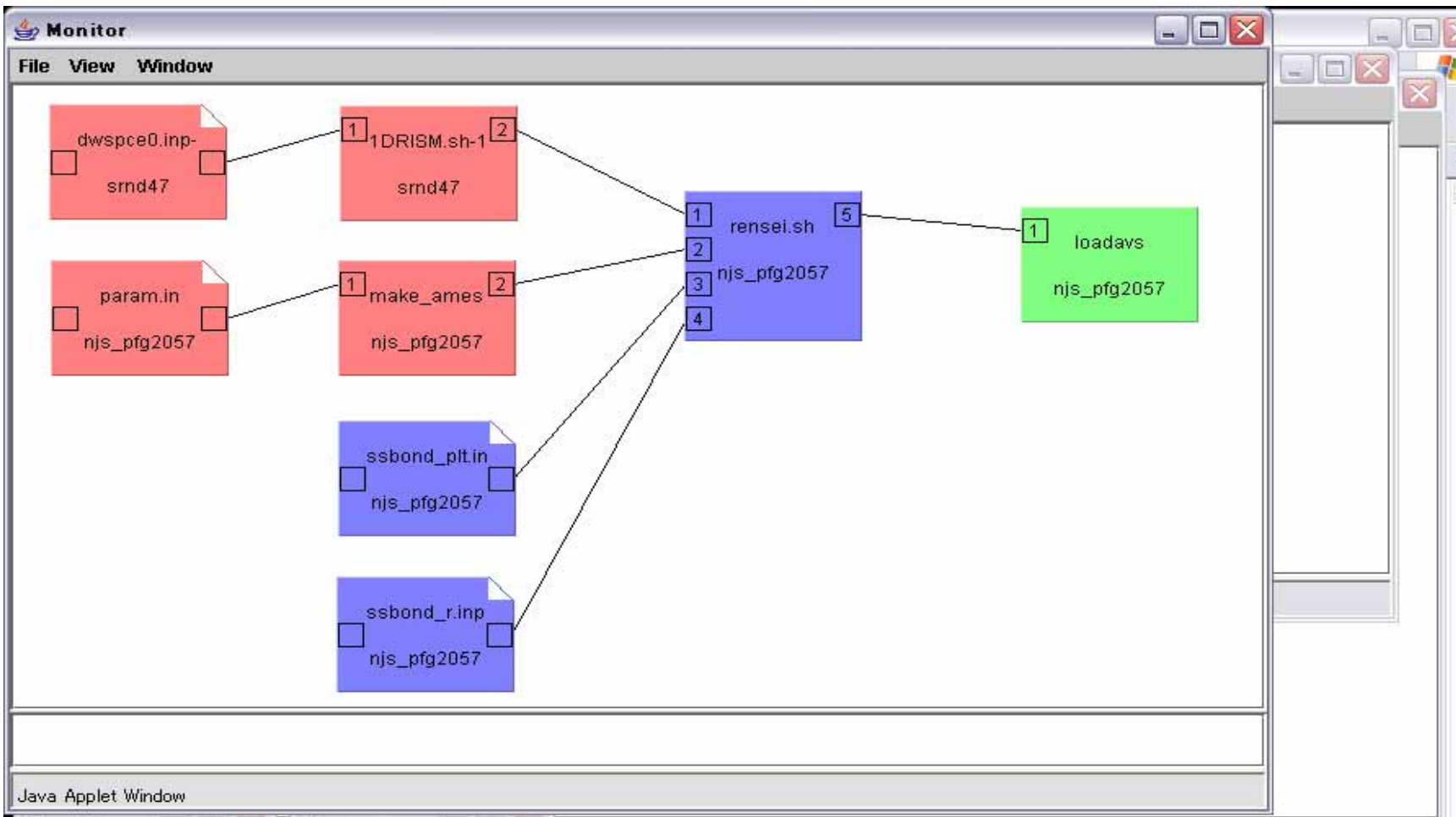
- (1) To develop a Grid Software System (R&D in Grid Middleware and Upper Layer) as the prototype of future Grid Infrastructure in scientific research in Japan
- (2) To provide a Testbed to prove that the High-end Grid Computing Environment (100+Tflop/s expected by 2007) can be practically utilized in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

Organization of NAREGI

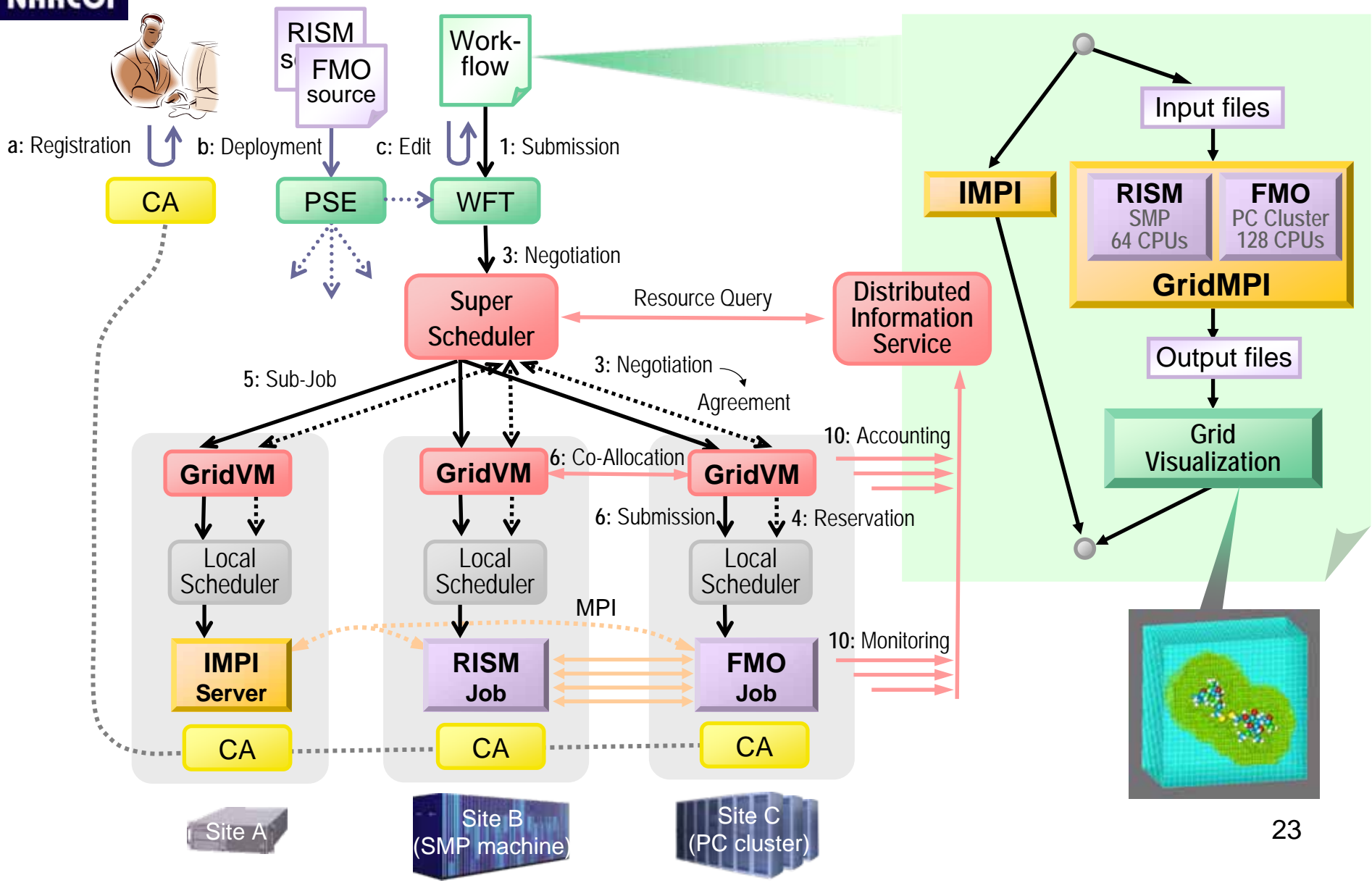


NAREGI Software Stack

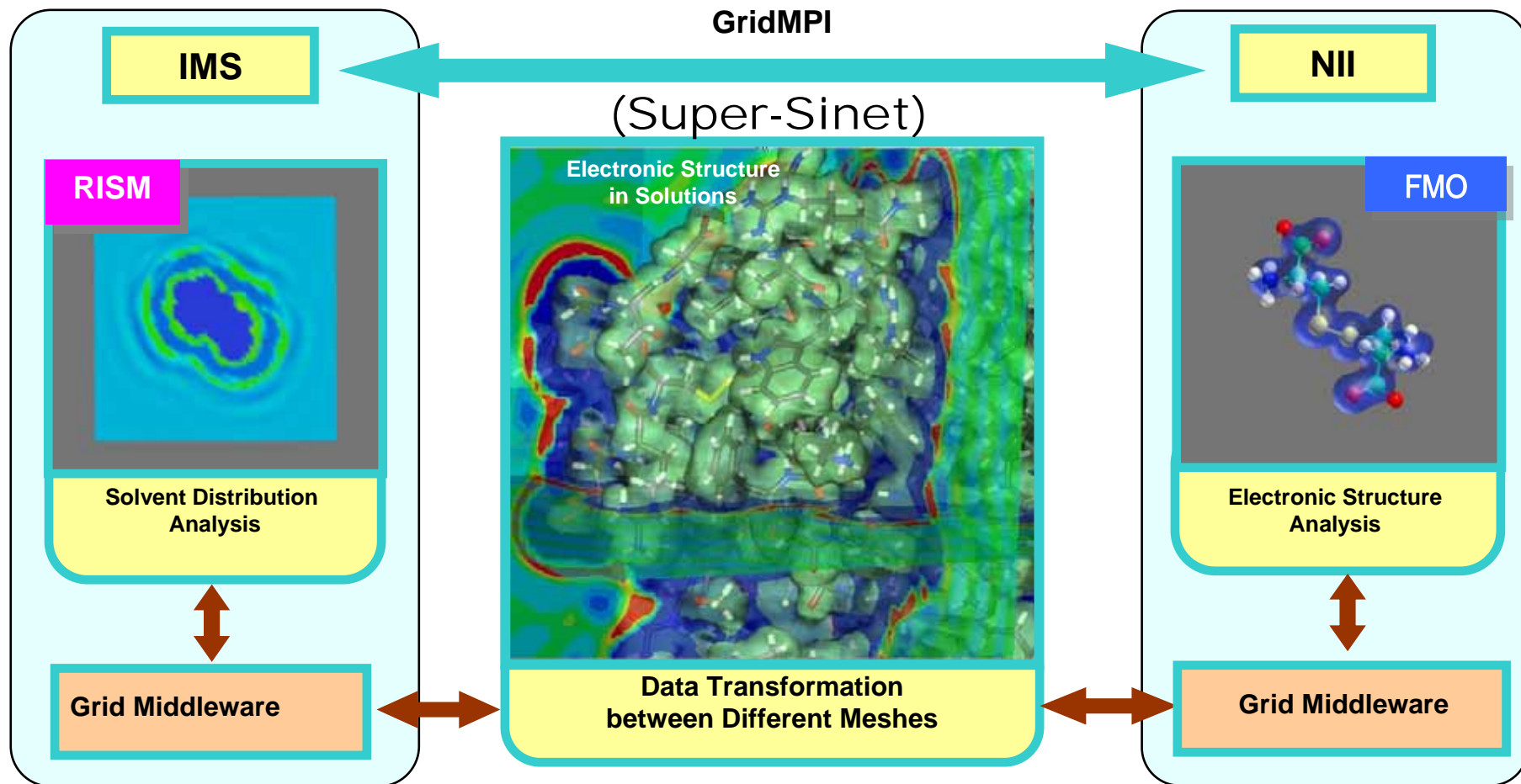




Scenario for Multi-sites MPI Job Execution



Adaptation of Nano-science Applications to Grid Environment



RISM

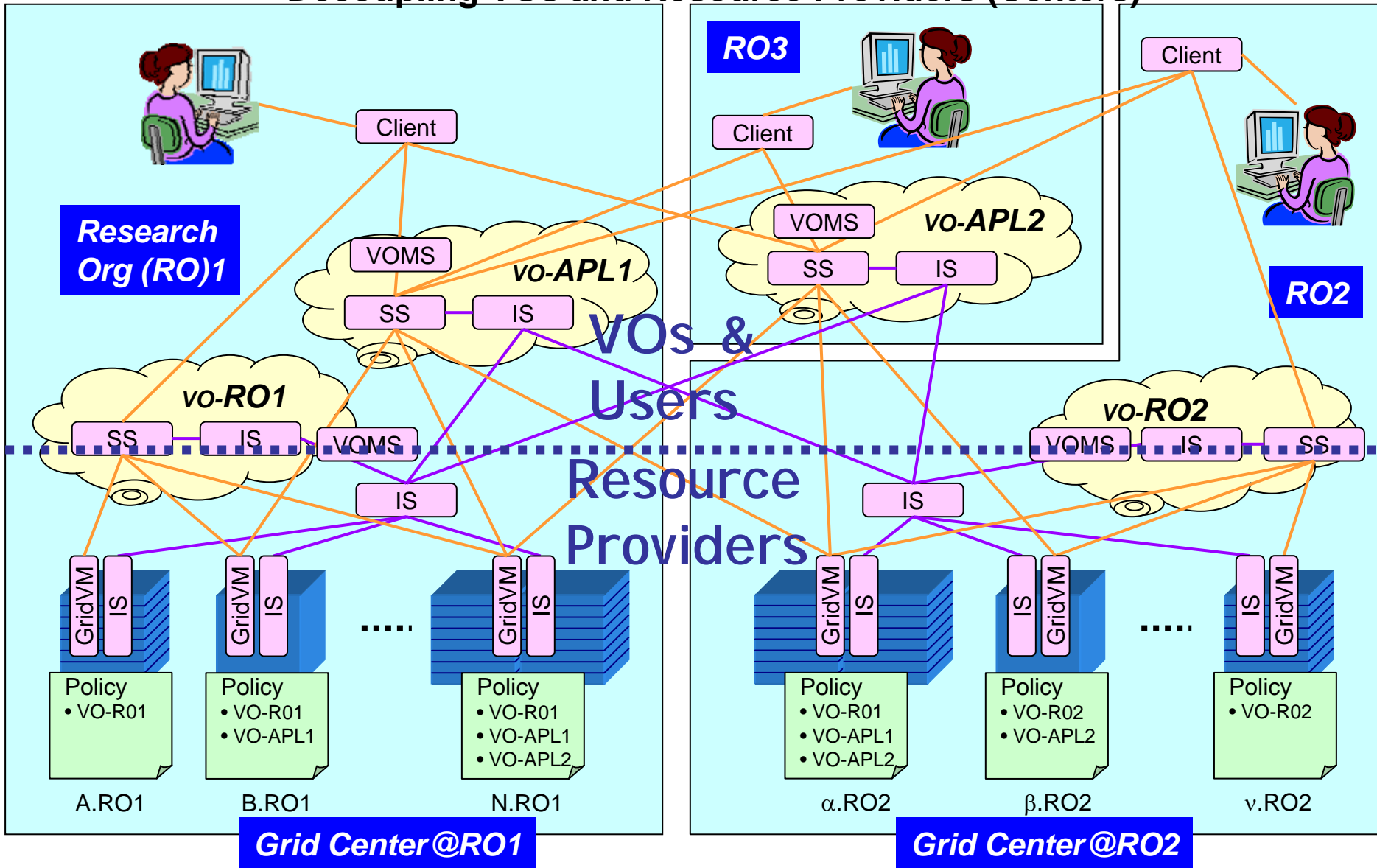
Reference Interaction Site Model

FMO

Fragment Molecular Orbital method

VO and Resources in Beta 2

Decoupling VOs and Resource Providers (Centers)



Collaboration in Data Grid Area

- High Energy Physics (GIN)
 - KEK
 - EGEE
- Astronomy
 - National Astronomical Observatory
(Virtual Observatory)
- Bio-informatics
 - BioGrid Project

Highlights of NAREGI β release (2005-6)

1. Resource and Execution Management

- GT4/WSRF based OGSA-EMS incarnation
Job Management, Brokering, Reservation based co-allocation, Monitoring, Accounting
- Network traffic measurement and control

The first incarnation
In the world (@ α)

2. Security

- Production-quality CA
- VOMS/MyProxy based identity/security/monitoring/accounting

NAREGI is operating
production level CA in
APGrid PMA

3. Data Grid

- WSRF based grid-wide data sharing with Gfarm

Grid wide seamless
data access

4. Grid Ready Programming Libraries

- Standards compliant GridMPI (MPI-2) and GridRPC
- Bridge tools for different type applications in a concurrent job

High performance
communication

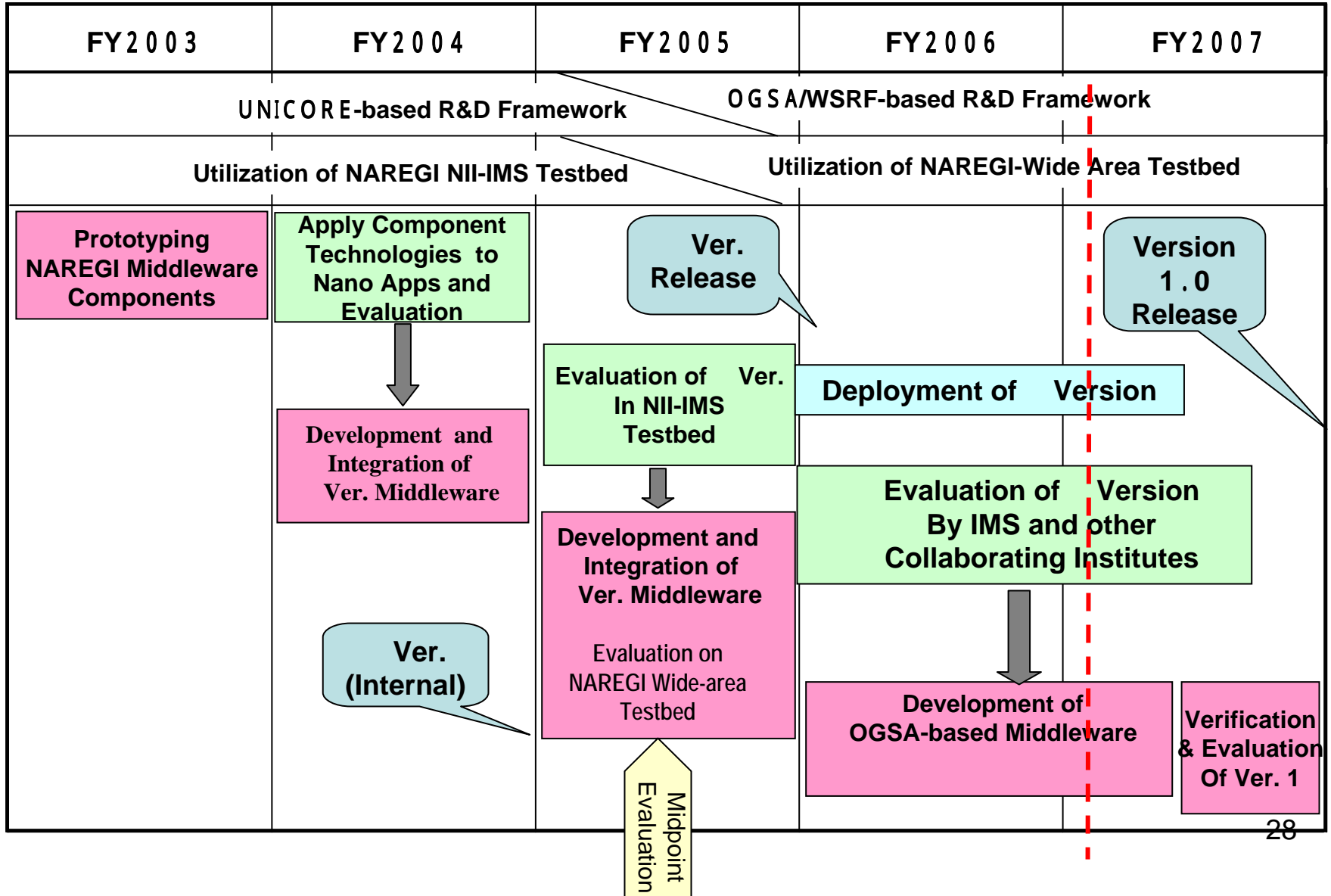
Support data
form exchange

5. User Tools

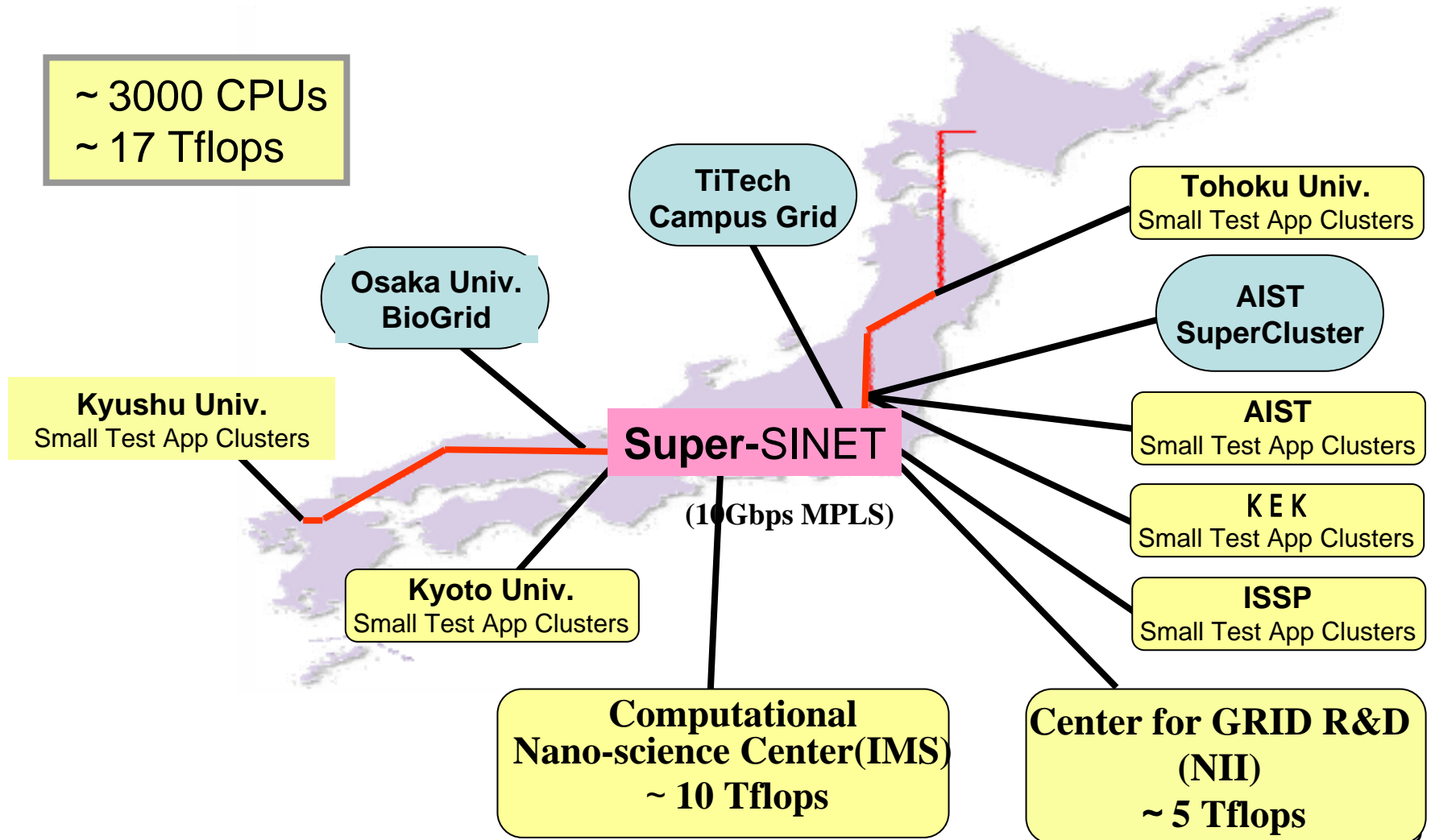
- Web based Portal
- Workflow tool w/NAREGI-WFML
- WS based application contents and deployment service
- Large-Scale Interactive Grid Visualization

A reference
implementation
of OGSA-ACS

Roadmap of NAREGI Grid Middleware

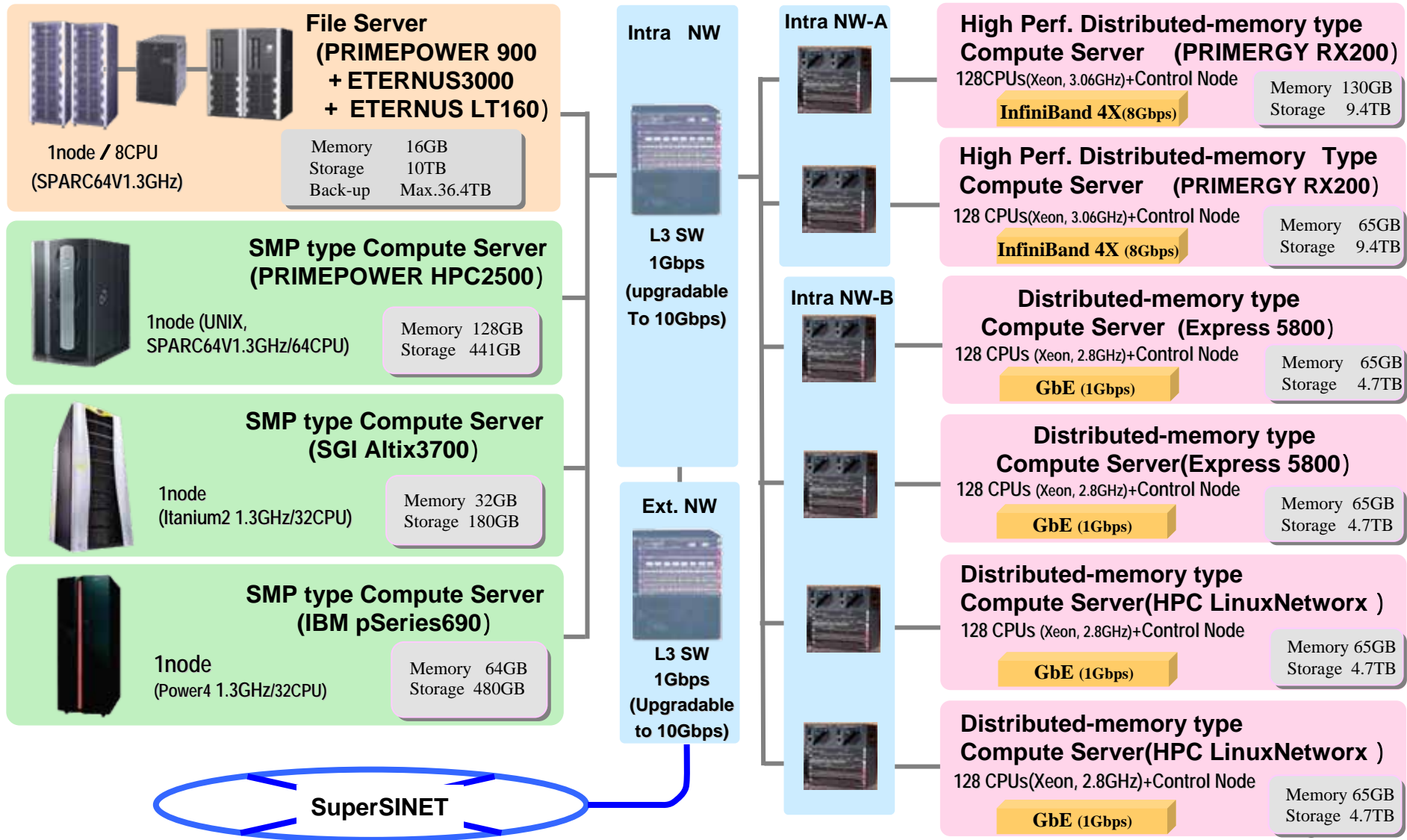


NAREGI Phase 1 Testbed



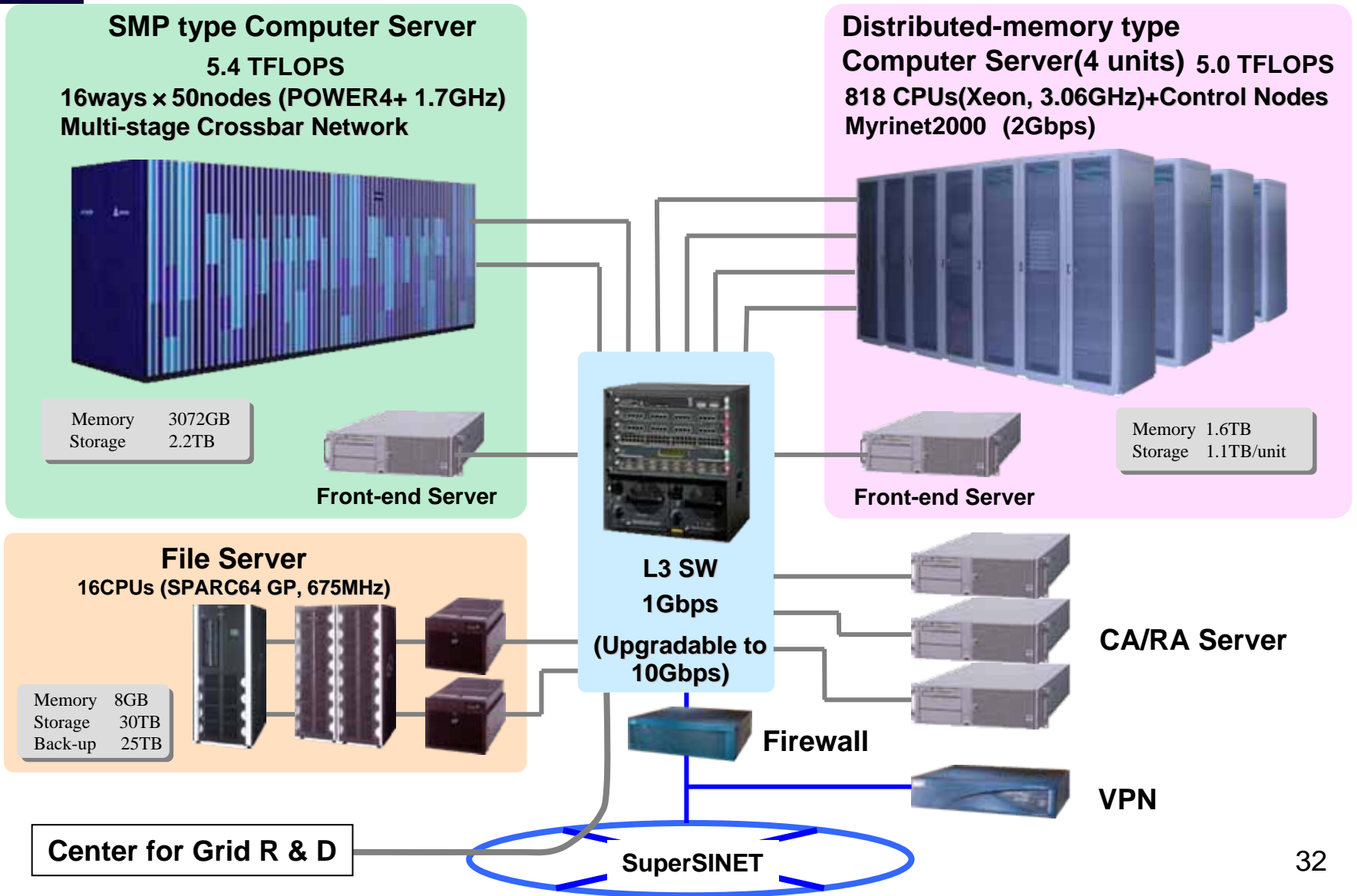


Computer System for Grid Software Infrastructure R & D Center for Grid Research and Development (5 Tflop/s , 700GB)



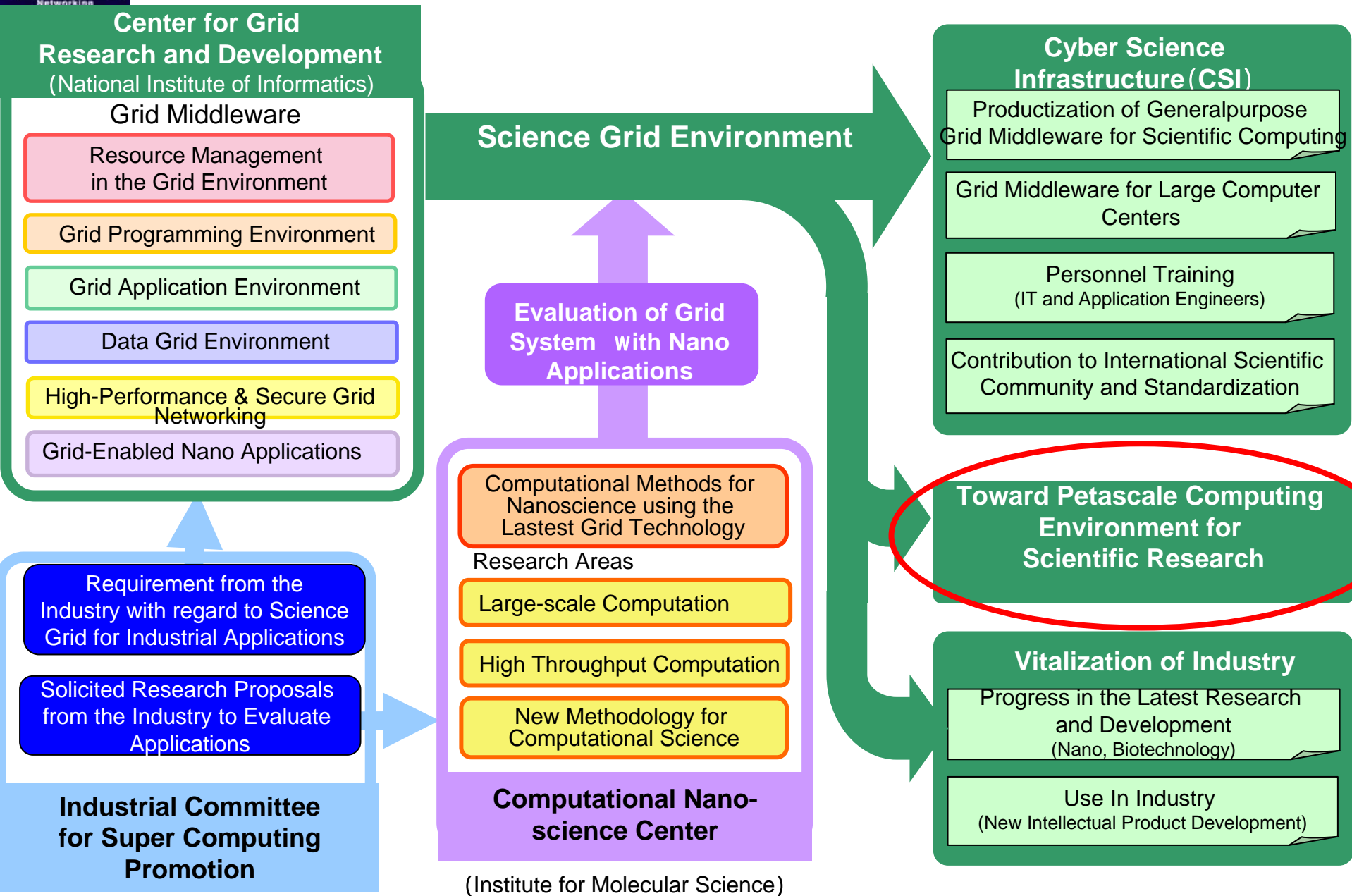
Computer System for Nano Application R & D

Computational Nano science Center (10 Tflop/s , 5TB)





Future Direction of NAREGI Grid Middleware



Current Schedule

FY		2006	2007	2008	2009	2010	2011	2012	
Operation						Start Operation	Full Operation		
	R&D								
Software	System Software	OS/Tools/GRID middleware Design & Production			Evaluation				
	Grand Challenge Application Software	Next Generation Nano-Science Simulation, Design & Production			Evaluation				
		Next Generation Life Science Simulation, Design & Production						Evaluation	
Hardware	Basic Design	Detail Design		Production		Enhancement			
File Systems and others			Design	Production		Enhancement			
Geographical investigation, Construction	Investigation	Design	Construction						



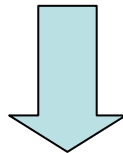
Outline

1. Next Generation Supercomputer Development Project
2. National Research Grid Initiative (NAREGI)
3. **Cyber Science Infrastructure (CSI)**

Cyber Science Infrastructure: background

- A new information infrastructure is needed in order to boost today's advanced scientific research.
 - **Integrated information resources and system**
 - Supercomputer and high-performance computing
 - Software
 - Databases and digital contents such as e-journals
 - “Human” and research processes themselves
 - **U.S.A: Cyber-Infrastructure (CI)**
 - **Europe: EU e-Infrastructure (EGEE,DEISA,....)**
- **Break-through in research methodology is required in various fields such as nano-Science/technology, bioinformatics/life sciences,...**
 - **the key to industry/academia cooperation:**

from ‘Science’ to ‘Intellectual Production’



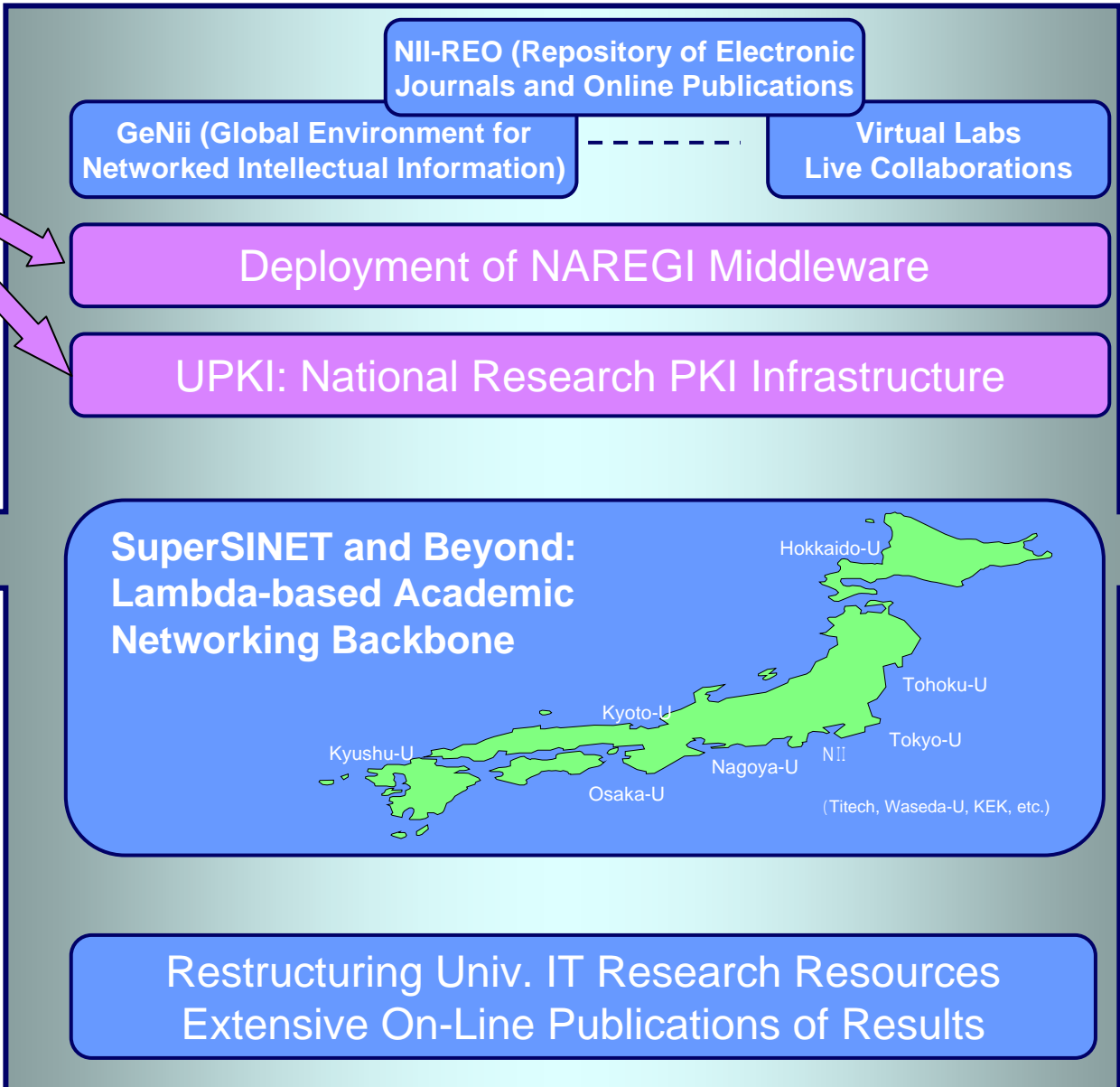
Advanced information infrastructure for research will be the key in international cooperation and competitiveness in future science and engineering areas

A new comprehensive framework of information infrastructure in Japan

Cyber Science Infrastructure

Cyber-Science Infrastructure for R & D

Cyber-Science Infrastructure (CSI)

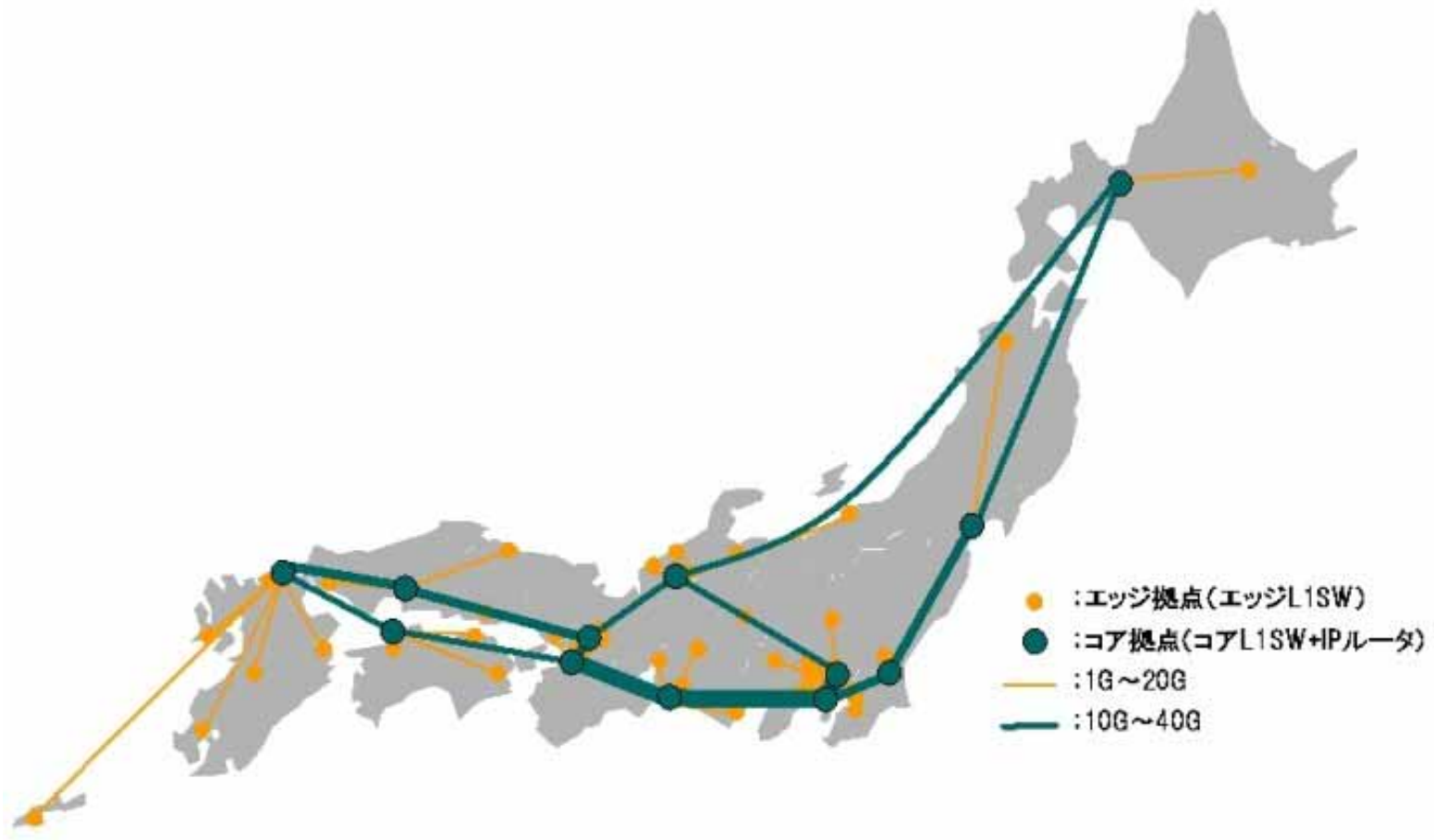


NAREGI
Outputs

Industry/Societal Feedback

International Infrastructural Collaboration

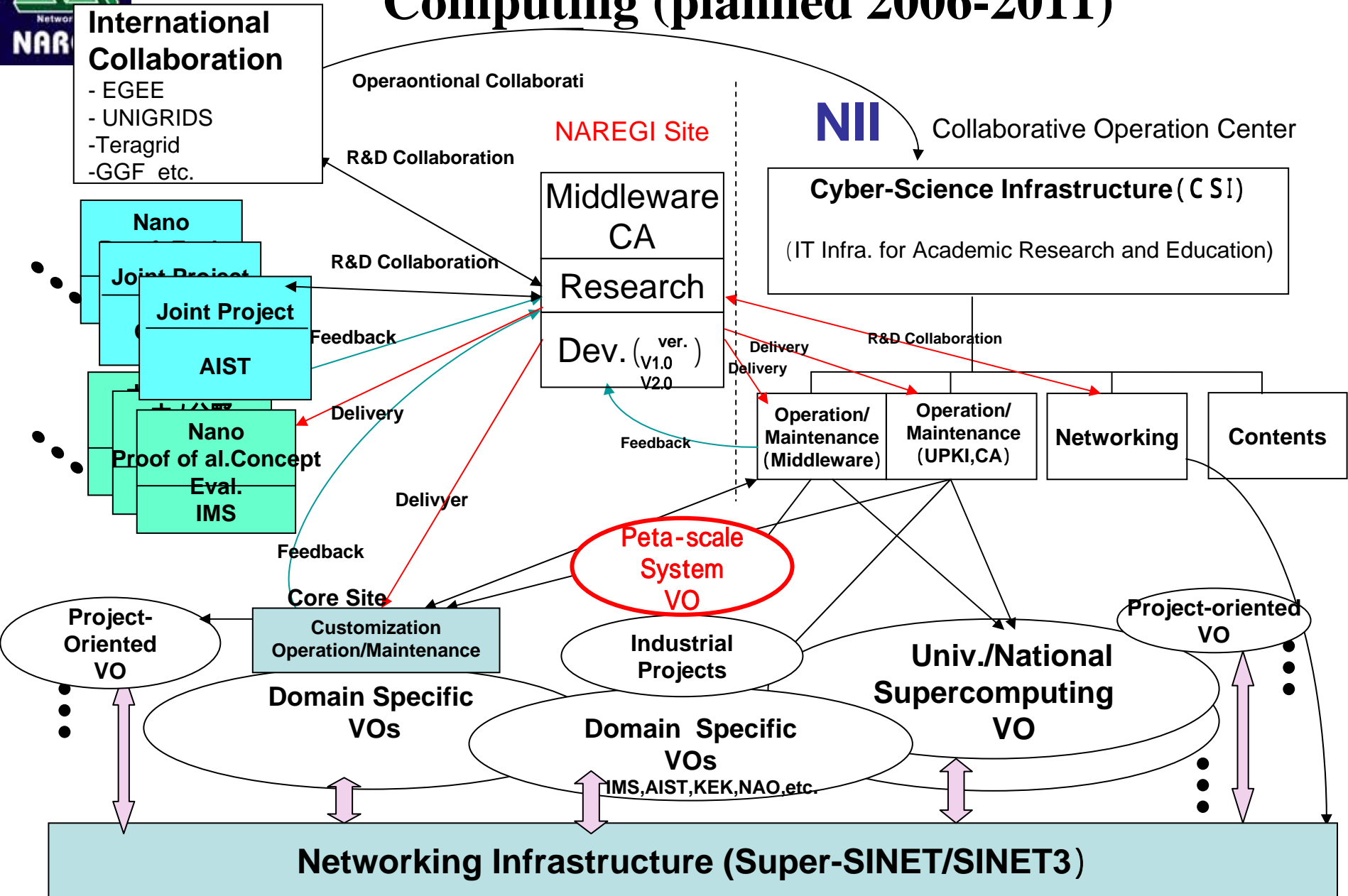
SINET3 Network Topology (FY2007 -)



10Gbps → 40Gbps



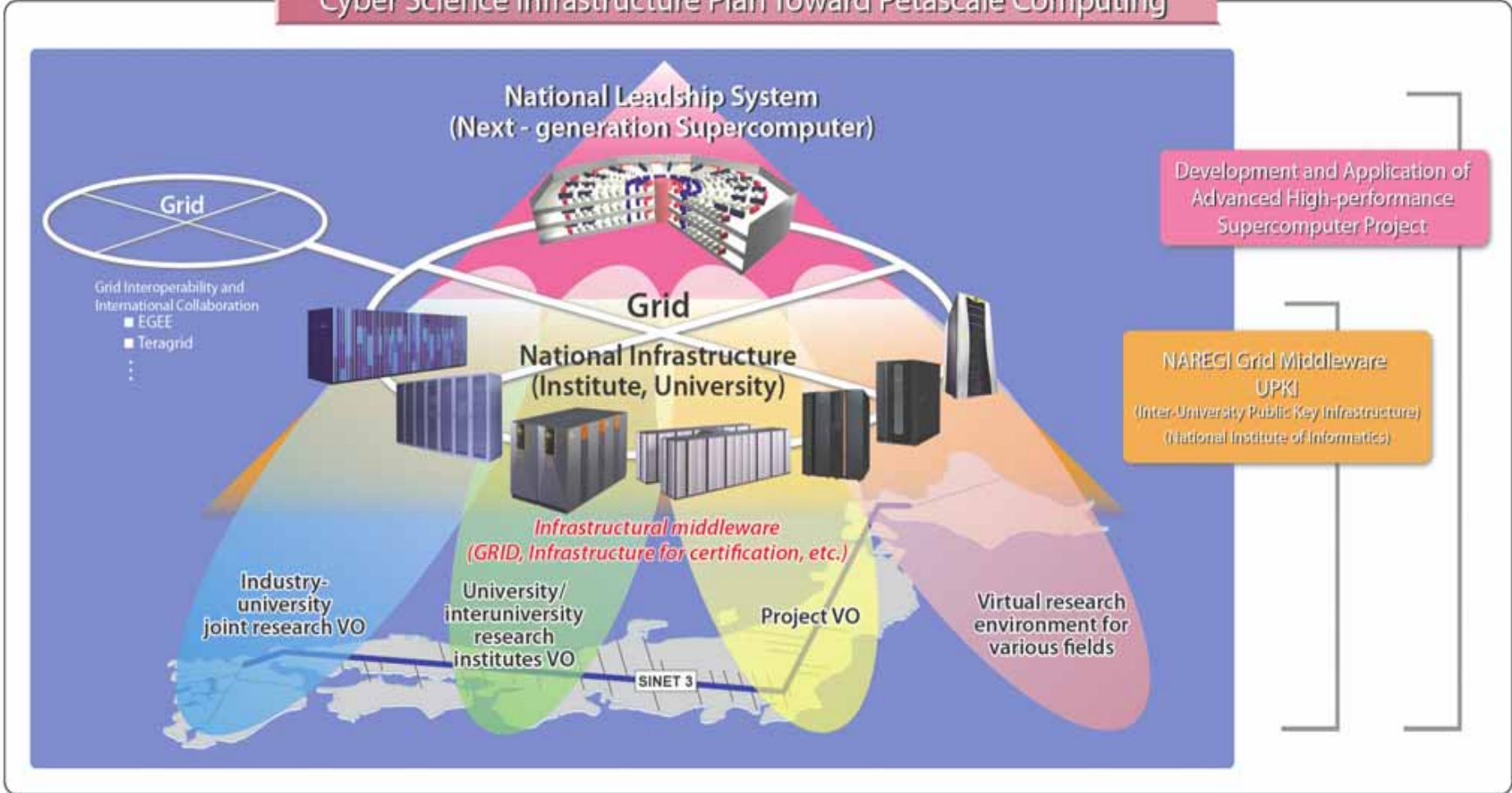
Cyber Science Infrastructure toward Petascale Computing (planned 2006-2011)



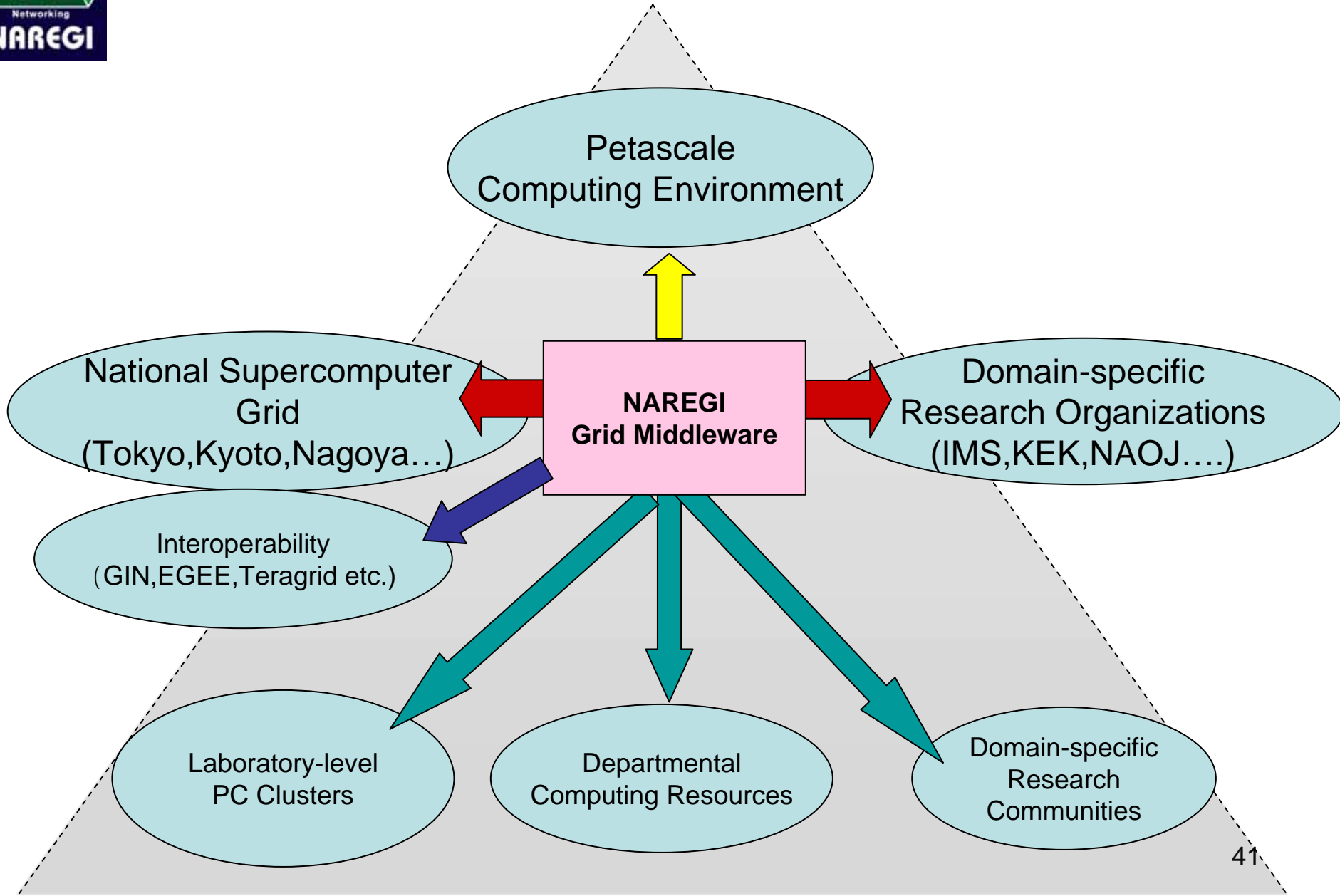
Note: names of VO are tentative)

Cyber Science Infrastructure

Cyber Science Infrastructure Plan Toward Petascale Computing



Expansion Plan of NAREGI Grid



Summary

- The **3rd Science and Technology Basic Plan** started in April 2006.
- The **Next Generation Supercomputer Project** (FY2006-2012, ~1B\$) is one of the high priority projects, aimed at the peta-scale computation in the key application areas.
- NAREGI Grid middleware will enable seamless federation of heterogeneous computational resources.
- Computations in Nano-science/technology applications over Grid is to be promoted, including participation from industry.
- NAREGI will provide the access and computational infrastructure for the **Next Generation Supercomputer System**.
- NAREGI Grid Middleware is to be adopted as one of the important components in the new **Japanese Cyber Science Infrastructure Framework**.



Thank you!



<http://www.naregi.org>