



NAREGI and Standards

- a View from appl. Developer -

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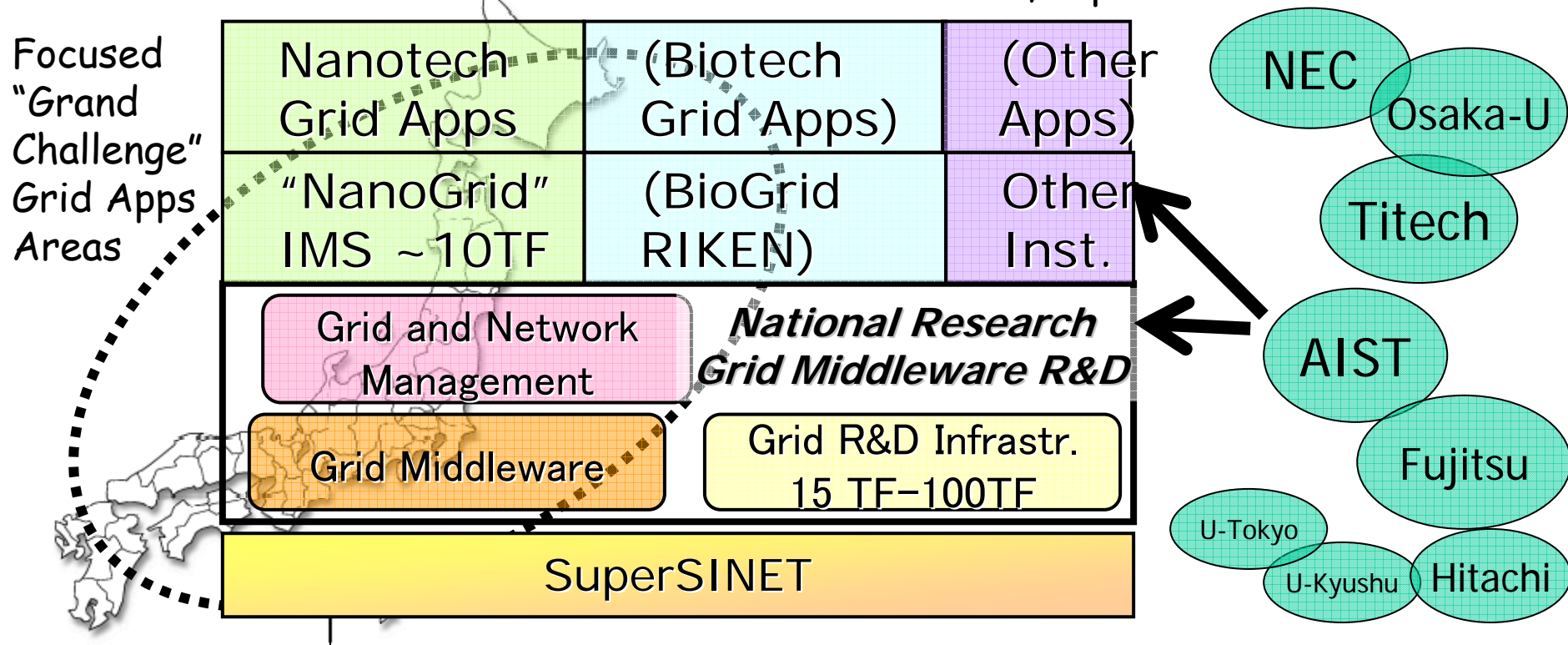
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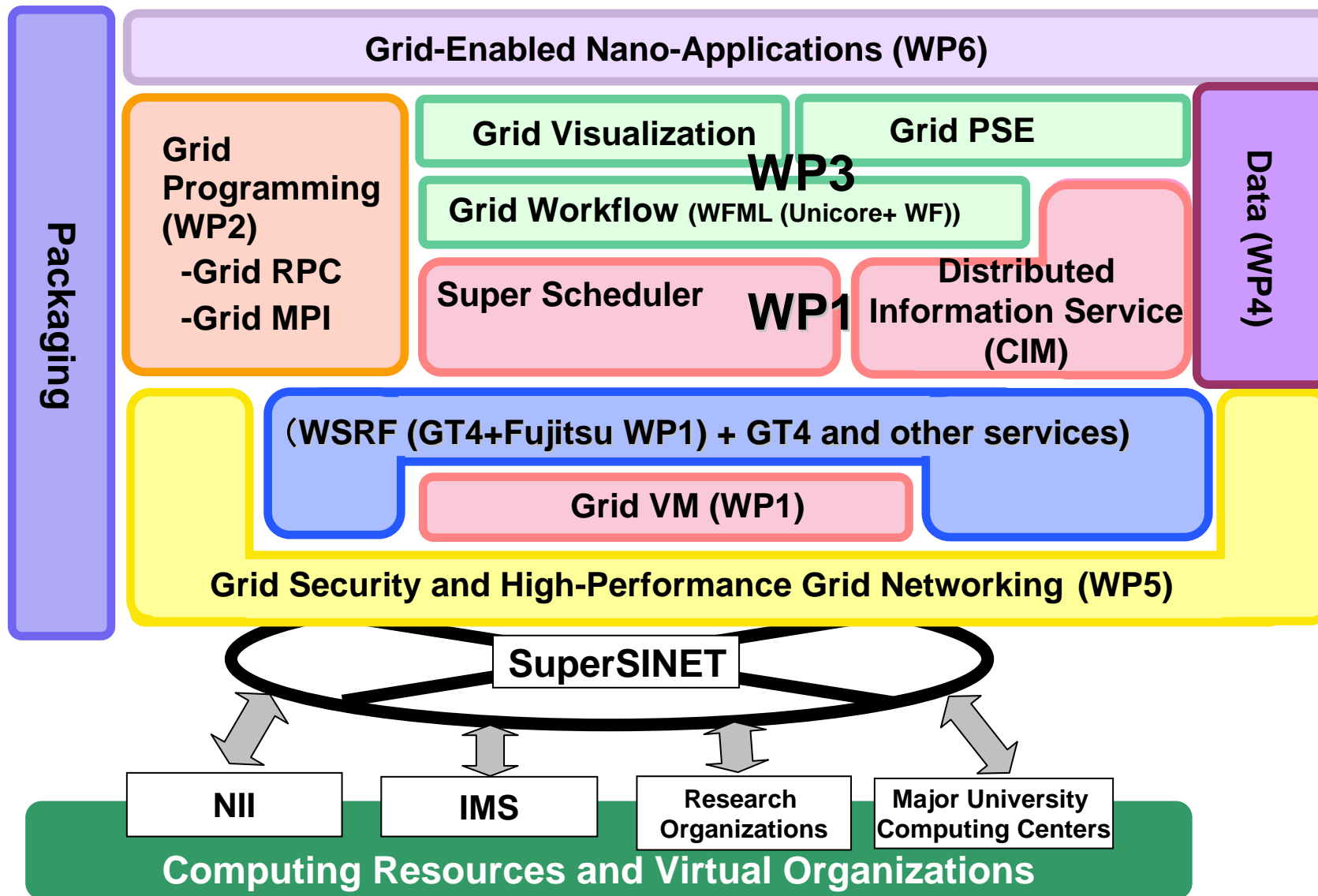
National Research Grid Infrastructure (NAREGI) 2003-2007

- Petascale Grid Infrastructure R&D for Future Deployment
 - \$45 mil (US) + \$16 mil x 5 (2003-2007) = \$125 mil total
 - Hosted by National Institute of Informatics (NII) and Institute of Molecular Science (IMS)
 - PL: prof. Ken Miura (Fujitsu → NII)
 - Sekiguchi(AIST), Matsuoka(Titech), Shimojo(Osaka-U), Aoyagi (Kyushu-U)...
 - Participation by multiple (>= 3) vendors, Fujitsu, NEC, Hitachi, NTT, etc.
 - Follow and contribute to GGF Standardization, esp. OGSA





NAREGI Software Stack (Beta Ver. 2006)





R&D in Grid Software and Networking Area (Work Packages)

- Work Package Structure :
 - Universities and National Labs: technology leadership
 - Vendors (Fujitsu, NEC, Hitachi, etc.): professional development
- WP-1: Resource Management:
 - Matsuoka(Titech), Nakada(AIST/Titech)
- WP-2: Programming Middleware:
 - Sekiguchi(AIST), Ishikawa(U-Tokyo), Tanaka(AIST)
- WP-3: Application Grid Tools:
 - Usami (new FY2005, NII), Kawata(Utsunomiya-u)
- WP-4: Data Management (new FY 2005, Beta):
 - Matsuda (Osaka-U)
- WP-5: Networking & Security
 - Shimojo(Osaka-u), Oie(Kyushu Tech.)
- WP-6: Grid-enabling Nanoscience Appls
 - Aoyagi(Kyushu-u)



Highlights of NAREGI Beta (May 2006, GGF17/GridWorld)

- Professionally developed and tested
- "Full" OGSA-EMS incarnation
 - Full C-based WSRF engine (Java -> Globus 4)
 - OGSA-EMS/RSS WSRF components
 - Full WS-Agreement brokering and co-allocation
 - GGF JSDL1.0-based job submission, authorization, etc.
 - Support for more OSes (AIX, Solaris, etc.) and BQs
- Sophisticated VO support for identity/security/monitoring/accounting (extensions of VOMS/MyProxy, WS-* adoption)
- WS- Application Deployment Support via GGF-ACS
- Comprehensive Data management w/Grid-wide FS
- Complex workflow (NAREGI-WFML) for various coupled simulations
- Overall stability/speed/functional improvements
- To be interoperable with EGEE, TeraGrid, etc. (beta2)

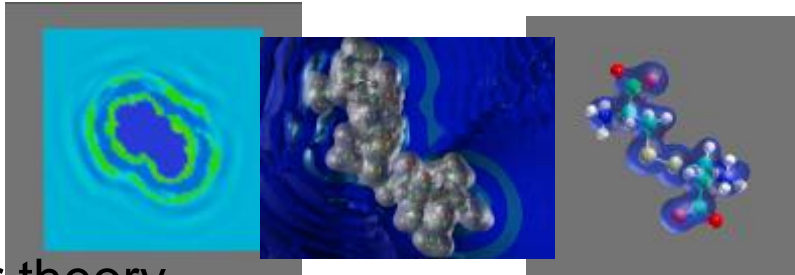


Nano-Science : coupled simulations on the Grid as the sole future for true scalability

--- Coupled Simulations as “Killer Apps” for Grid ---

Material physics
(Infinite system)

- Fluid dynamics
- Statistical physics
- Condensed matter theory



Molecular Science

- Quantum chemistry
- Molecular Orbital method
- Molecular Dynamics

...

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Limit of Idealization

Multi-Physics
Multi-Resolution

Limit of Computing Capability

Old HPC environment:

- decoupled resources,
- isolated users,
- special software, ...
- no coupling!

Coordinates decoupled resources on Grid;

Meta-computing,
High throughput computing,
Multi-Physics simulation

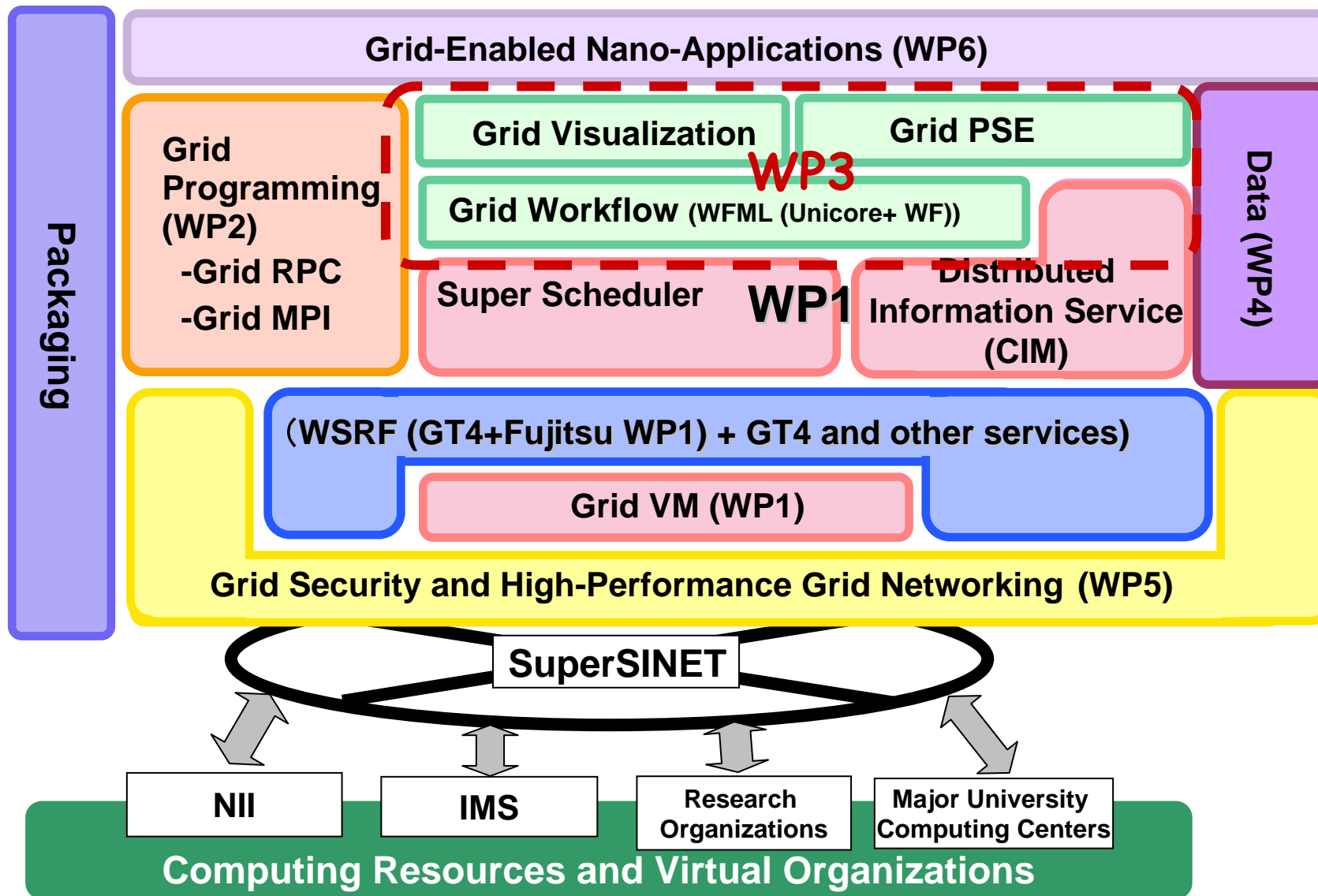
w/ components and data from different groups
within VO composed in real-time



The only way to achieve true scalability!

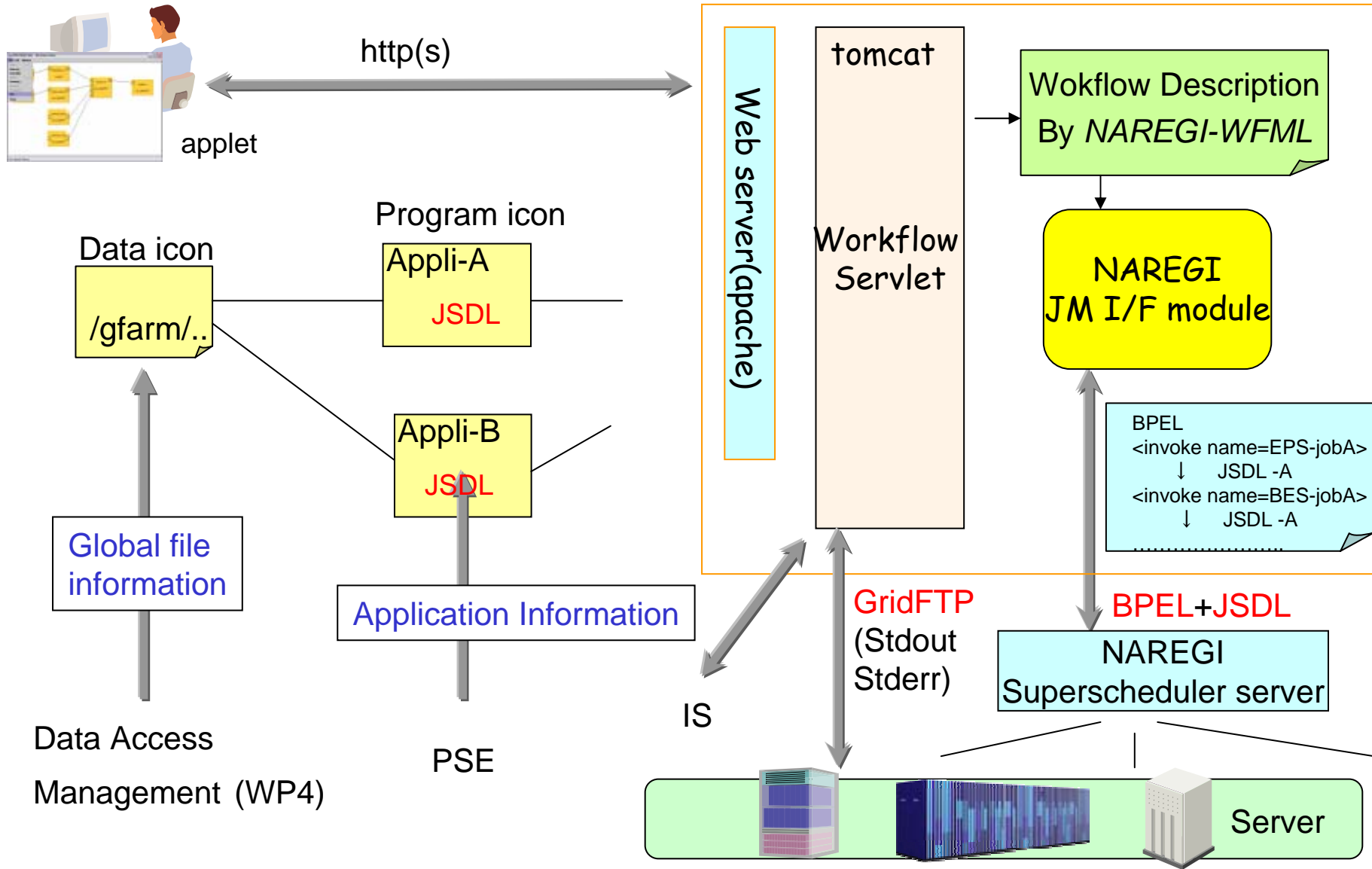


NAREGI Software Stack (Beta Ver. 2006)



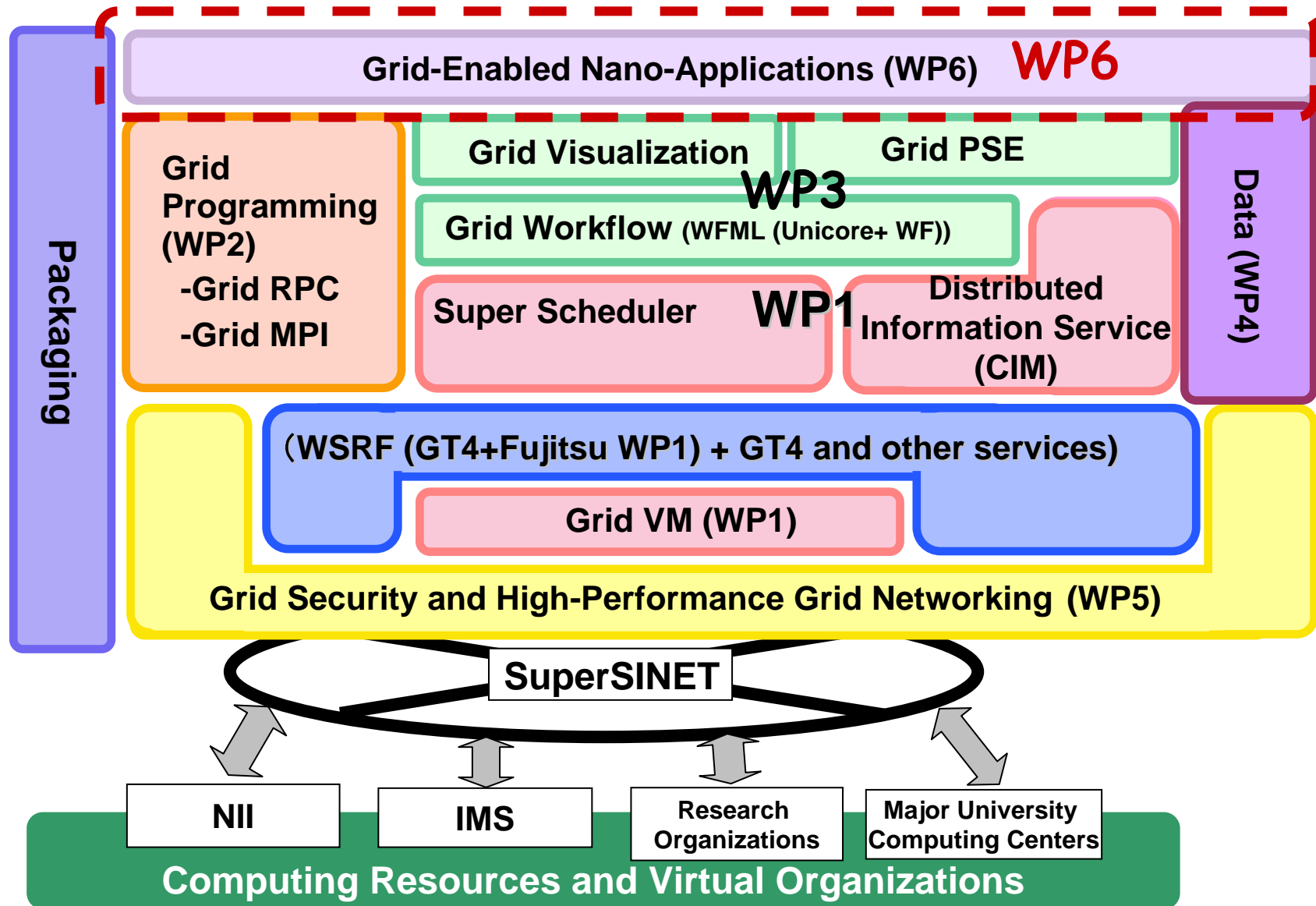


NAREGI WP3 Workflow Tool





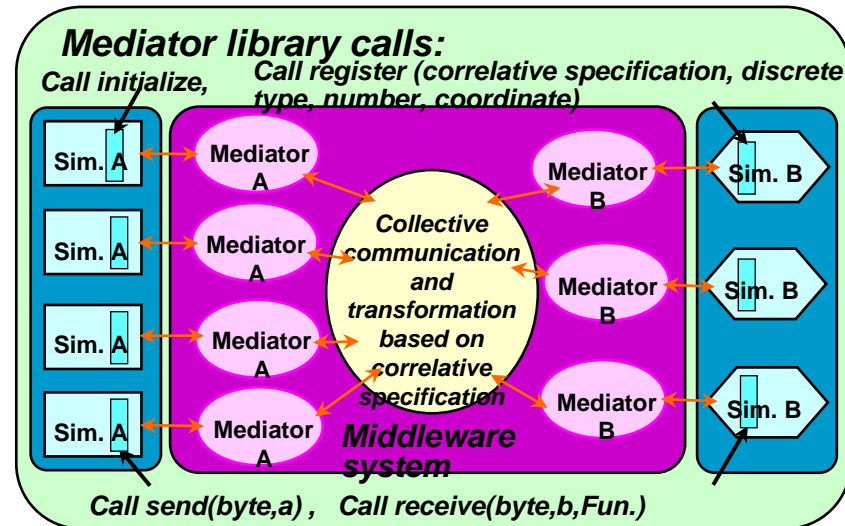
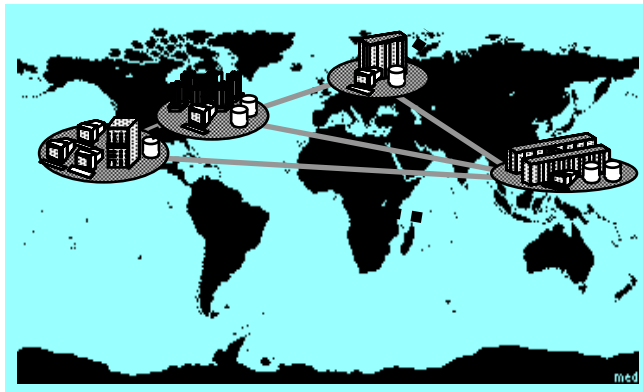
NAREGI Software Stack (Beta Ver. 2006)





Mediator: Grid middleware for Coupled Simulations

A new grid middleware is developed which allows various kinds of Nano-application softwares to be coupled efficiently for solving **multi-scale and multi-physics problems**.



Respect Independency of each application prog.

Reduce the barriers to construct grid-ready appl.



NAREGI Application Mediator (WP6) for Coupled nano-science simulations

Mediator Components

*Support data exchange
between coupled simulation*

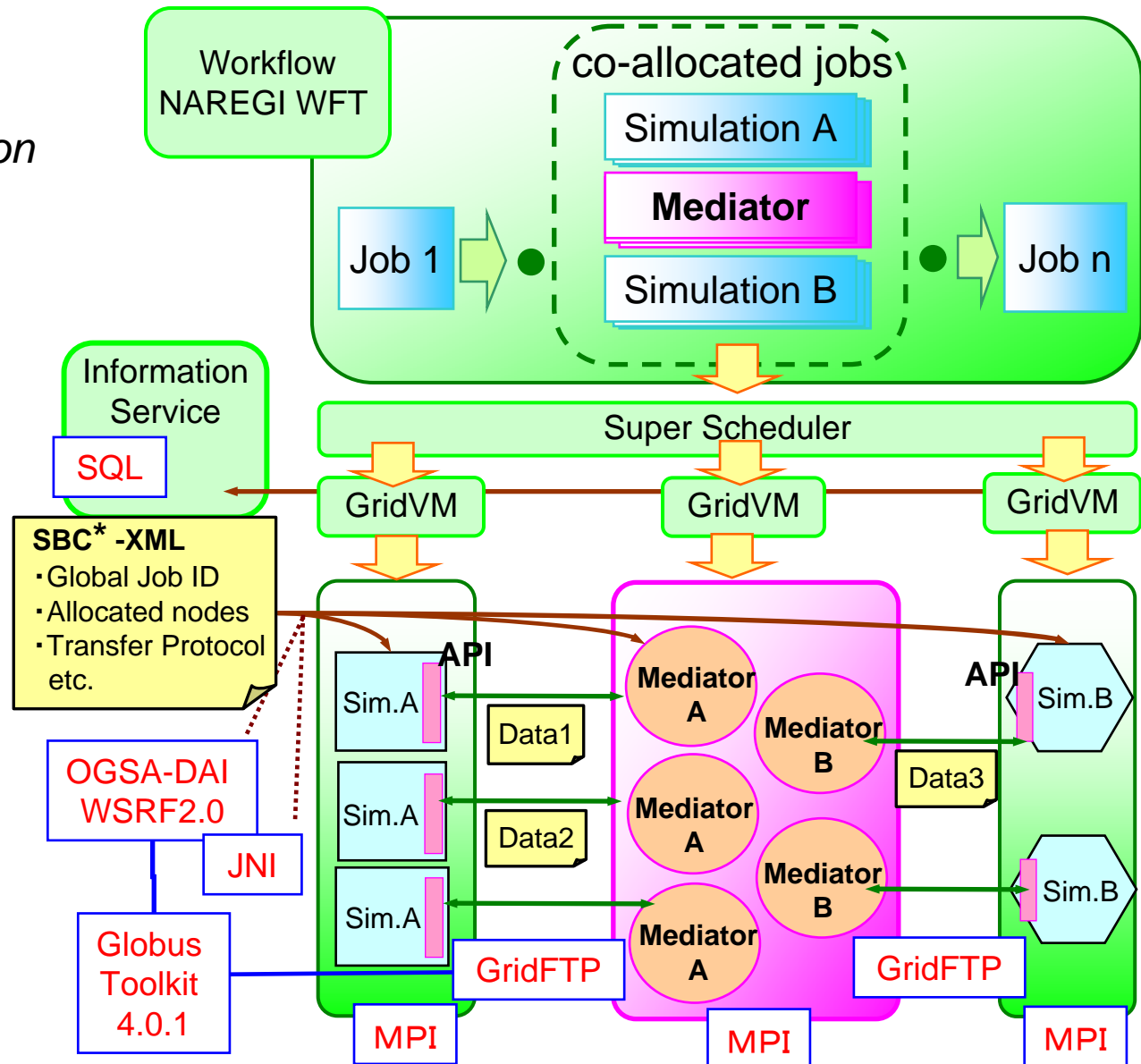
Data transfer management

- Synchronized file transfer
- Multiple protocol GridFTP/MPI

Data transformation management

- Semantic transformation libraries for different simulations
- Coupled accelerator

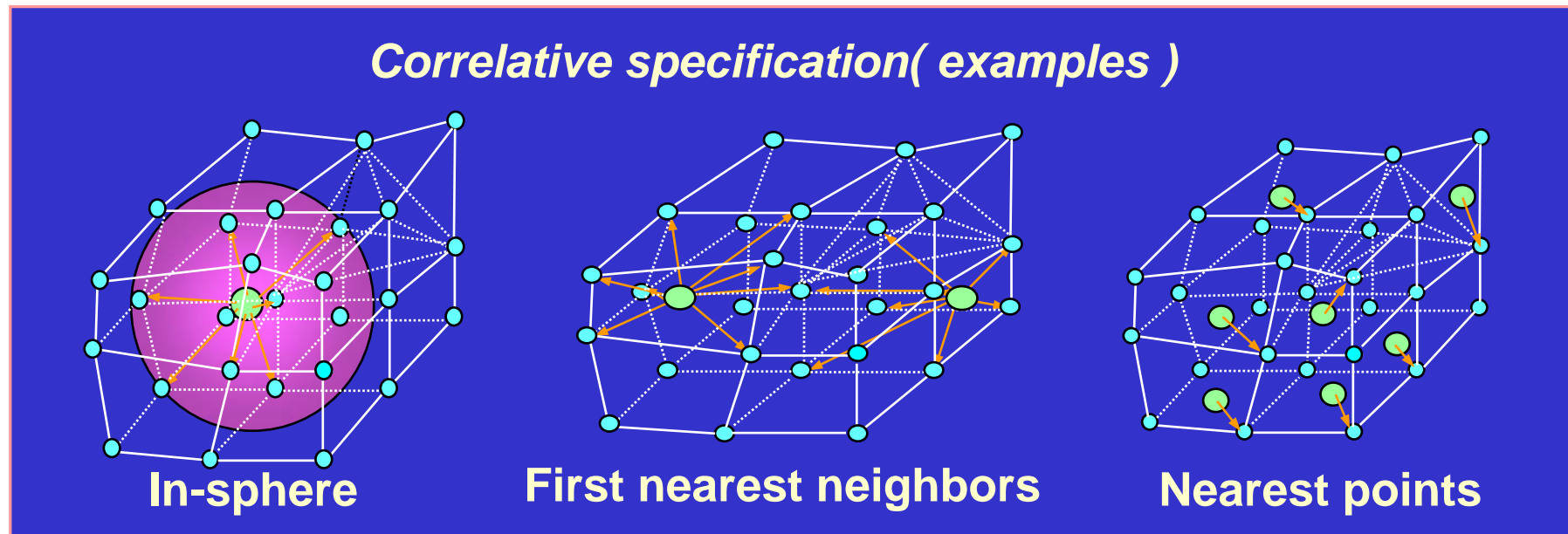
*SBC: Storage-based communication





Mediator: Tools for Coupled Simulations

The mediator provides high-level transparency in data communication between different discretization methods associated with a model specific spatial and temporal scale based on our physical requirements.

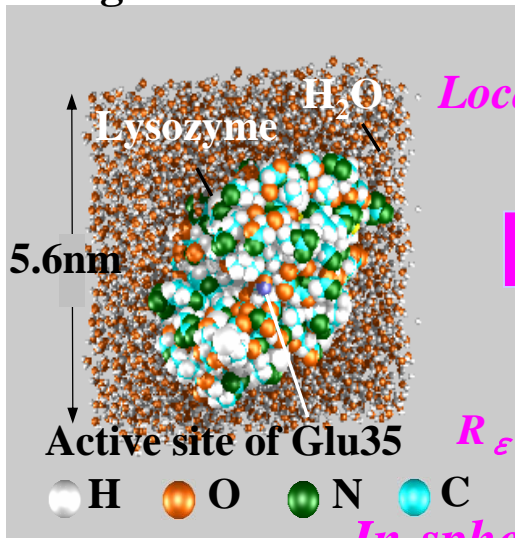


Other correlation specification can be defined as user-plug-in.

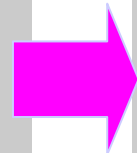
Ex1: Mediator based Molecular dynamics(MD) and Poisson–Boltzmann(PB) coupled simulation(1)

Method of Simulation

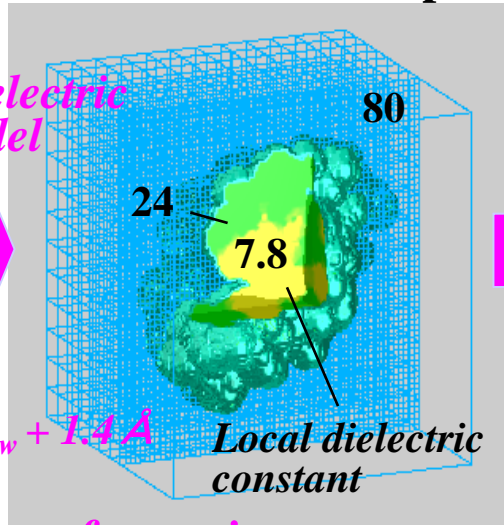
Hydrate structure using MD simulation



Local dielectric model



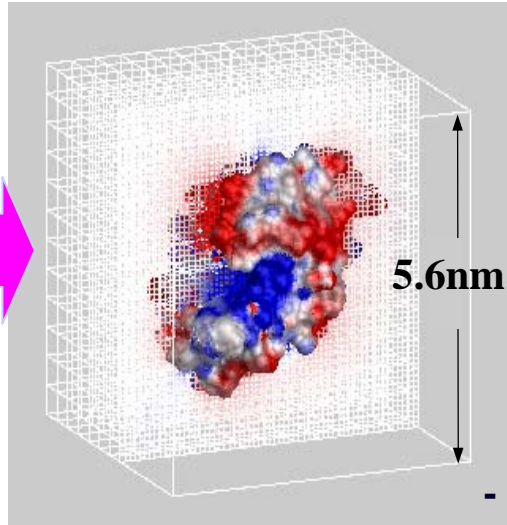
Distribution of dielectric constant over mesh point



Local dielectric constant



Electrostatic potential simulation using PB

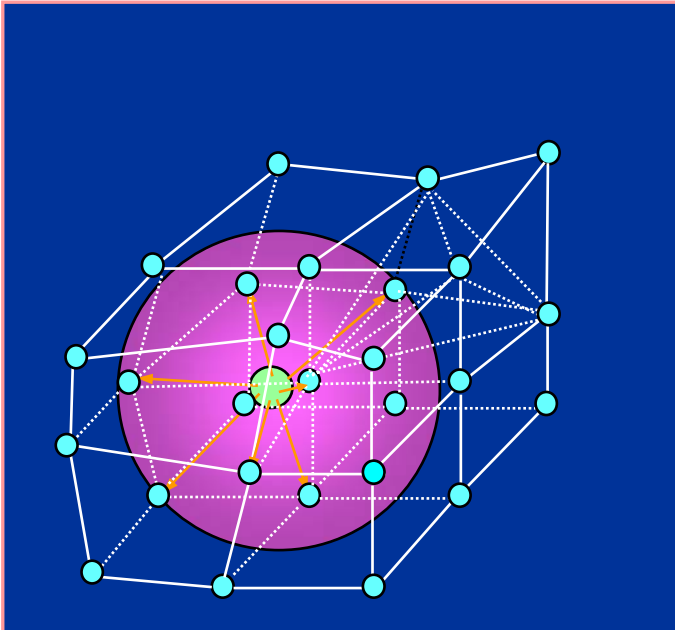


In-sphere transformation used

Roughly estimate “Active Site” of lysozyme and H-Dissociation energy at Glu35.

Efficient Data Transfer on Different Discretization models

- Particle (MD) / Mesh (FDM)



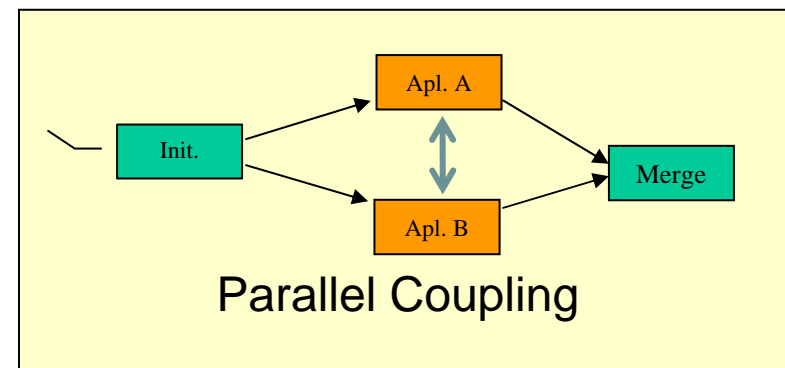
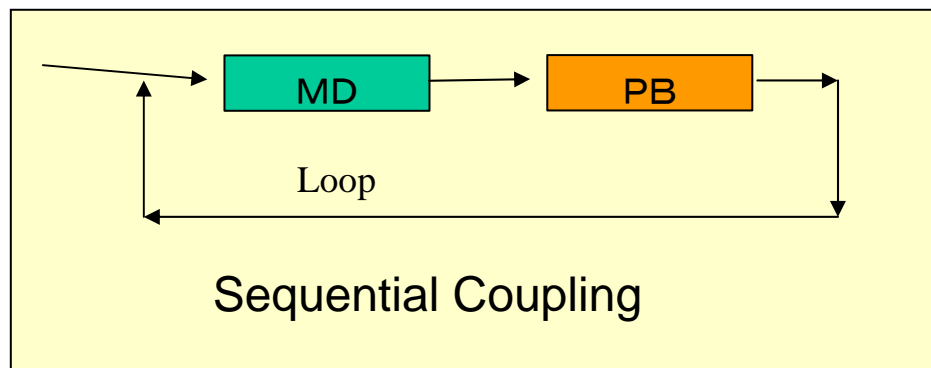
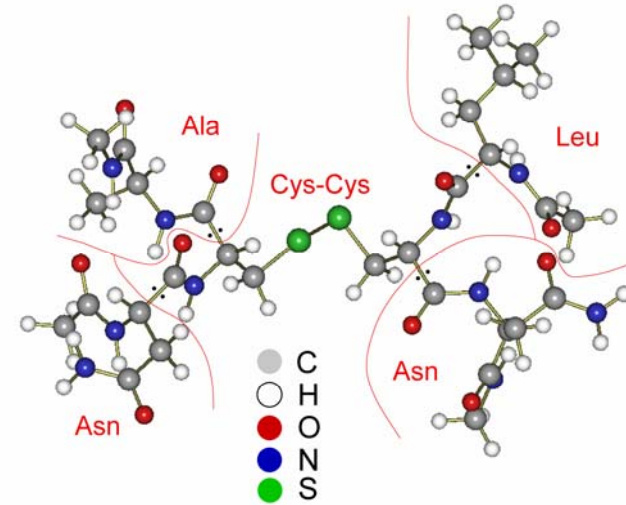
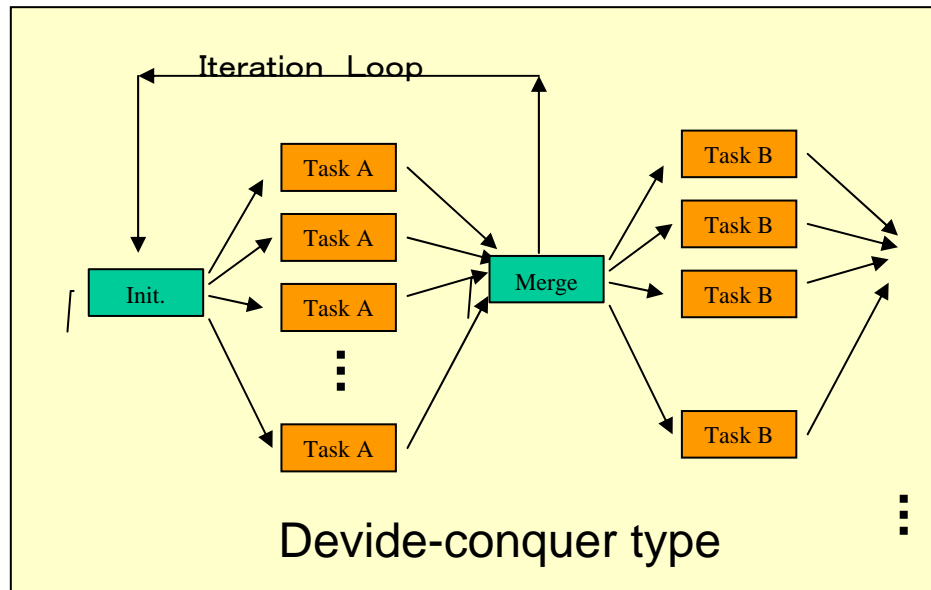
Mediator automatically
generates the correlation
relation over different
discretization models:

Dipole moment of particles
⇔ Distribution of dielectric
constant over mesh points

To keep transportabilities and independencies of APLs,
Semantic transformation required in coupled simulations
should be achieved in the third component as Mediator,
not in the application components themselves.

Classification of Workflow

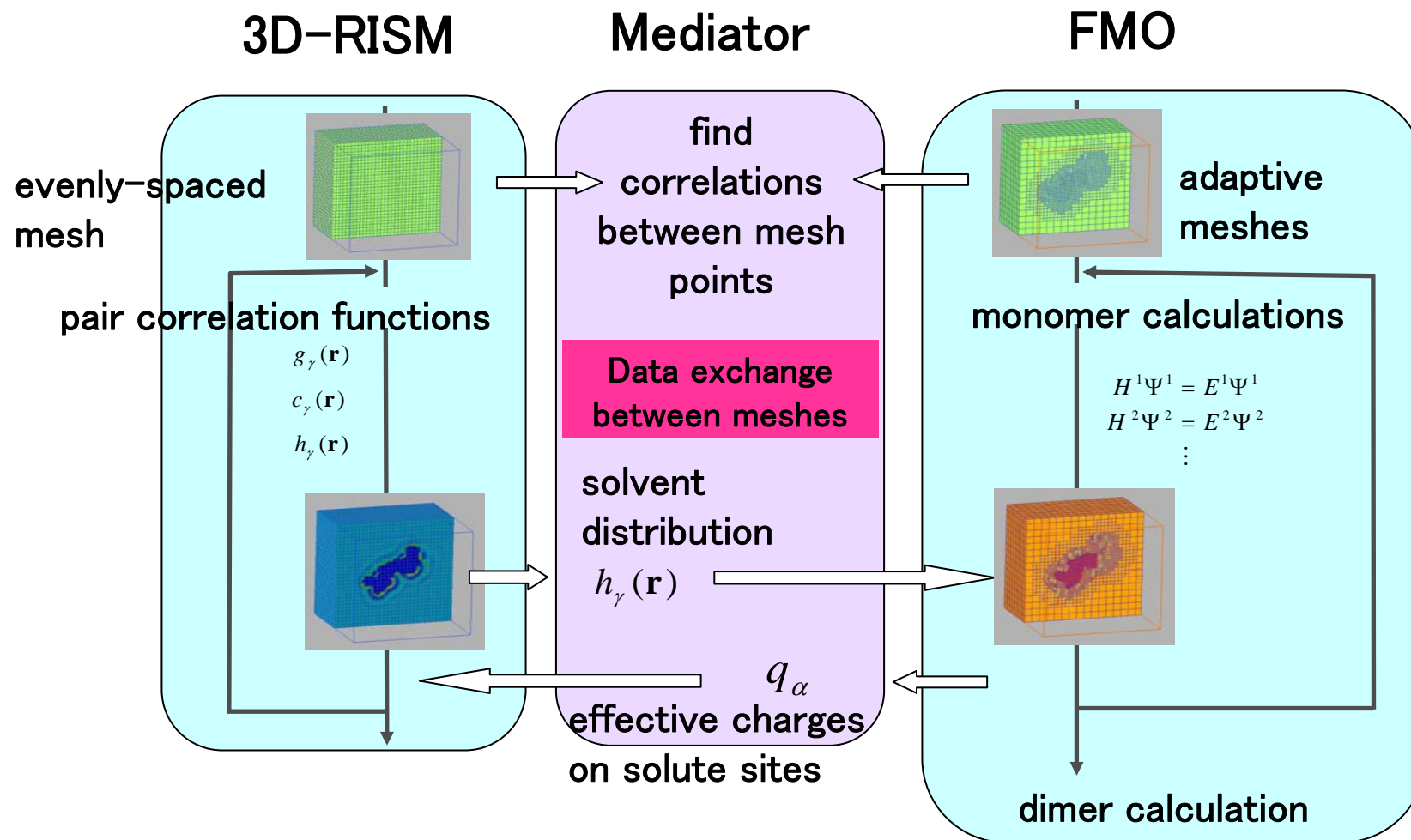
Modularize in consideration of granularity, communication overhead, latency awareness, portability, etc



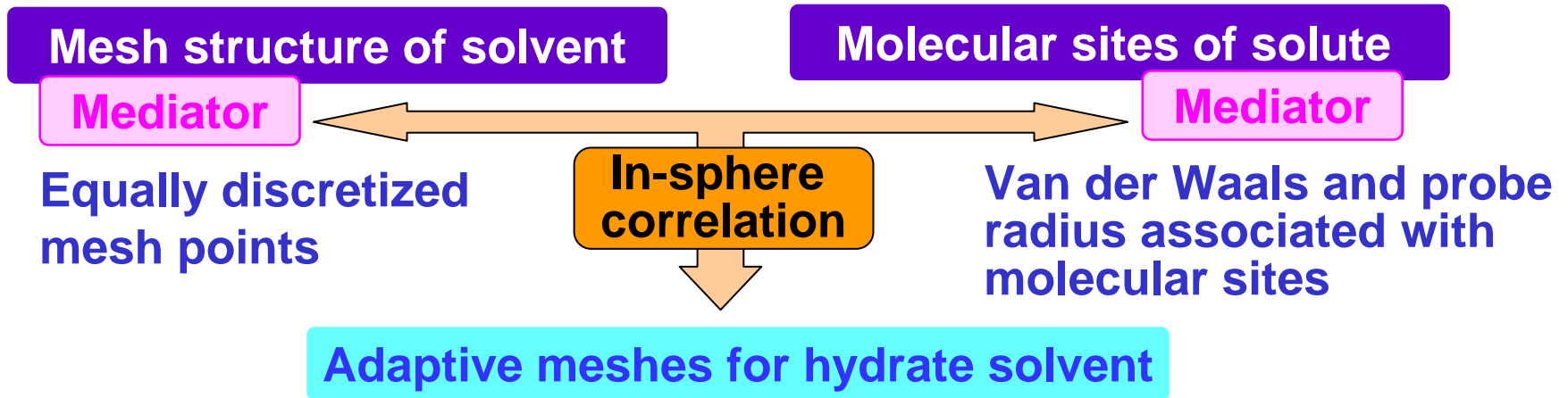


2nd Example: RISM-FMO coupled Simulation

Outline of workflow:

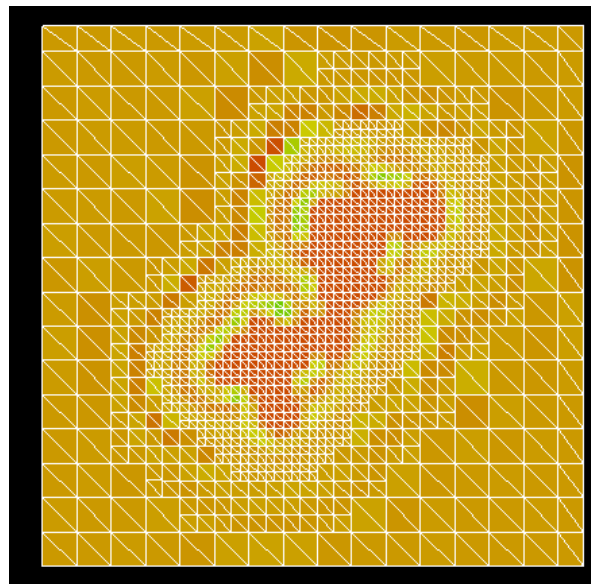


Data Exchanges in RISM-FMO



We respect
Independency of
developing each
Application.

Mediator facilitate
customization
processes of original
application program for
coupled simulations.



Mediator treats with
Data exchange on
different discretization
scheme of apl. A and apl.
B.



Coupled simulation model

Coupled simulation	RISM-FMO	MD-PB
Discretization method	FDM / Irregular point	Particle / FDM
Physical quantities to be transformed	Solvent charge density to charge on solvent atoms	Dielectric distribution, Charge on atoms to charge density
Correlation specification	In-rectangular	In-sphere
Transformation function	Weighted function conserving charge	Weighted function equalizing electric field
Programming style	Sequential / Master-Worker	Master-Worker / Sequential
Communication paradigm	Two-way iterative communication	One-way, Variable communication
Interconnection	GridMPI, MPICH-G2, GridFTP, MPICH, Score	MPICH, MPI2, Stampi
Server machines	Hitachi SR8000, AIX, Linux, Alpha clusters	Hitachi SR8000, SR2201, DEC, Sun clusters



Grid enabling of the GAMESS FMO prog.

GAMESS

The General Atomic and Molecular Electronic Structure System (GAMESS) is a general ab initio quantum chemistry package.

GAMESS is maintained by the members of the Gordon research group at Iowa State University.

[Summary of program capabilities](#)

[How to get GAMESS](#)

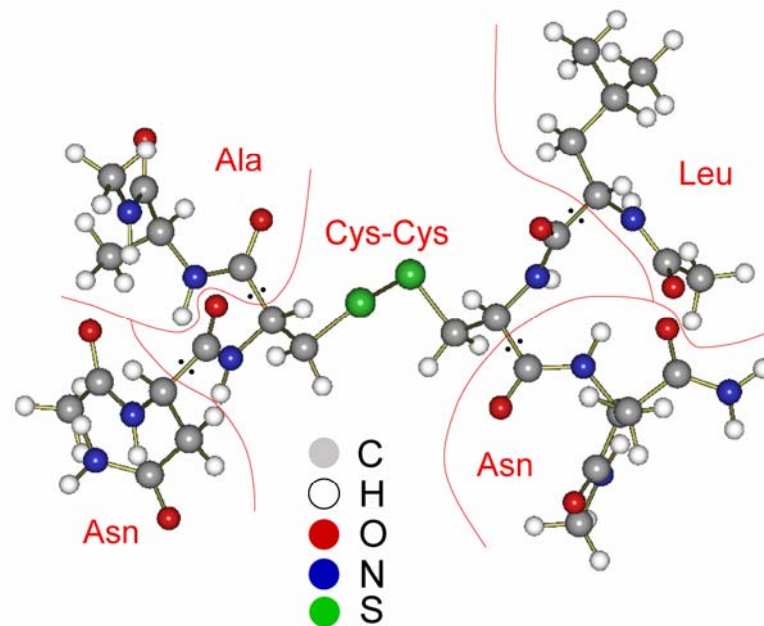
[GAMESS documentation](#)

[Chemistry graphics programs](#)

[A version history of GAMESS](#)

[The Gordon Research Group](#)

[Security and Privacy Notice](#)

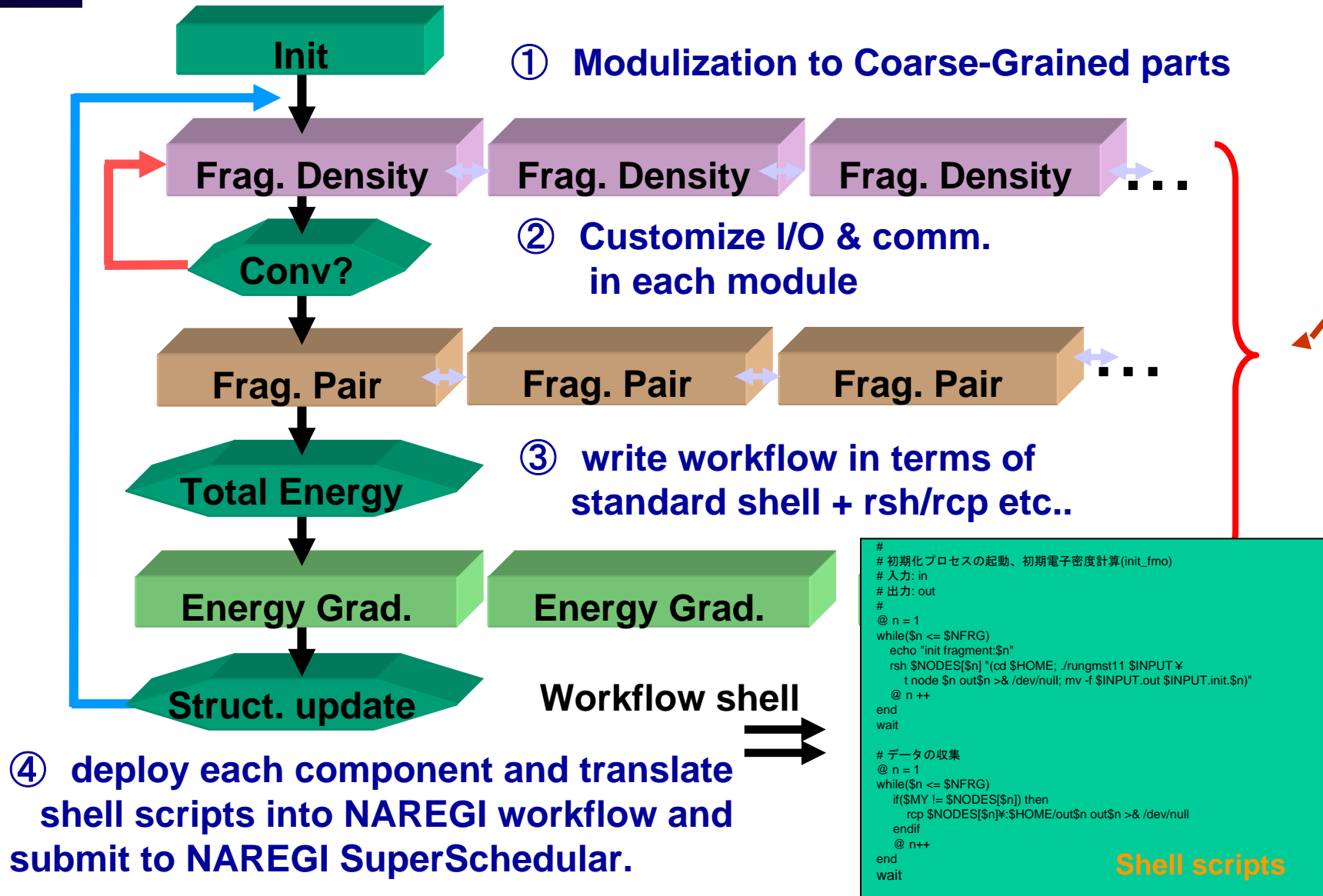


<http://www.msg.ameslab.gov/GAMESS/GAMESS.html>

One of the most popular open-source program used in the world-wide nano science community.



Grid enabling of the GAMESS FMO prog.

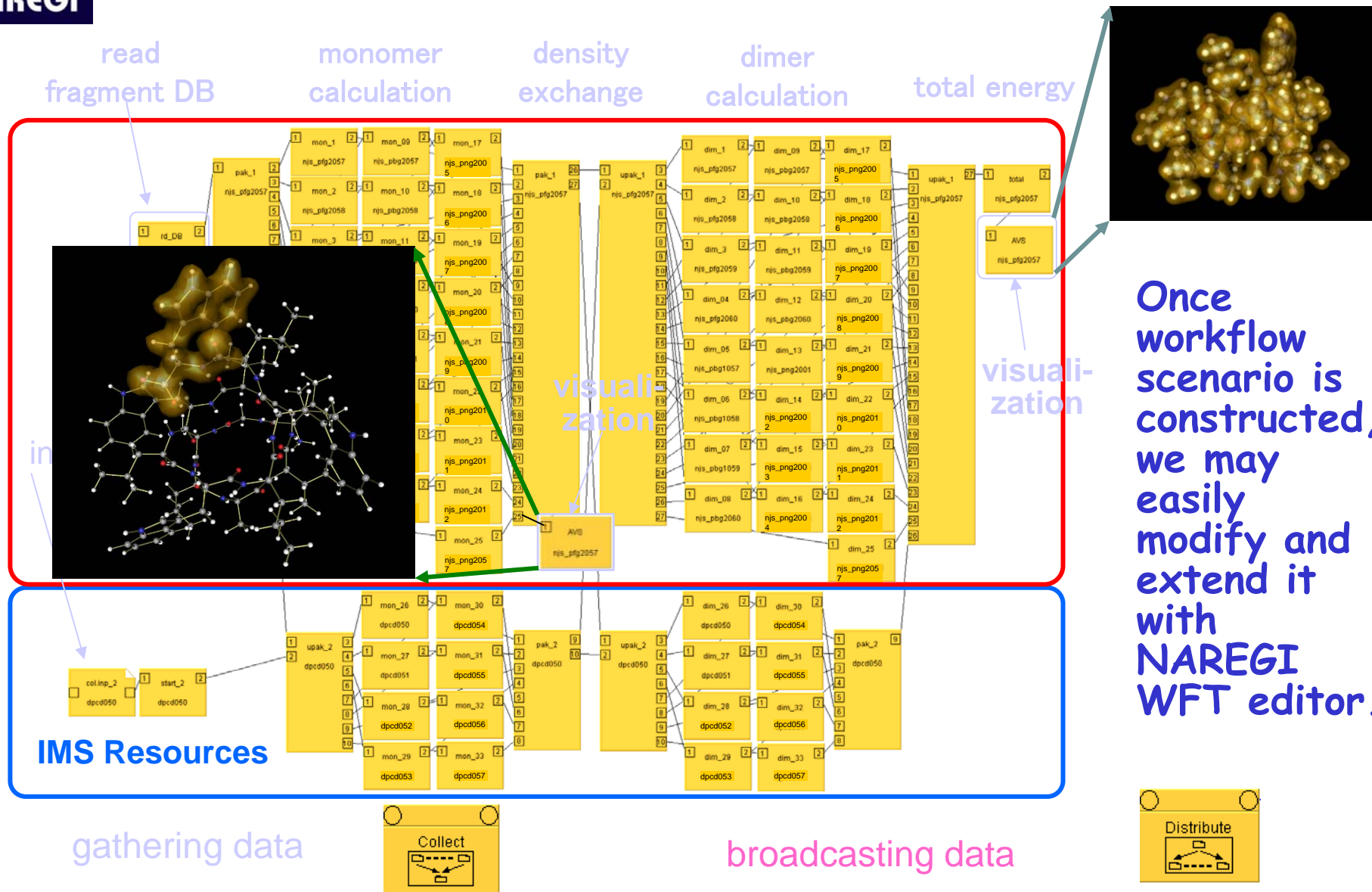


Workflow based distributed computing for Grid FMO Simulations of protein





Fragment Electron Density in Grid FMO



Computer Resources for demonstration



NII



CPU: Dual Xeon 2.8GHz (Memory 1GBytes) x 8
OS: RedHat Linux 9 (kernel 2.4.21 SMP)
Host: png1043.naregi.org



CPU: IBM Power4 1.3GHz (32 way SMP)
OS: AIX Version 5.2.0.75
Host: sig0001.naregi.org

Kyushu Univ.

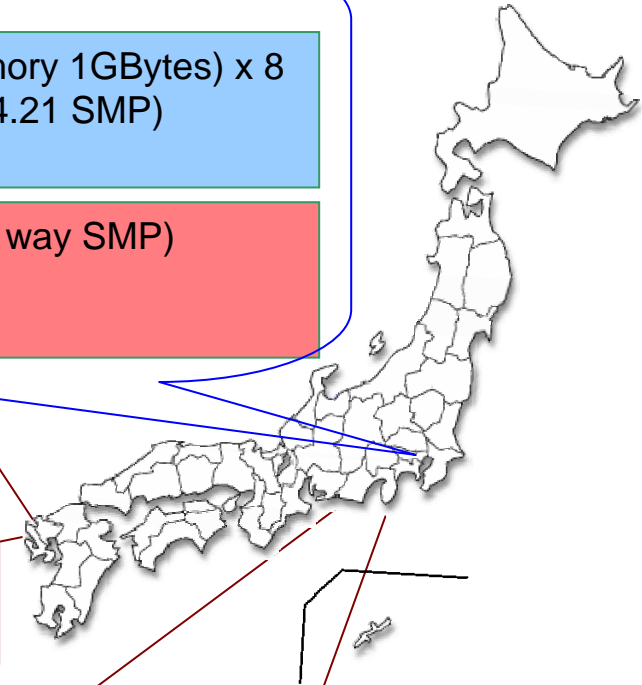


CPU: Dual Xeon 3.0GHz (Memory 2GBytes) x 4
OS: RedHat Linux 9 (kernel 2.4.21 SMP)
Host: nrgb01.cc.kyushu-u.ac.jp

TiTech



CPU: Dual Xeon 3.4GHz (Memory 2GBytes) x 5
OS: RedHat Linux 9 (kernel 2.4.21 SMP)
Host: demo1.cc.titech.ac.jp

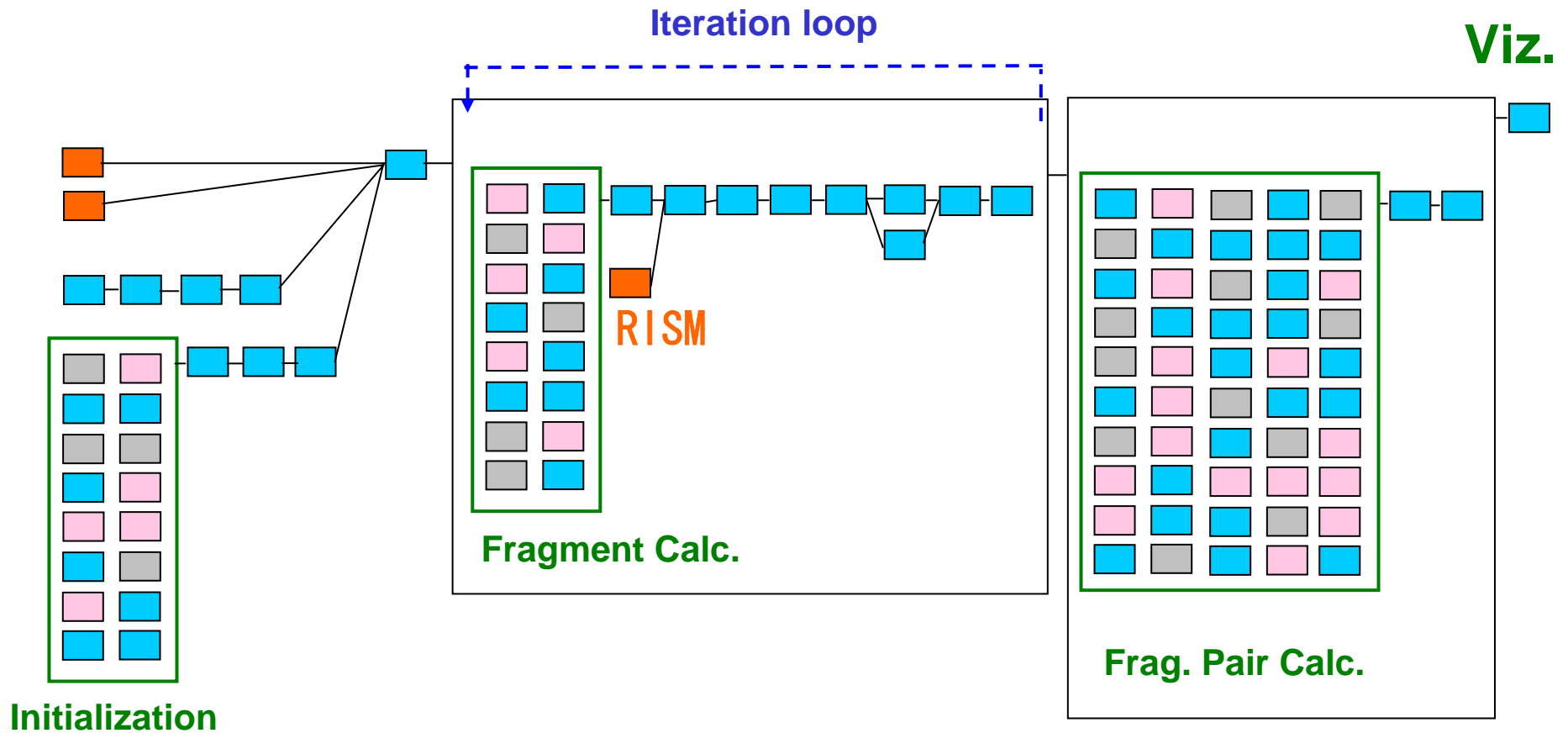




Distributed Computing through NAREGI SS & WFT

- NII (IBM AIX)
- NII (Cluster)

- Kyushu Univ. (Cluster)
- TiTech (Cluster)





NAREGI ...

- Is THE National Research Grid in Japan
 - Part of CSI and future Petascale initiatives
- Has extensive commitment to WS/GGF-OGSA
 - Entirely WS/Service Oriented Architecture
 - Set industry standards e.g. 1st impl. of OGSA-EMS
- Will work with EU/US/AP counterparts to realize a "global research grid"
 - Various talks have started, incl. SC05. SC06.. interoperability meeting
- Just delivered first public beta in May 2006 @ GGF17/GridWorld in Tokyo



Summary

- Interoperability is the key for grid adoption
- NAREGI believes, as a major national grid project, that committing to standards is the best bet for interoperation and industry adoption
 - Will be working next 2 years to set and adopt more standards
- Will be working with other parties, within and outside GGF to achieve common standards