Building the CyberScience Infrastructure Community in NAREGI

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Tokyo Inst. Technology
& NAREGI Project National Inst. Informatics

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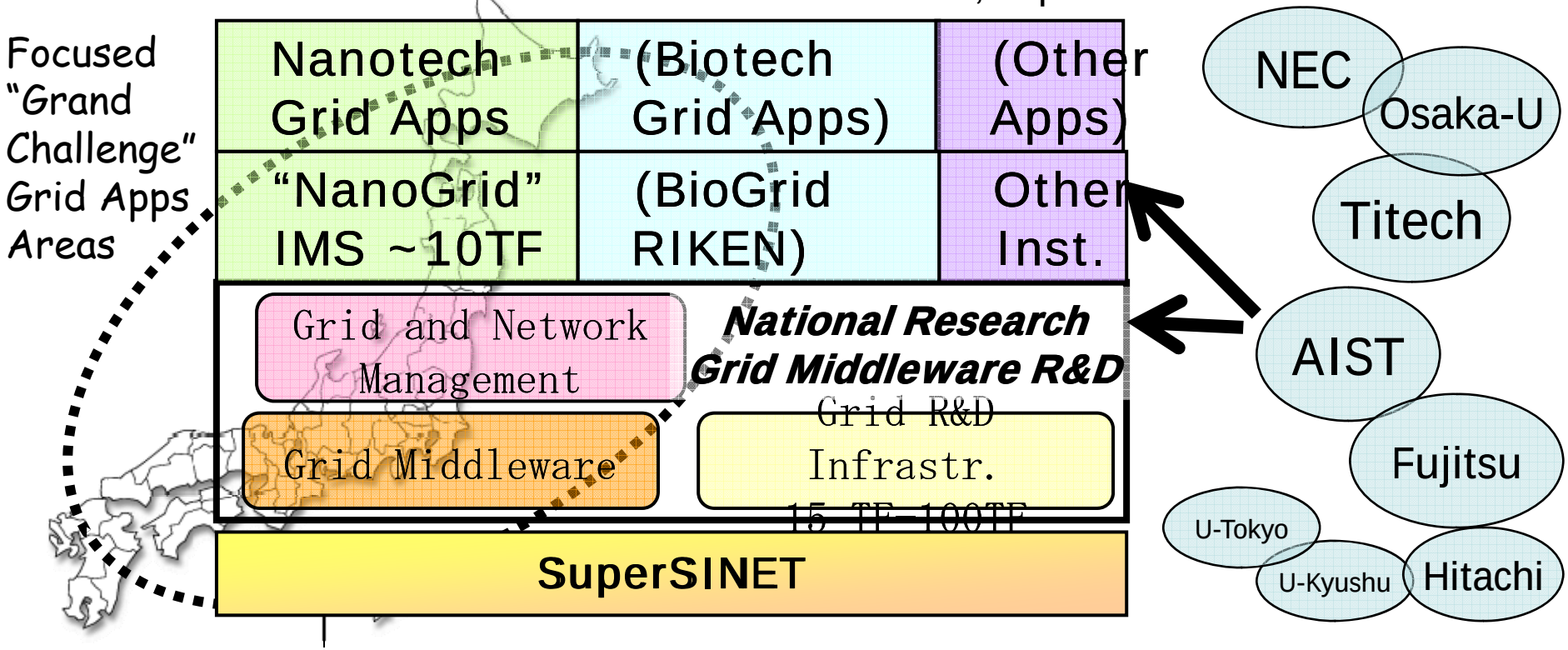
OGF20 Campus & Community Grid Workshop
Manchester, UK

TSUBAME (Swallow)

National Research Grid Infrastructure (NAREGI) 2003-~~2007~~ 2010

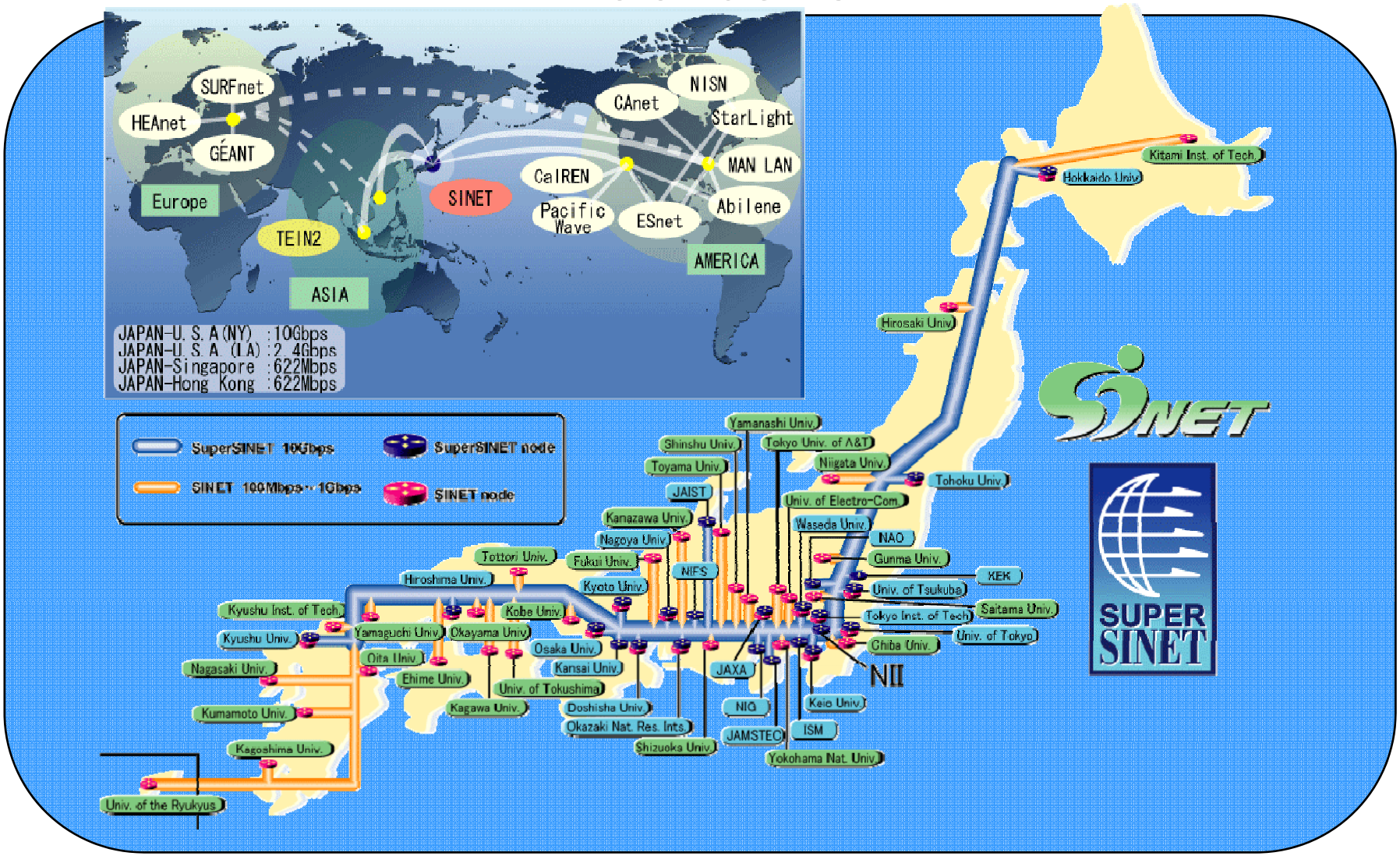
--- A Core of Japanese CyberScience Infrastucture (CSI) ---

- Petascale Grid Infrastructure R&D for Future Deployment
  - > $120 mil total over 8 years
  - Now part of Japanese 10 petascale computing initiative
  - Hosted by National Institute of Informatics (NII)
  - PL: Ken Miura (NII), Co-PI: Kento Aida (new) (NII), S. Sekiguchi(AIST), S. Matsuoka(Titech), S. Shimojo(Osaka-U), M. Aoyagi (Kyushu-U)…
  - Participation by multiple (>= 3) vendors, Fujitsu, NEC, Hitachi, NTT, etc.
  - Follow and contribute to GGF Standardization, esp. OGSA

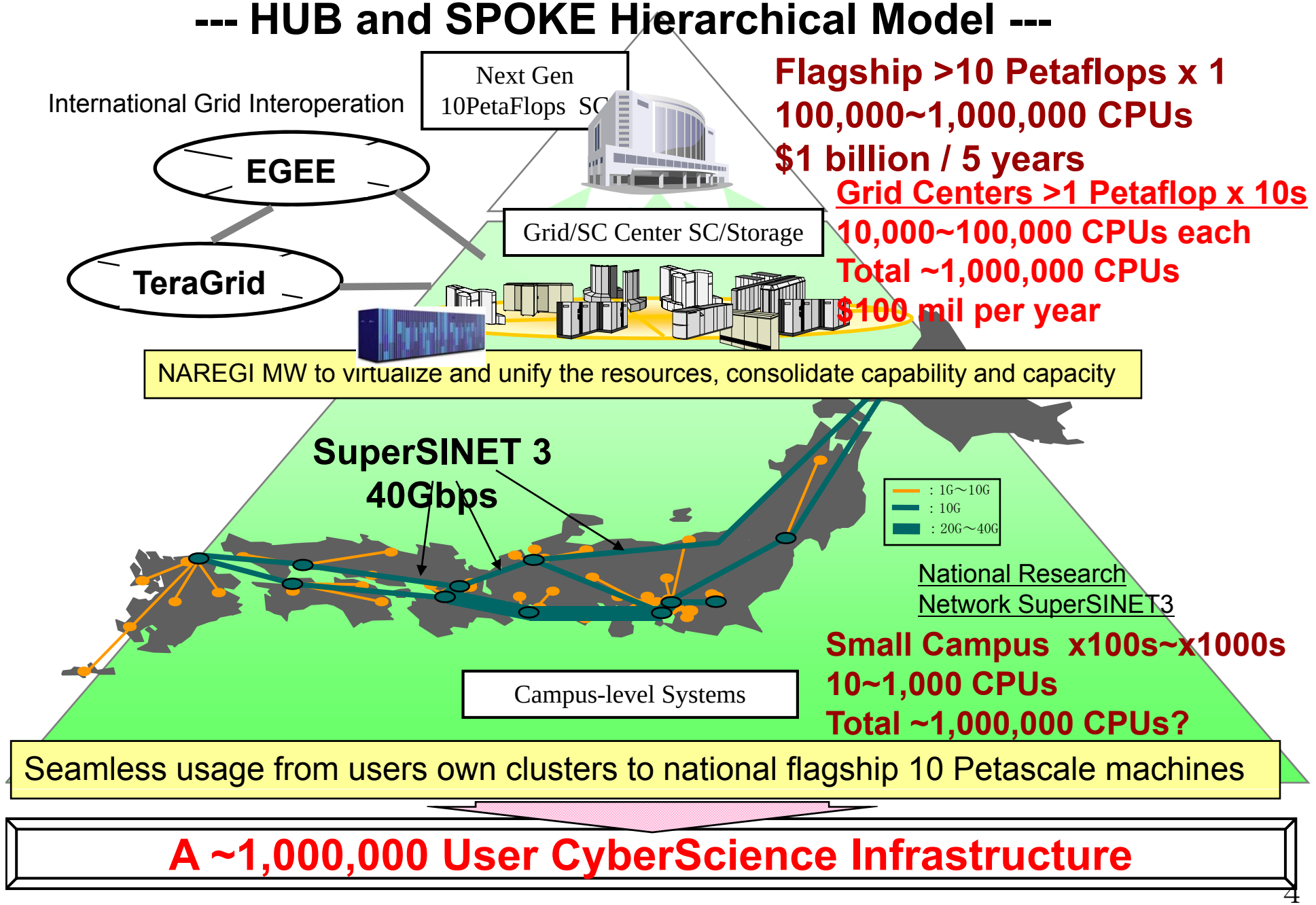


Super SINET3 (new!)

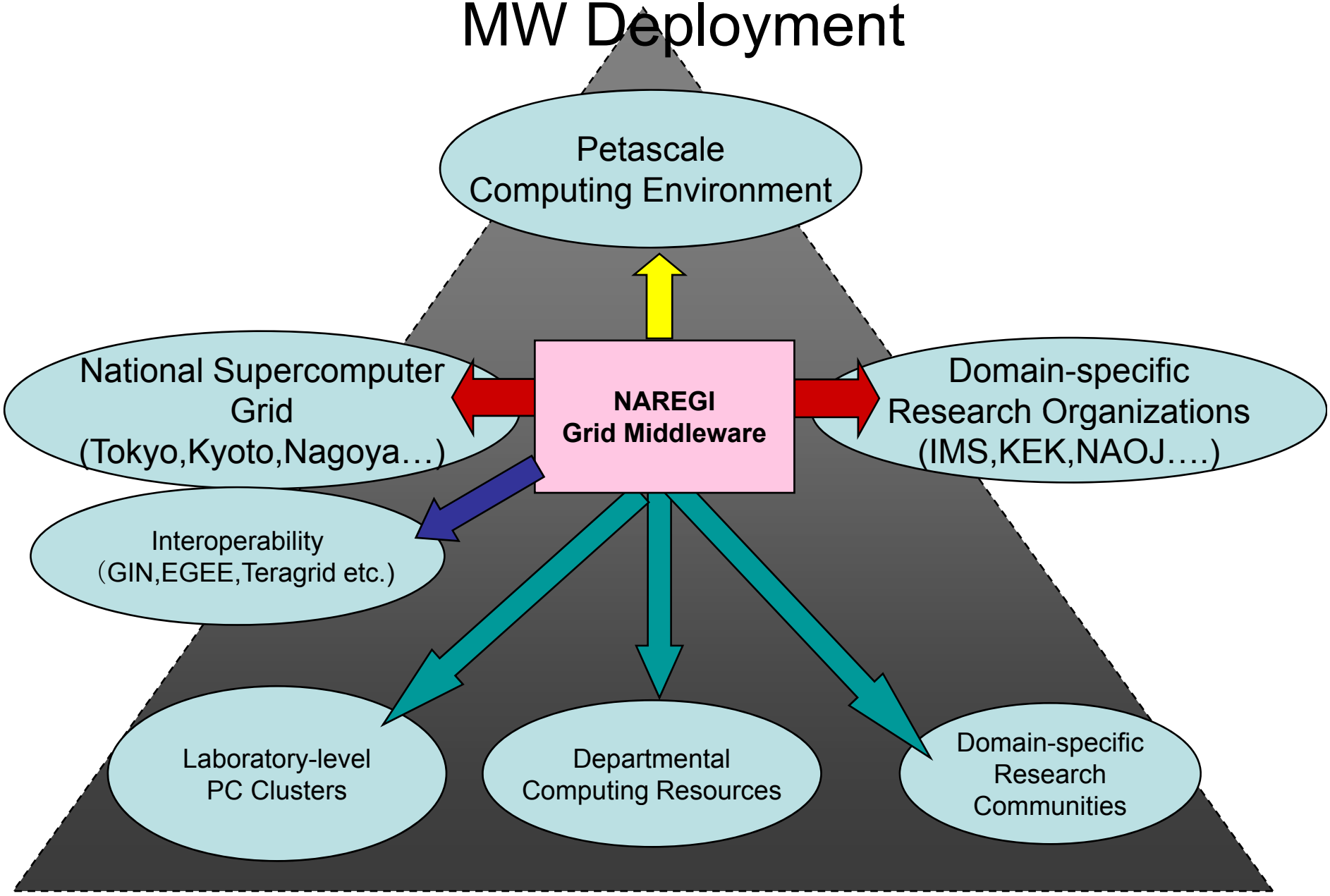
Dynamic L1/L2/L3 provisioning 40 Gbps Backbone



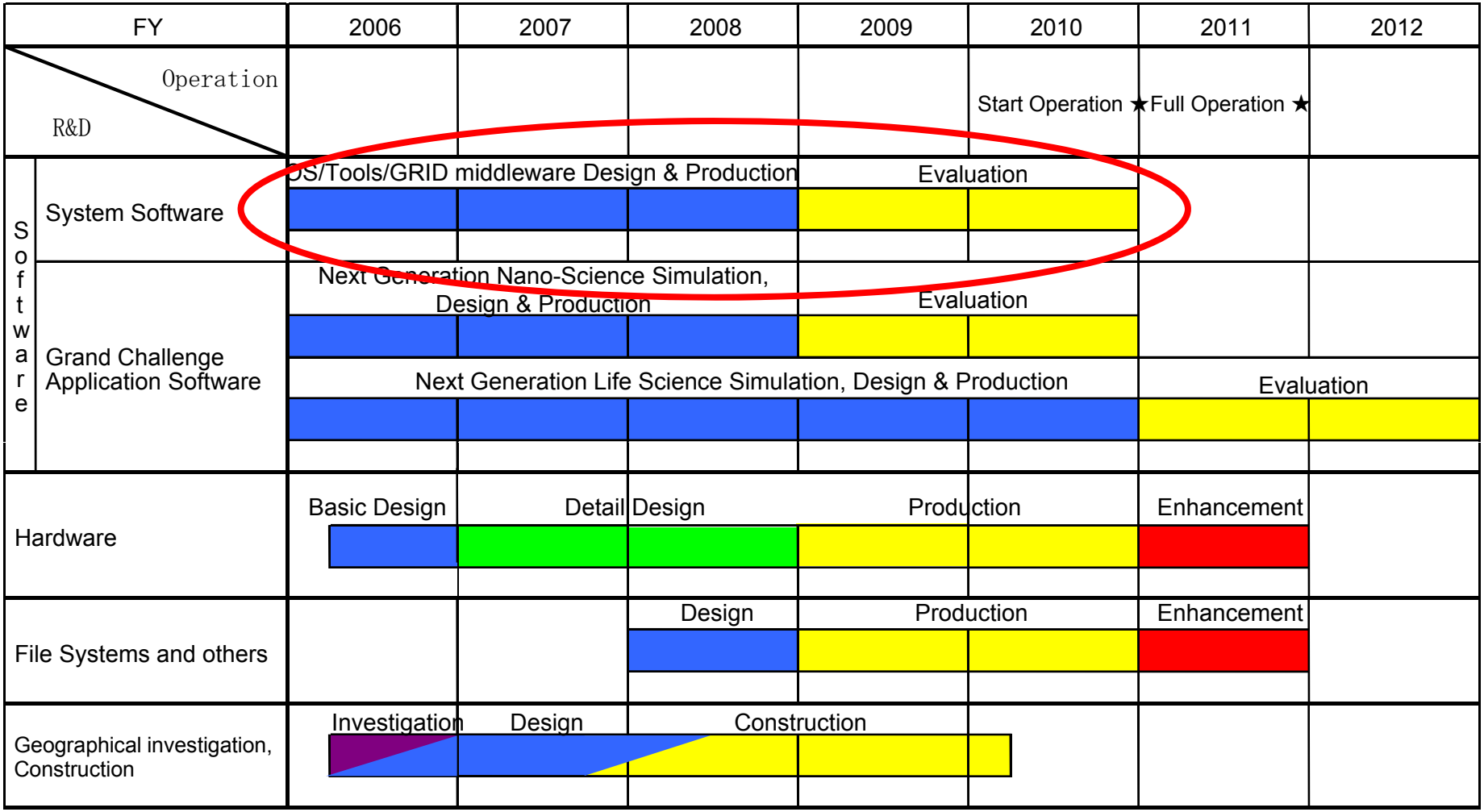
CSI Tier-Model of Next Generation Grid/SC Infrastructure
--- HUB and SPOKE Hierarchical Model ---



CyberScience Infrastrucuture and NAREGI MW Deployment

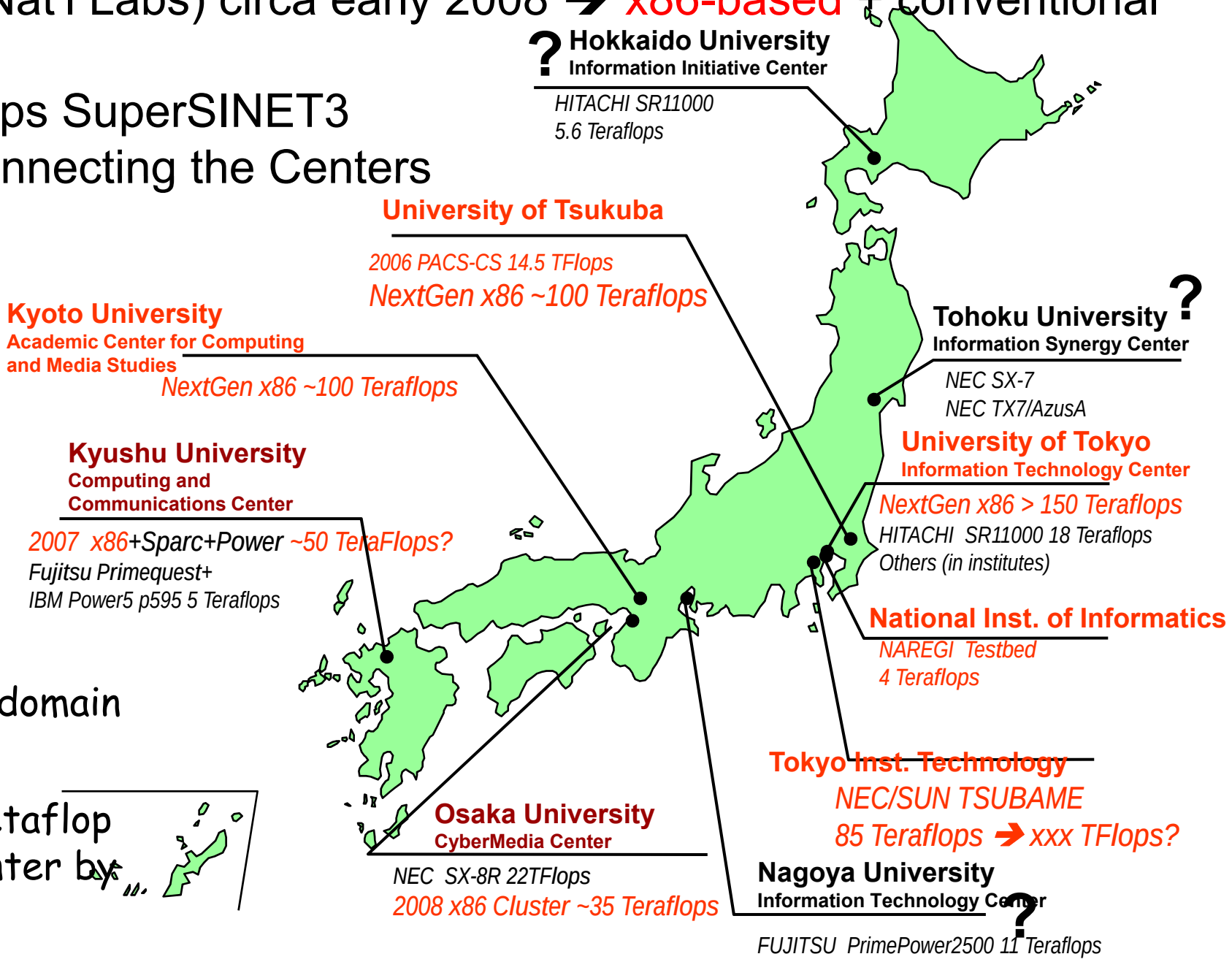


Next Generation Supercomputer Development Project (Current Schedule)



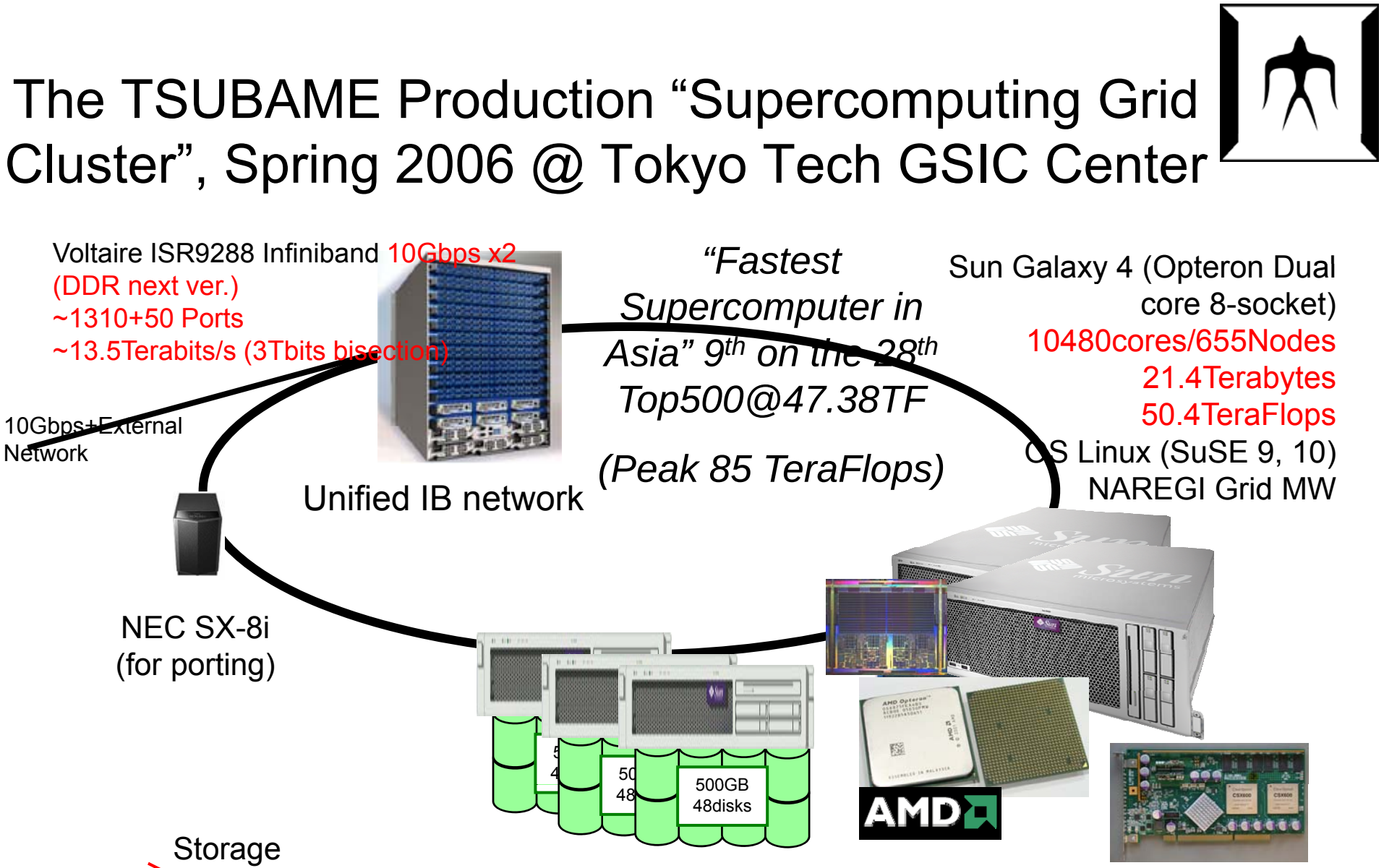
Japan's 9 Major University Computer Centers (excl. Nat'l Labs) circa early 2008 ➔ x86-based + conventional

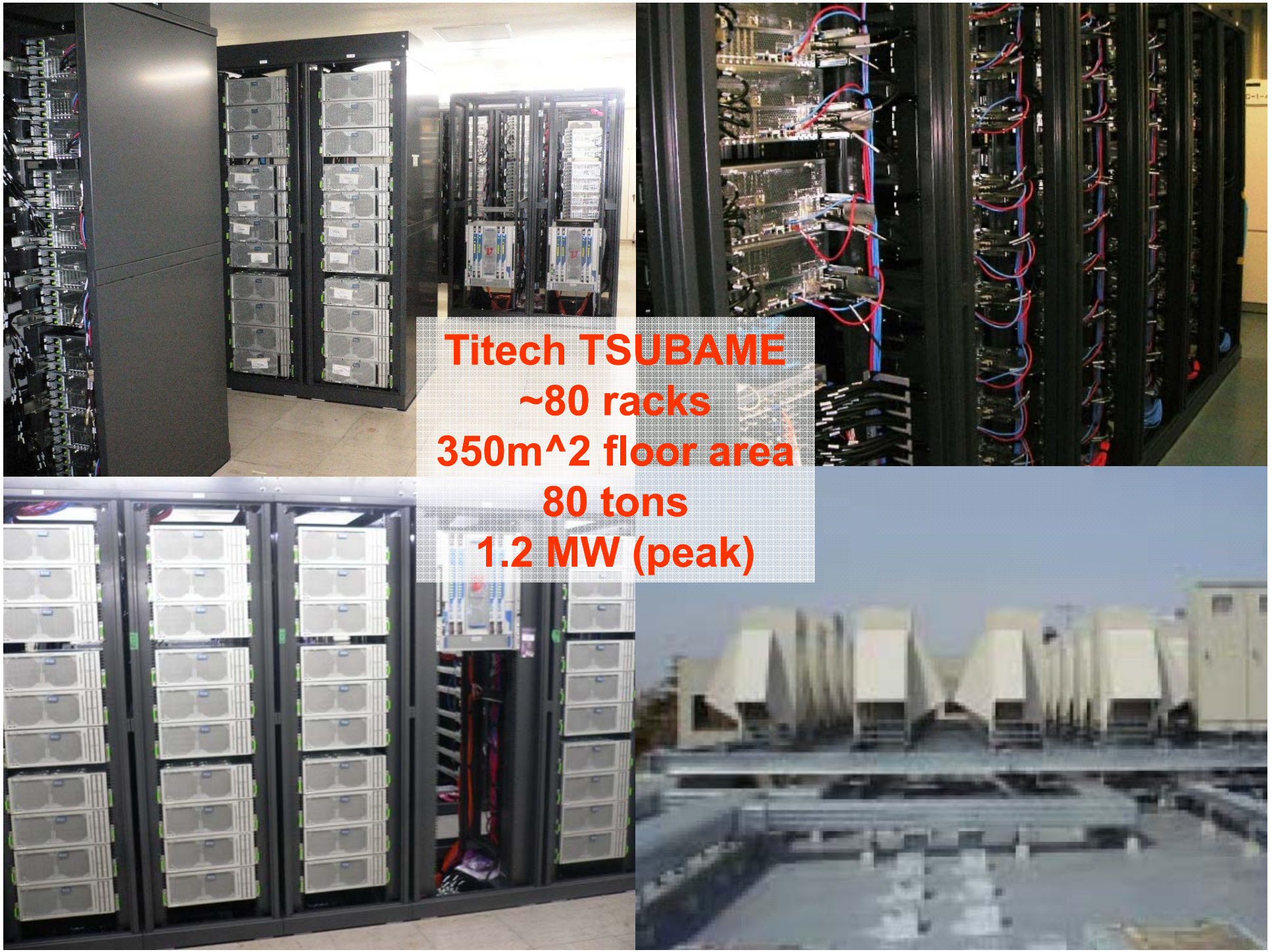
>40Gbps SuperSINET3 Interconnecting the Centers



- Other domain centers
- ~ 10 Petaflop NLP center by 2012

The TSUBAME Production "Supercomputing Grid Cluster", Spring 2006 @ Tokyo Tech GSIC Center




Titech TSUBAME
~80 racks
350m^2 floor area
80 tons
1.2 MW (peak)

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TITECH GRID

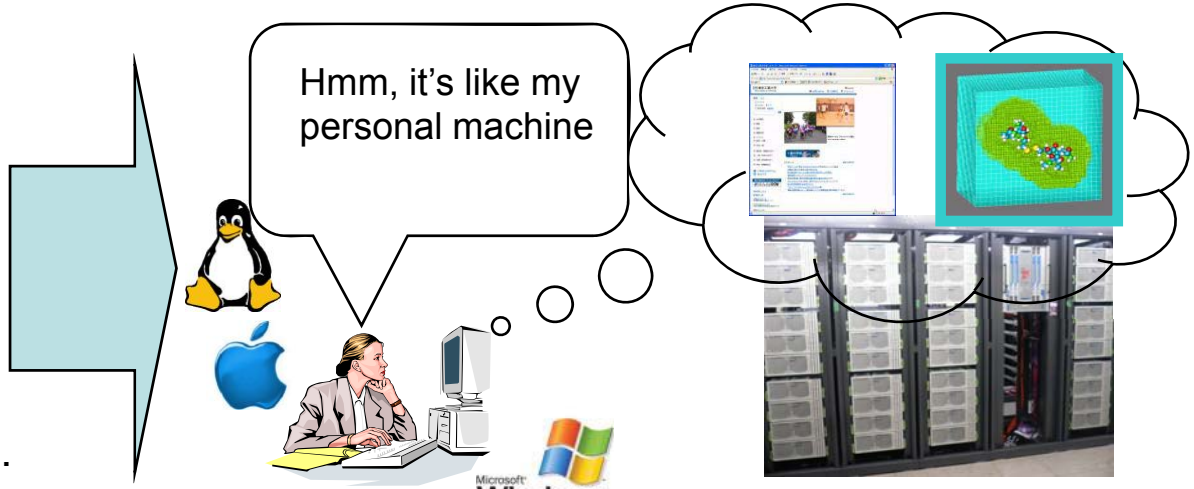
"Everybody's Supercomputer" as core of Campus Grid and IT Consolidation

Isolated High-End

Massive Usage Env. Gap

- Different usage env. from
- No HP sharing with client's PC
- Special HW/SW, lack of ISV support
- Lack of common development env. (e.g. Visual Studio)
- Simple batch based, no interactive usage, good UI

Seamless integration of SCs with *end-user and Enterprise Env.*



"Everybody's Supercomputer"

Seamless,Ubiquitous access and usage

=>Breakthrough Science through Commoditization of Supercomputing and Grid Technologies

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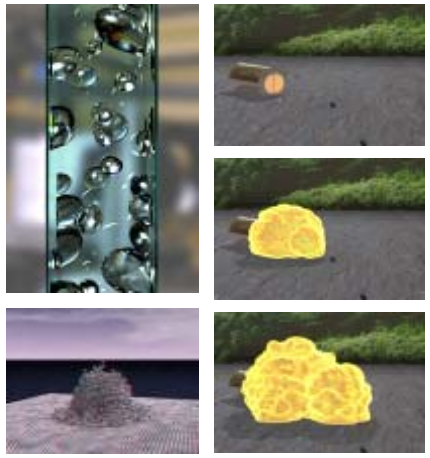
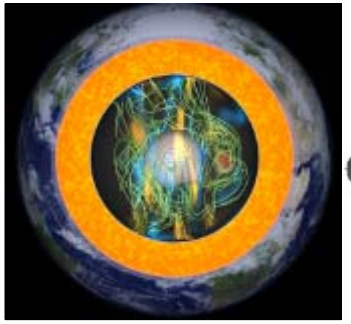
Grand Challenge Supercomputing @ Titech

100 Teraflops-scale computing with Petascale Storage

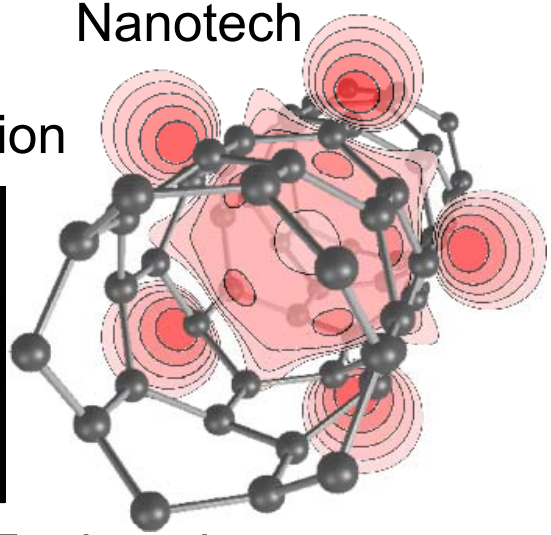
CFD



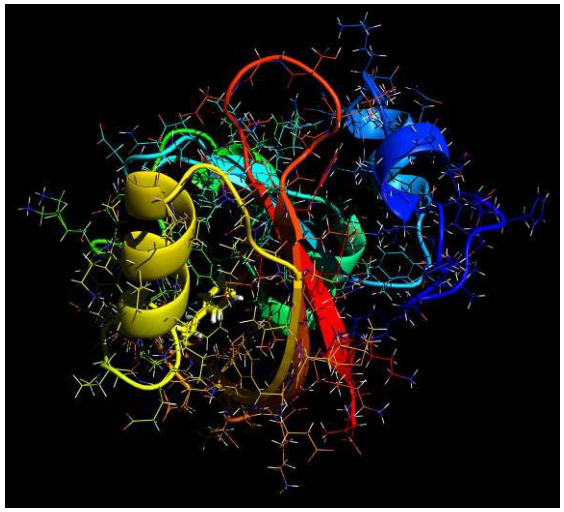
EMF Simulation



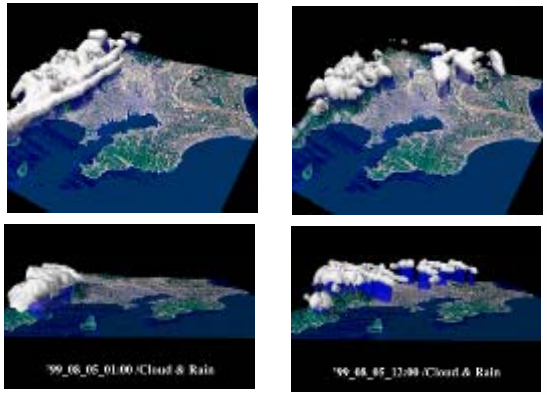
Nanotech



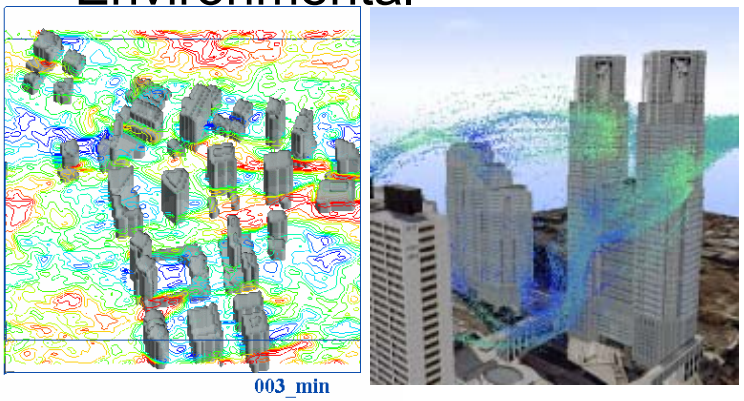
Bioinformatics



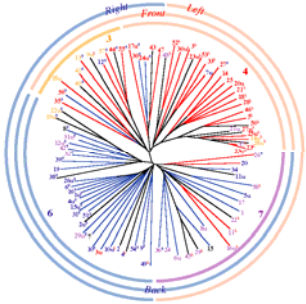
Weather Prediction



Civil Engineering
Environmental



Bio-simulation
+ Bioinformatics



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TITECH GRID

TSUBAME General Purpose DataCenter Hosting

As a core of IT Consolidation

All University Members == Users

No more private servers & clusters in closets

> 10,000 users on campus

- Various Application Portals for Edu and Research
- Campus-wide AAA Sytem (April 2006)
  - 50TB (for email), 9 Galaxy1 nodes
- Campus-wide Storage Service (NEST)
  - 10s GBs per everyone, Research Reposit
- CAI, On-line Courses (OCW)
- Administrative Hosting (VEST)

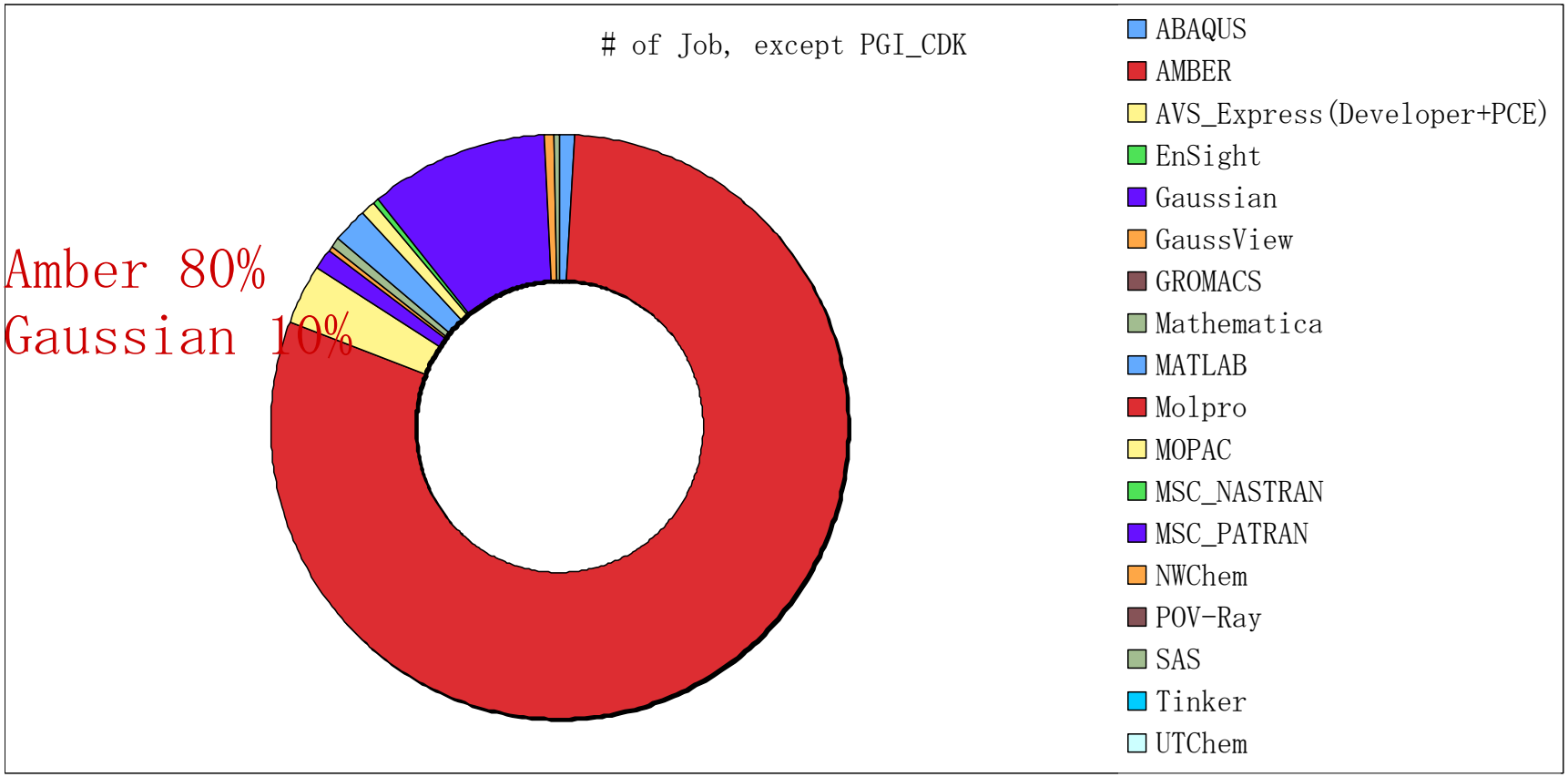
Titech Campus Grid 2006
- An x86 “DataCenter” Grid -

- **~13,000 CPUs, 90 TFlops, ~26 TBytes Mem, ~1.1 PBytes HDD**
- ***All Hosted at GSIC: No more private servers & clusters in closets, same as the modern Internet***

TSUBAME Application Profile

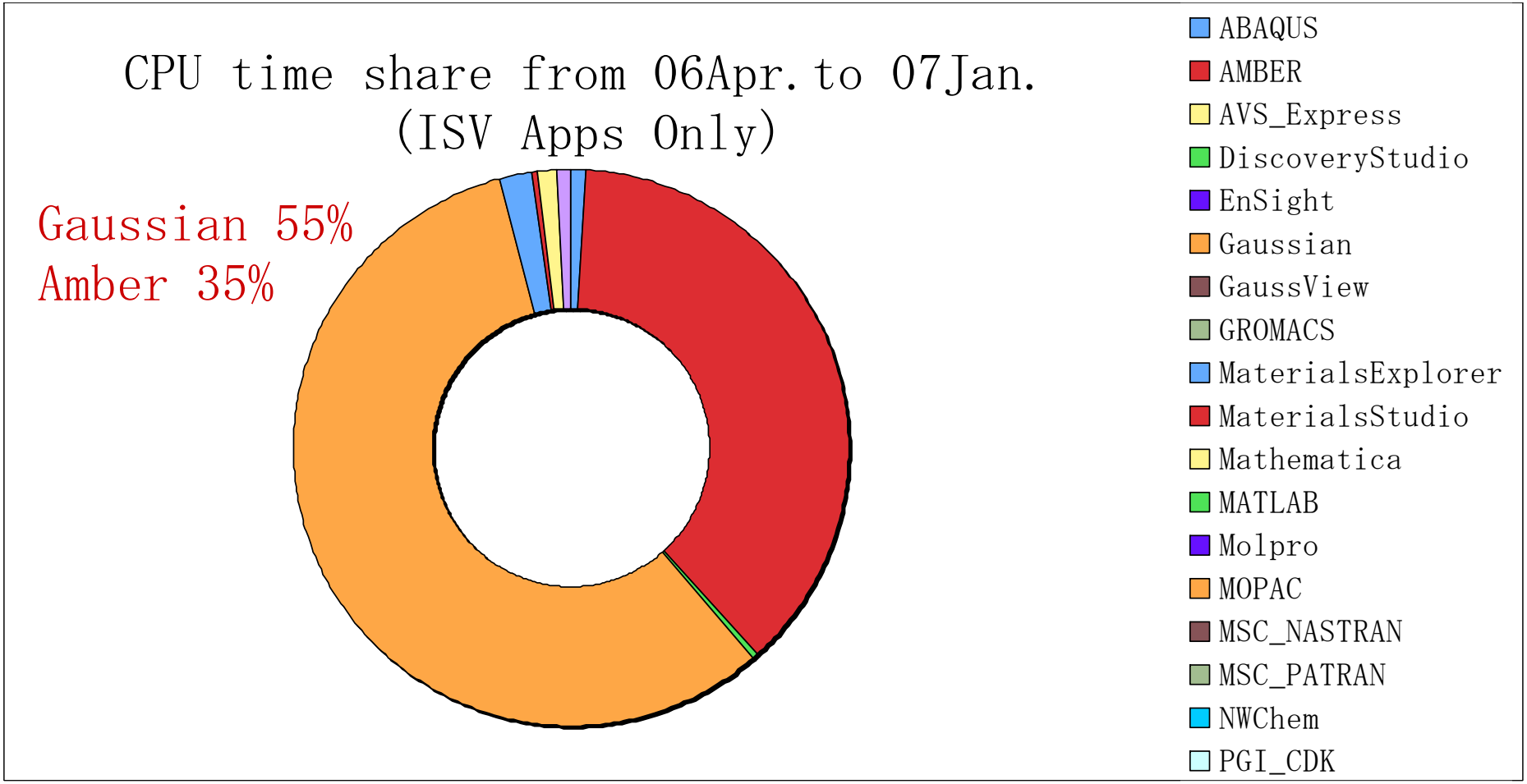
- Large scale codes, e.g. port from the Earth Simulator
  - Simple porting is easy
  - Tuned Vector code into cache-friendly "normal code" takes more time.
- Large-Scale (>1,000~10,000 instances) Parameter Survey, Ensemble, Optimization, …
- Lots of ISV Code---Gaussian, Amber, …
- Storage-Intensive Codes --- Visualization
- => Often Limited by Memory, not CPUs
- Must Give users both EASE and COMPELLING REASON to use TSUBAME and the Grid Infrastructure thereof

TSUBAME Job Statistics for ISV Apps (# Processes)



1,363,374 Processes (ISV only, excl. PGI_CDK)
Approx. 5000~10,000/day (via Sun GridEngine)

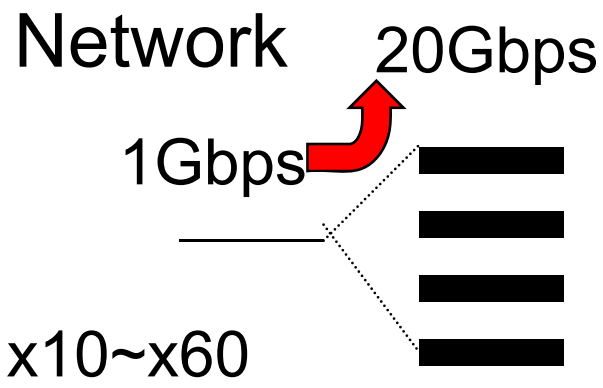
TSUBAME Job Statistics for ISV Apps (# CPU Timeshare)

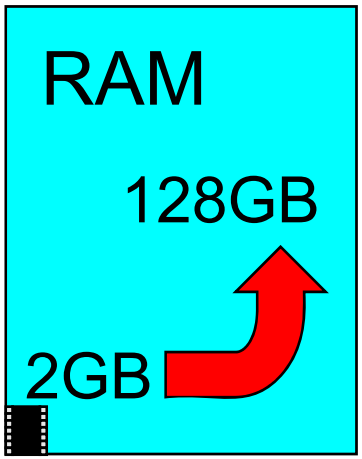


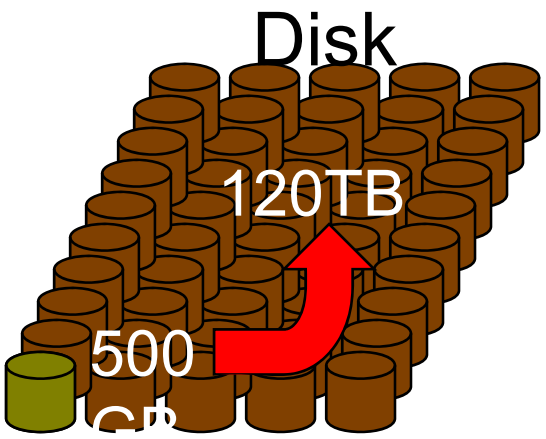
Why Industries are interested in TSUBAME (and other SCs on Grid)?

- Standard Corporate x86 Cluster Env. vs. TSUBAME -

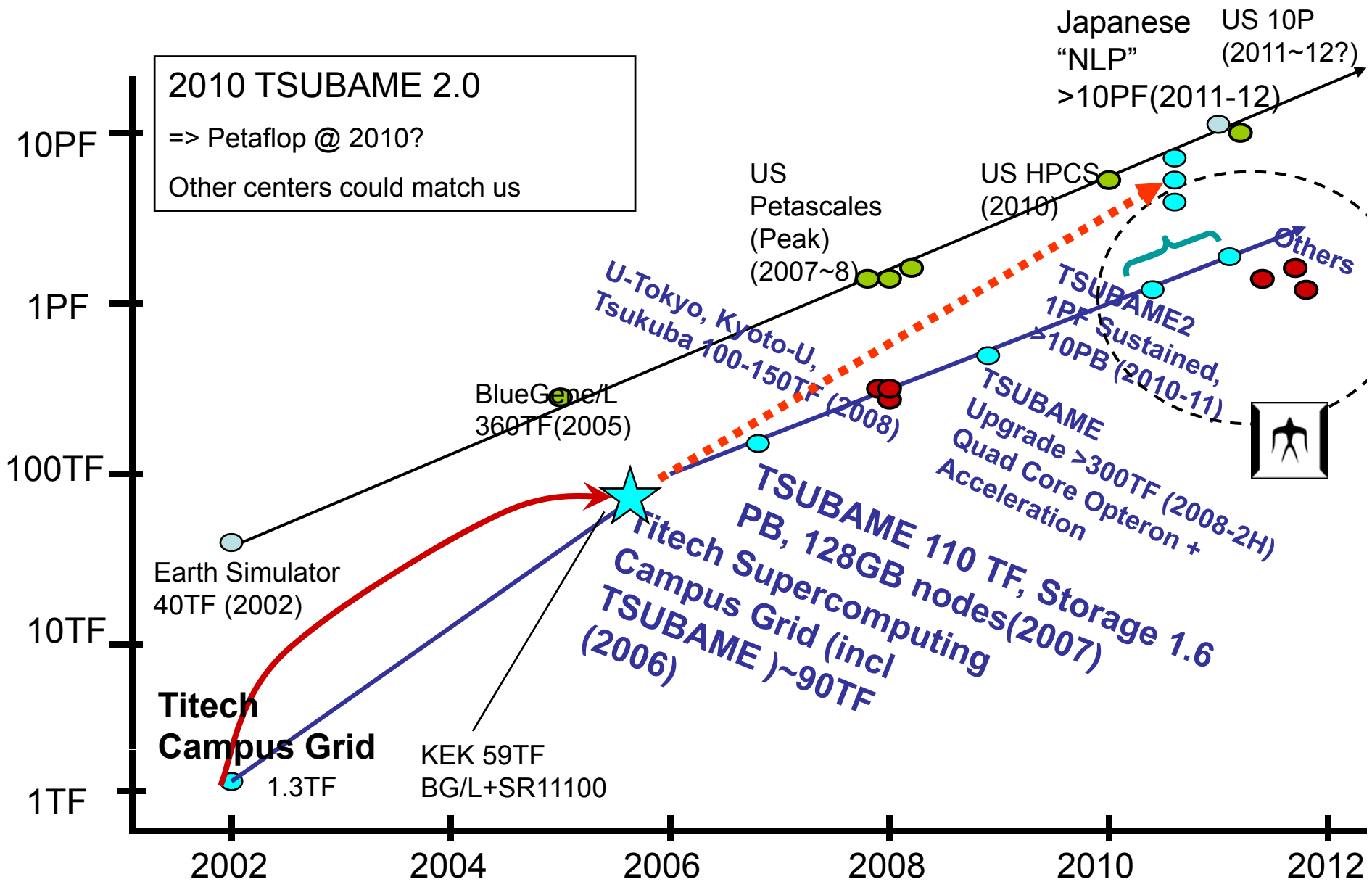
	CPU Core	Network	RAM	Disk(Cap, BW)
Std.	2~4 (node) 32~128 (job)	1Gbps 32Gbps	2~8GB 128GB	500GB, 50MB/s 10TB(NAS), 100MB/s
TSUBAME	16 (node) 1920 (job)	20Gbps 2.5Tbps	32~128GB 3840GB	120TB, 3GB/s 120TB, 3GB/s







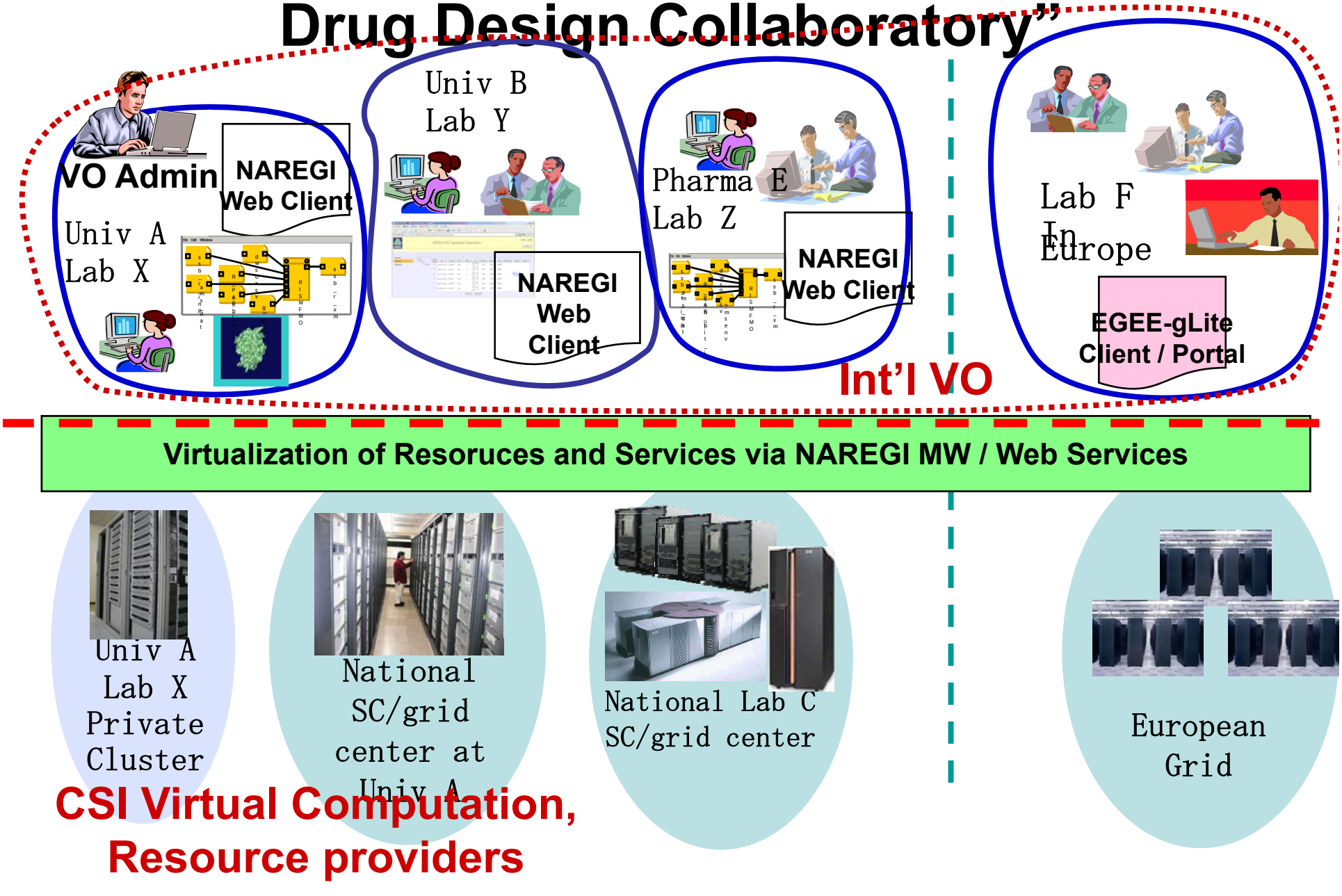
Scaling Towards Petaflops



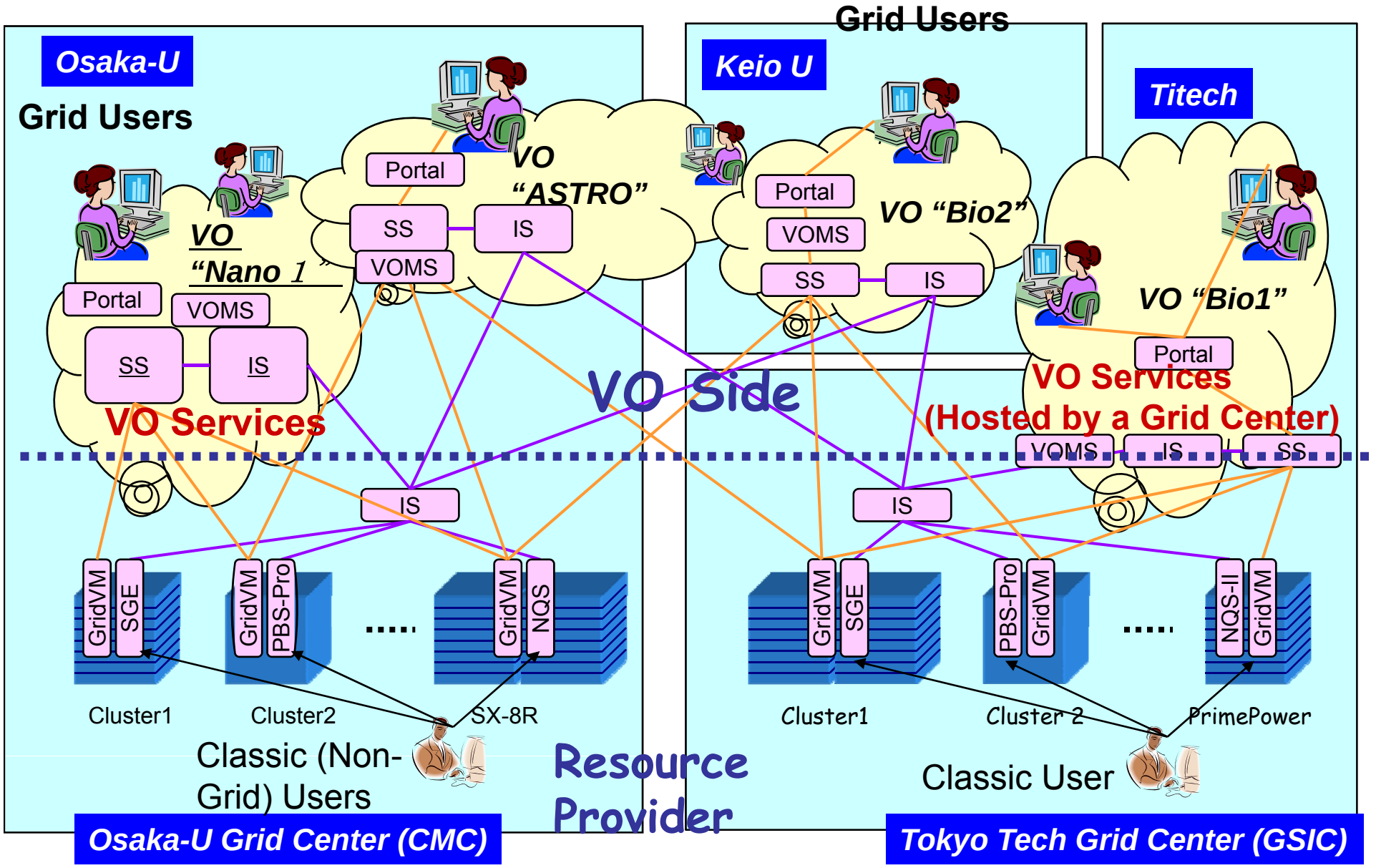
VO Operations in the CyberScience Infrastructure (CSI)

- A individual-globally identifiable ID
  - Everyone MUST have a verifiable electrical ID
  - UPKI (University PKI) effort in CSI, Shibboleth, etc.
- VO's register with a designated grid centers, just as one would register domains
  - Most cases, Grid centersw would host VO services
- I.e., SC/grid centers are resource providers as well as service providers for generic & VO-specific VO services (Web Services, Web DB, Web Portalなど)
  - Web 2 and beyond community hosting vision

CSI VO Vision Examle: “Int’l Computational Drug Design Collaboratory”



NAREGI β2 Operational Model



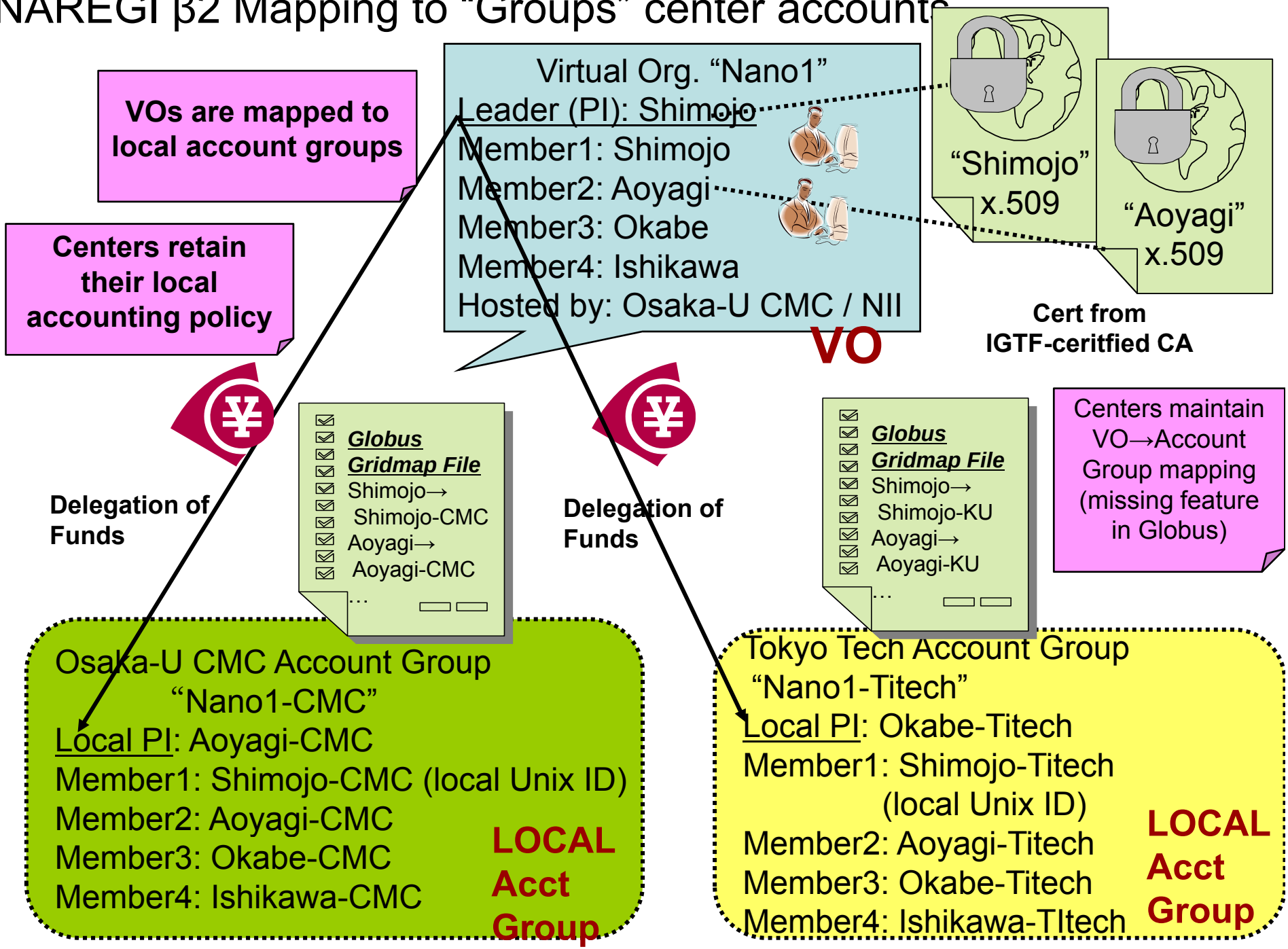
NAREGI β1 – Release May, 2006

- **Objective：Functional test for ver.1.0**
- Platform Shift (Unicore=> Globus 4-WSRF)
  - Set of WSRF (Web Services Resource Framework) Components
- OGF OGSA-EMS based resource management
  - Reservation/Co-Allocation/Co-Scheduling framework
- VO management built on EGEE-VOMS
- OGF-ACS WS application deployment
- Data grid features based on grid filesystem (GFarm)
- NAREGI-WFML description of complex workflow
  - Including co-scheduled resources
- GridMPI/GridRPC and other programming frameworks
- MyProxy-based Security and ID management w/session management, IGTF “ready”
- Being test-deployed, currently release 1.0.2
- Many many patches / bug fixes applied ☺

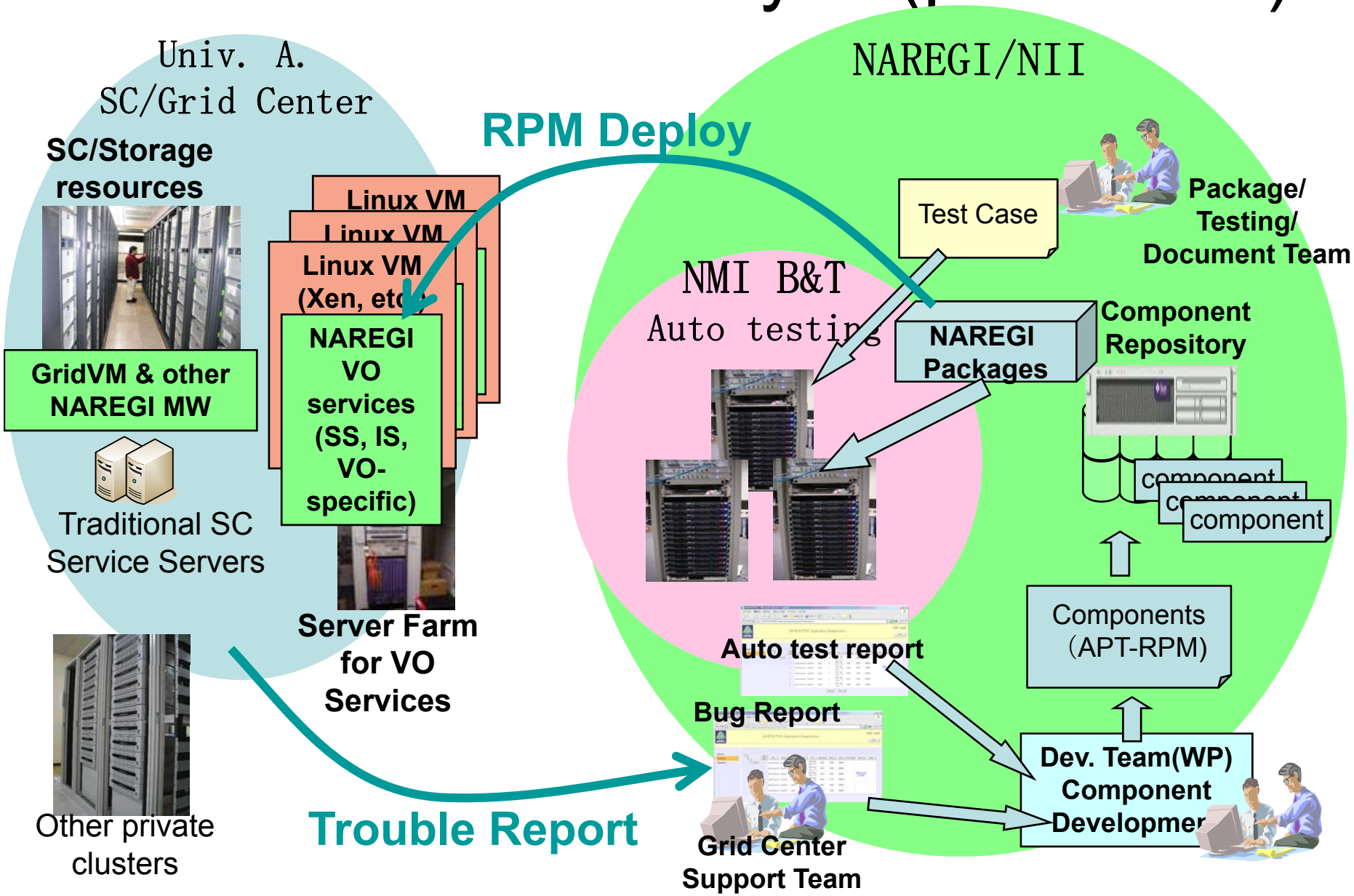
NAREGI Beta 2 - v.1.0 Highlights

- Beta2-Production Release Candidate (3Q 2007)
- Lots of bug, performance & stability fixes
- Stable WS(RF) components and APIs (+ Globus 4.0.3)
- RPM and Dynamic, VM-based deployment
- VO and “Resource Provider” decoupling for multiple VO management by VOs and Centers
- Integration of NAREGI WF and Ninf-G GridRPC
- More BQ and systems support (+PBS Pro, LoadLeveler)
  - NEC SX-NQS, SGE, Fujitsu NQS II… (Condor?)
- Flexible Job submission and WF management
  - Non-grid jobs, non-reserved jobs, various WF tools
- Various Data Tools and Infrastructures (w/EGEE interop)
- EGEE-GIN Interoperation (new)
- Various Administration and Logging Tools
- Support from dedicated NAREGI/NII support team
- Large-scale deployments @ Osaka-U, Titech... (beta2)

NAREGI β2 Mapping to "Groups" center accounts



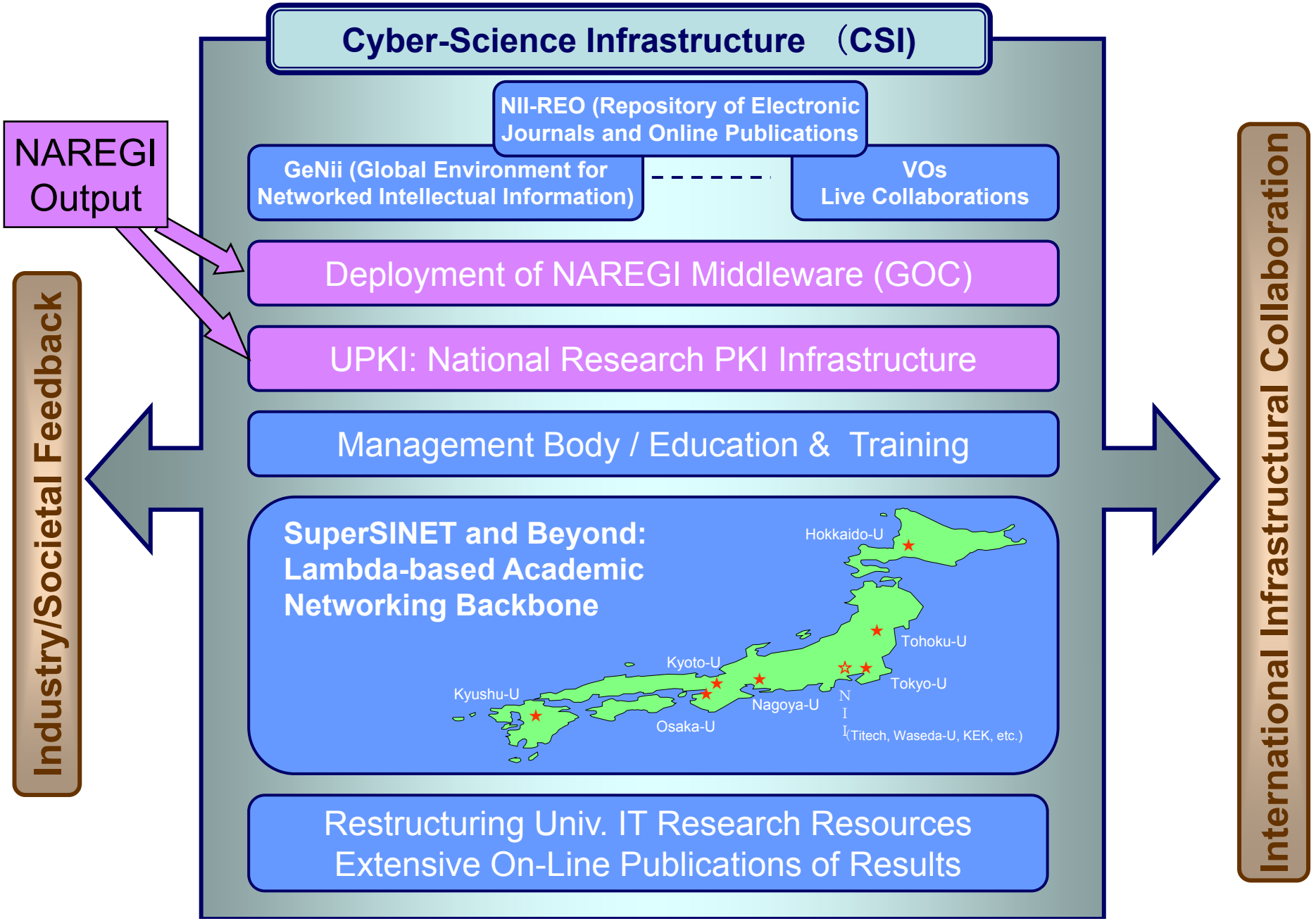
NAREGI MW Lifecycle(β2 and v1)



NAREGI EGEE Interoperation

- GLite ⇔ NAREGI MW Interoperation component as standard in NAREGI beta2 distribution
- Results of GIN Interoperation Efforts

Japanese CyberScience Infrastructure Project



Upscaling the Resources to a Petascale Grid

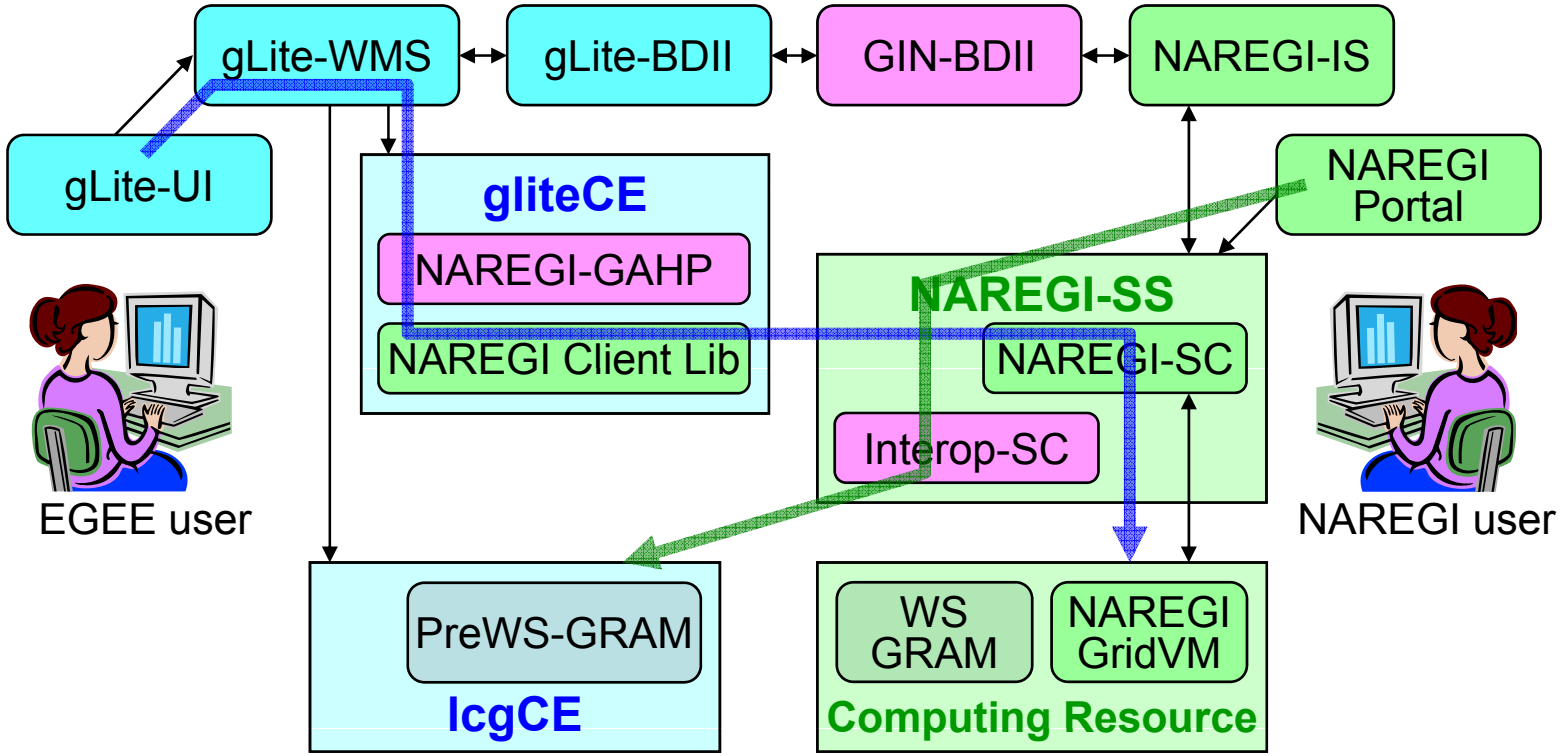
Backup Slides

GIN (Grid Interoperation Now)

- An activity of OGF for interoperation among production grids
- Major grid projects are participating
  - EGEE, NAREGI, UK National Grid Service, NorduGrid, OSG, PRAGMA, TeraGrid, ...
- Trying to identify islands of interoperation between production grids and grow those islands
- Areas
  - GIN-auth: Authorization and Identity Management
  - GIN-data: Data Management and Movement
  - GIN-jobs: Job Description and Submission
  - GIN-info: Information Services and Schema
  - GIN-ops: Operations Experience of Pilot Test Applications

GIN-jobs: NAREGI-EGEE Architecture

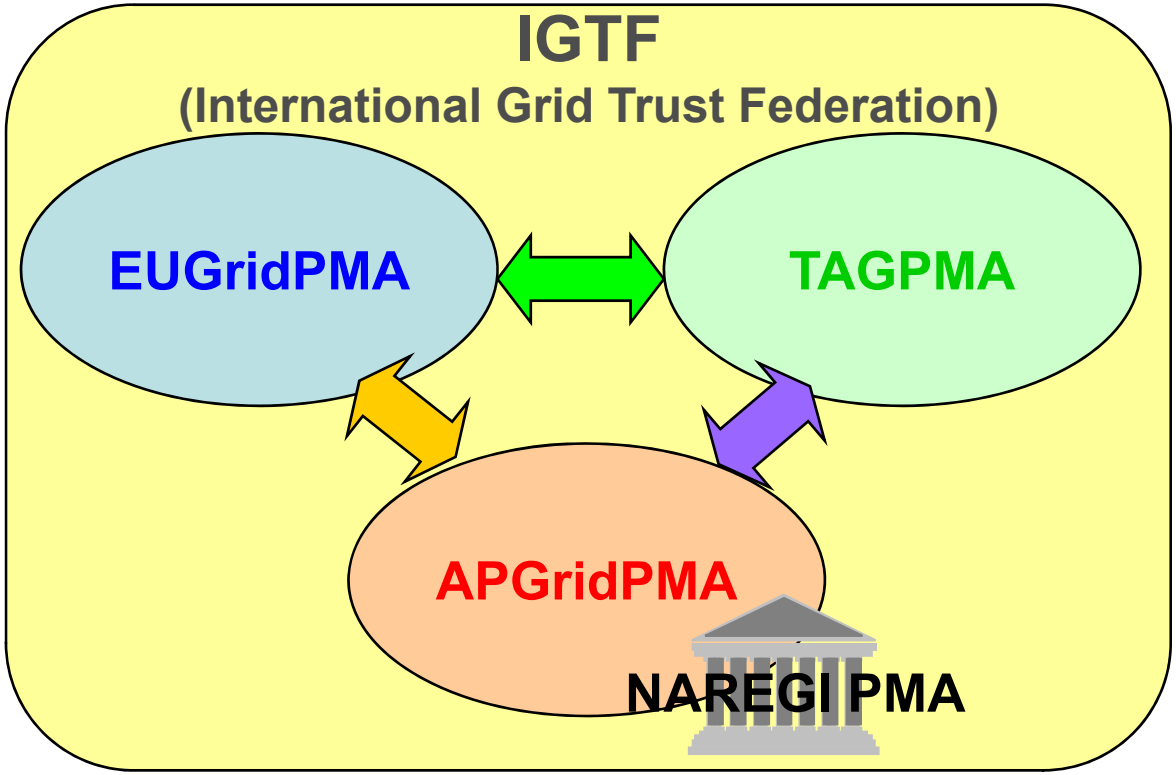
- Architecture



- Demo
  - NAREGI → EGEE: using NAREGI Workflow
  - EGEE → NAREGI: using glite WMS commands

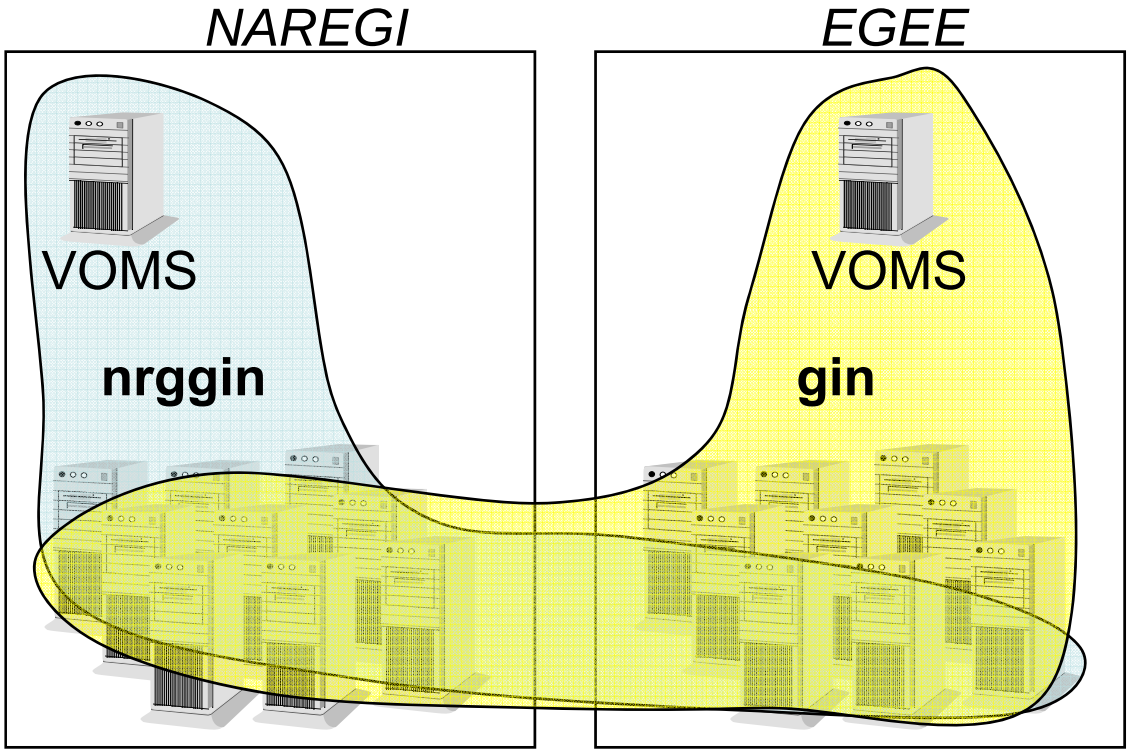
Authentication

- IGTF is framework of International Grid Trust Federation.
- IGTF consists of APGridPMA, EUGridPMA and TAGPMA.
- NAREGI CA joined the APGrid PMA.
- NAREGI CA has been approved as a production-level CA by APGridPMA.
- GSI compliant with x.509 proxy certificates for authentication.
- It has become available to use grid computing easily on the worldwide Internet by IGTF.



VO Management

- The GIN VO is a VOMS service.
- NAREGI uses VOMS as VO management system.
- Transport of supported authorization attributes via VOMS extensions.
- VO names are expected to abide by the VO naming conventions described in GIN VO Naming in order to avoid name conflicts between grids.
- All members of GIN VO should observe AUP(Acceptable Use Policy).

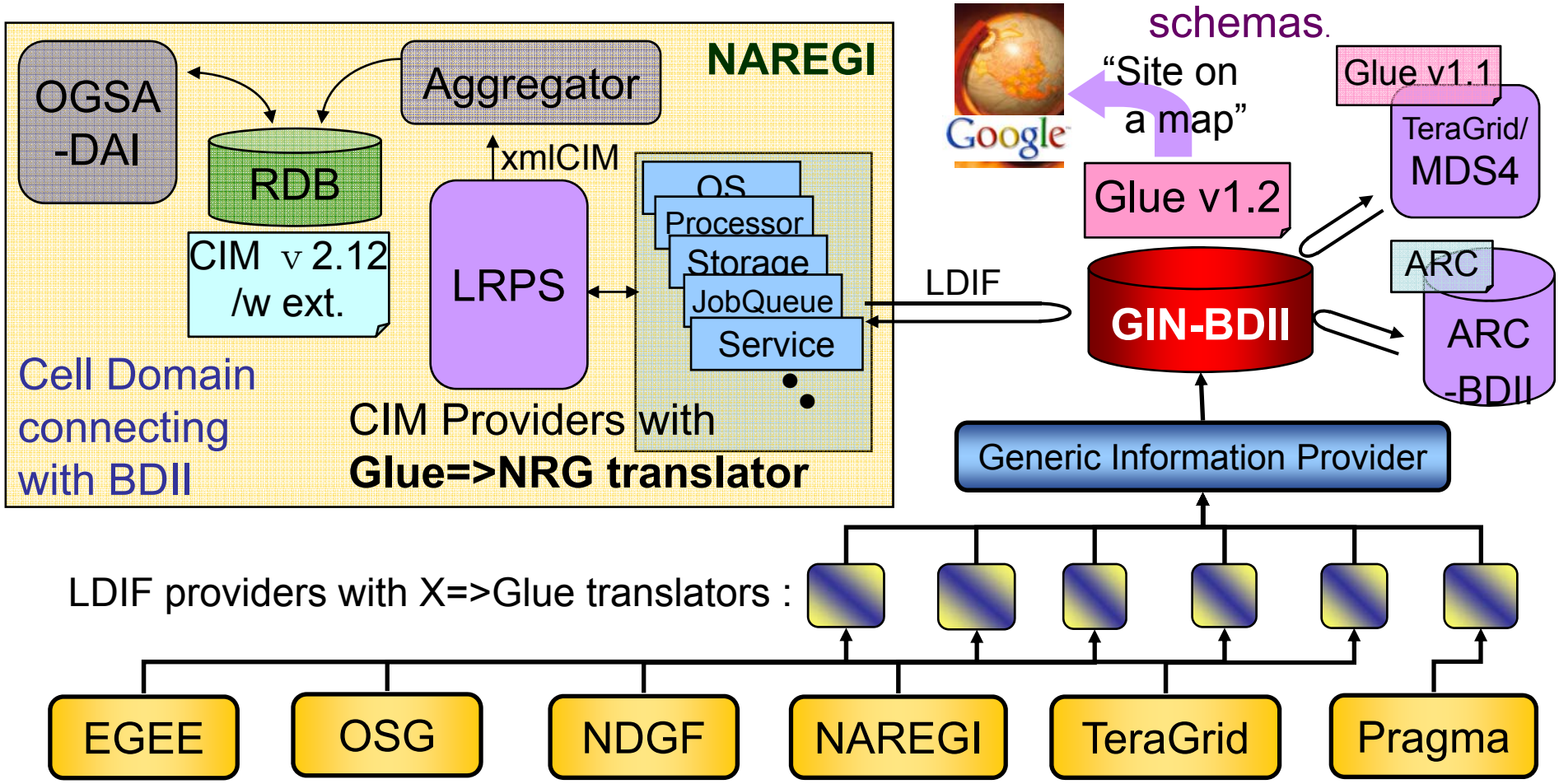


reference
http://forge.gridforum.org/sf/wiki/do/viewPage/projects.gin/wiki/GINAuth

GIN-info: Architecture

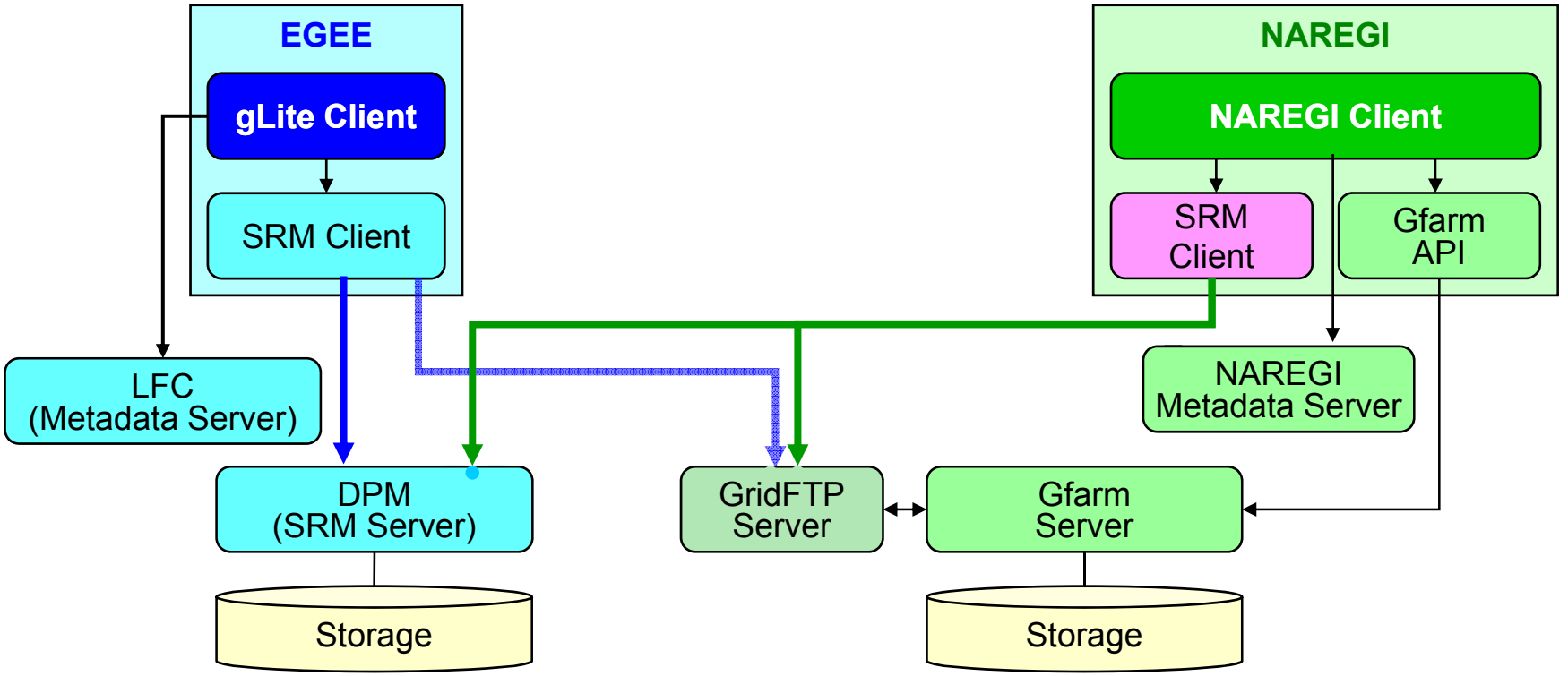
All of grid information can be retrieved by each of grid in its fashion WRT resource description schema, data format, query language, client API, …

Each information service in grid acts as an information provider for the other and translator embedded in the provider performs conversion between different schemas.



GIN-data: Architecture

- NAREGI and EGEE gLite clients can access to both data resources (e.g., bi-directional file copy) using SRM interface.
- GridFTP is used as its underlying file transfer protocol.
- File catalog (metadata) exchange is planned.



NAREGI GIN Summary

- NAREGI developed EGEE-NAREGI island as an activity of GIN
  - Bilateral information exchange
  - Bilateral job submission
  - Bilateral file exchange
  - Interoperable security properties
- Next steps
  - Improve interoperation interfaces and functions
    - WS-GRAM, BES, JSDL, …
  - Grow the island with other EGEE partners
  - KEK will use NAREGI-EGEE interoperation environment for their high energy physics calculations

CSI / NAREGI VO Communities

- ~= User Groups, unit of resource policies
- Various Vo Examples

Full Blown Reseach SNS

  - International Research Consortium
  - A research area and SC user group thereof
  - Members of (large) research grants
  - Industry-Academia collaboration group
  - User group of a particular application hosted by a center
  - A research lab in a university
  - Students of across-Institutional class
  - ○ ○ ○

SC Usage bu Individuals

↓

Group based social networks

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TITECH GRID

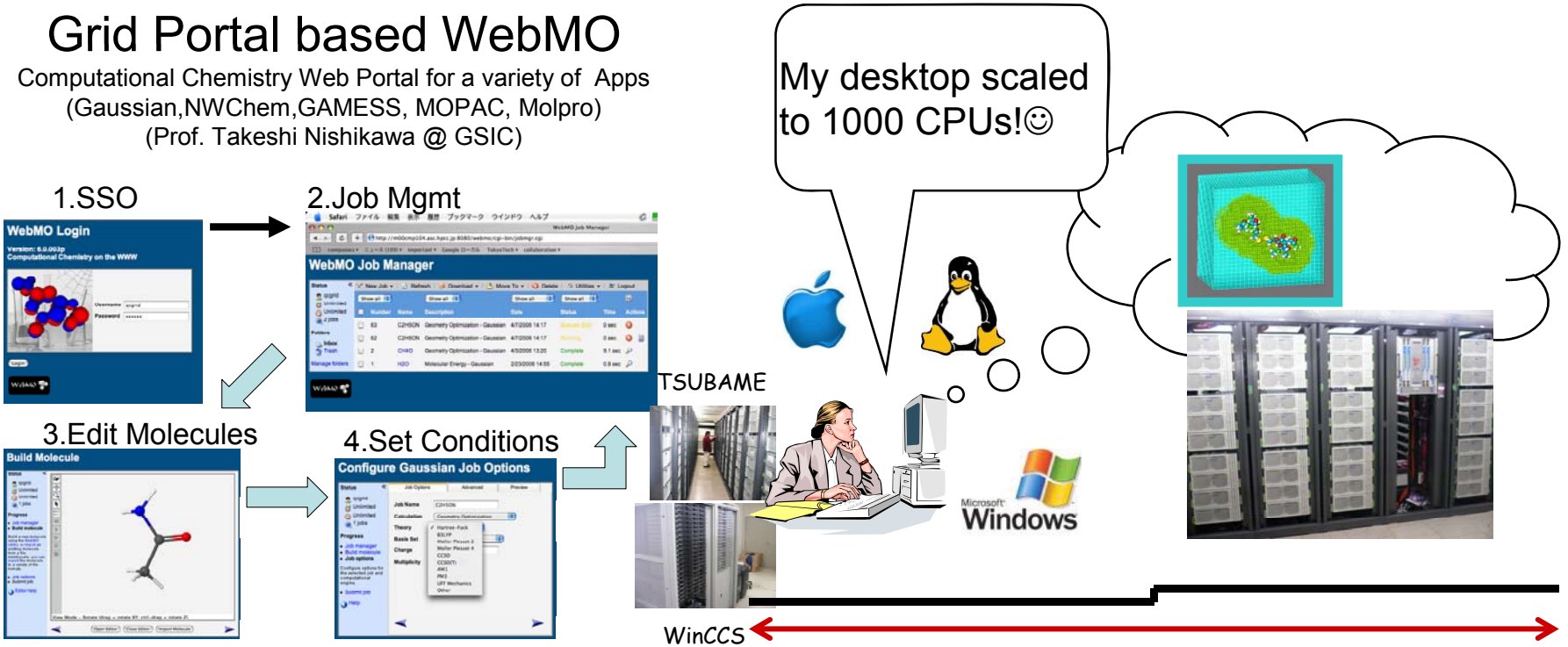
Supercomputing in All Educational Activities

Over 10,000 users

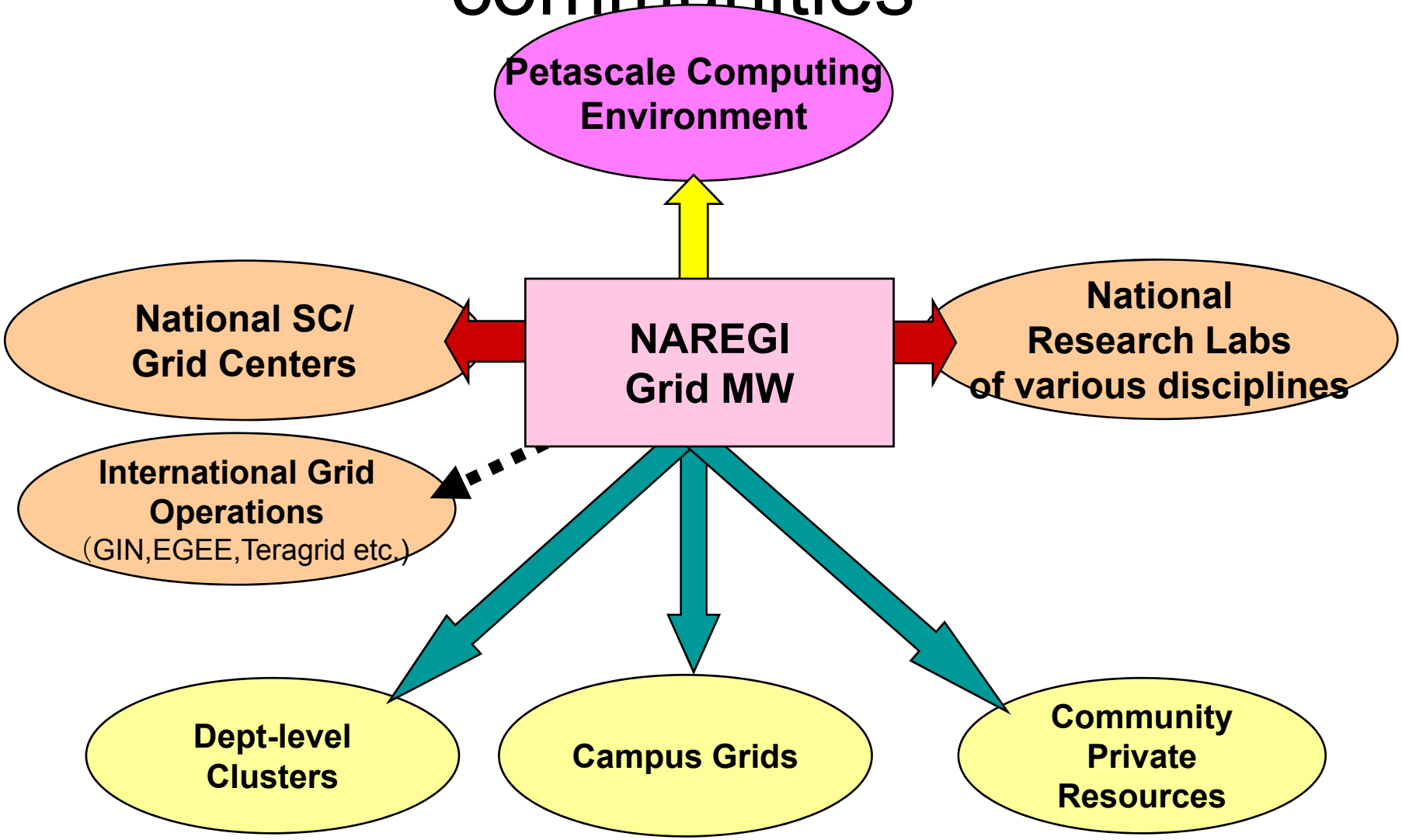
- High-End education using supercomputers in undergrad labs
  - High end simulations to supplement “physical” lab courses
- Seamless integration of lab resources to SCs w/grid technologies
- Portal-based application usage

Grid Portal based WebMO

Computational Chemistry Web Portal for a variety of Apps
(Gaussian,NWChem,GAMESS, MOPAC, Molpro)
(Prof. Takeshi Nishikawa @ GSIC)



NAREGI's outreach to all research communities



NAREGIβ2 and V.1.0

- New Features
  - EGEE gLite-LCG interoperation support
  - Workflow support in GridRPC (& GridMPI)
  - Non-reserved jobs and bulk job submissions
  - Direct support of Globus WS-GRAM as side-interface
  - Multiple VO support and sharing of resources
  - Various batch queue support w/reservation emulation
    - PBS Pro (β1), LoadLeveler, NEC NQSII (β1), & Job Manipulator on SX and clusters, Sun GE(β2), Fujitsu NQS(v.1.0), Condor…
  - Various management tools
  - Private address support

- Performance and stability
  - Various fault tolerancy, e.g., support of failed workflows
  - Much better scalability and performance due to feedback from beta 1, profiling, bug fixe, etc.
  - Distributed Information Service management of system info everything from applications to system faults