



# **Science Gateways: Common Community Interfaces to Grid Resources**

## **Grid Enabling of Nano-Science Applications in NAREGI**

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**Kyushu Univ.**

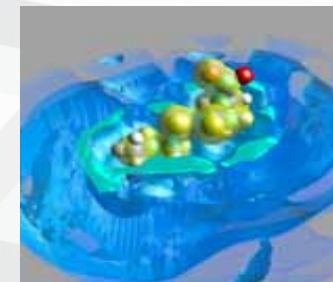
**aoyagi@cc.kyushu-u.ac.jp**  
**Head of Grid-Enabling Team&**  
**Sub-Leader of NAREGI(JAPAN)**

# Outline

## 1. Grid-Enabling by Mediator/GridMPI

**Application to Solvent interactions  
in hydrolysis of Lysozyme**

**MD-PB and RISM-FMO coupled simulations**

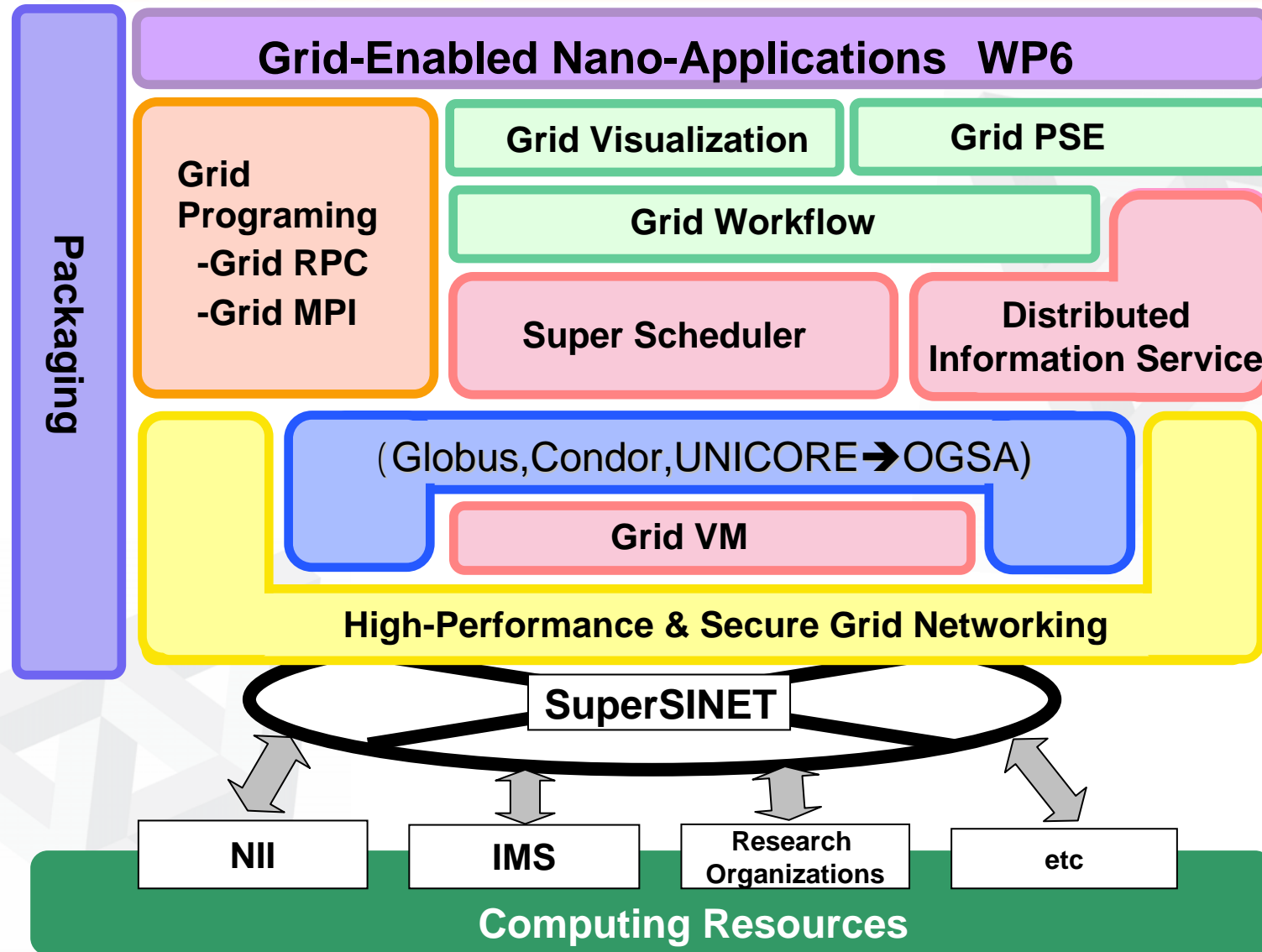


## 2. Grid-Enabling by NAREGI middlewares

**Use of Loosely Coupled Components**

**Applications to GAMESS-FMO&TINKER**

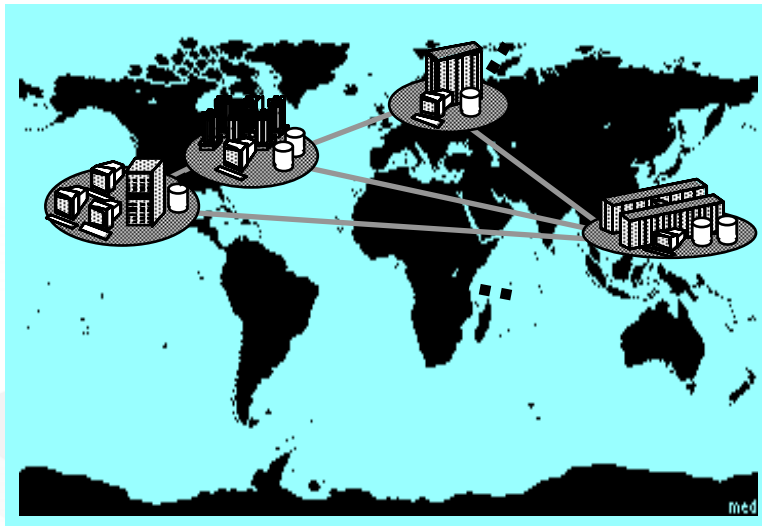
# NAREGI Software Stack



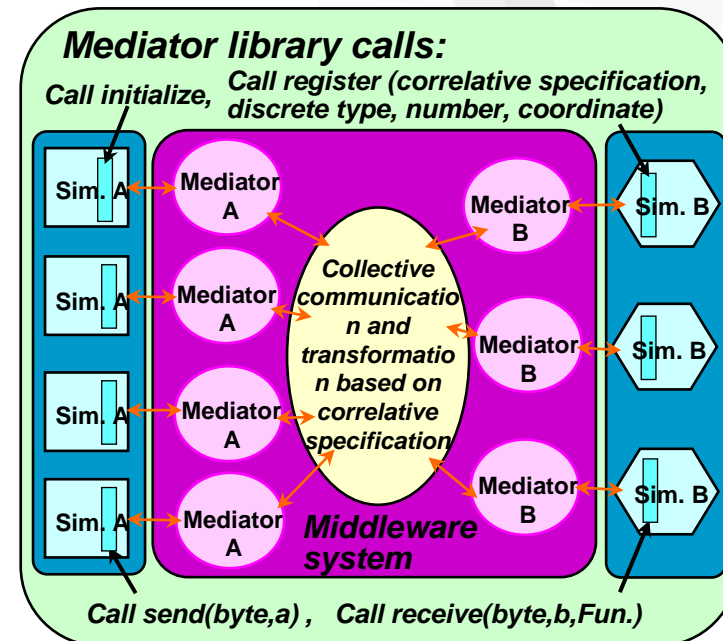
# Mediator: Grid middleware for Coupled Simulations

## For Multi-Scale and Multi-Physics Simulations

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



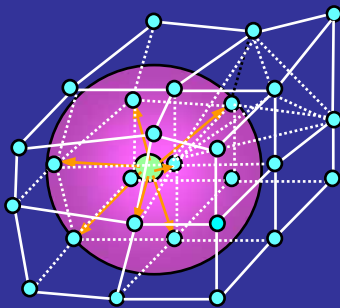
Respect Independency of each application prog.



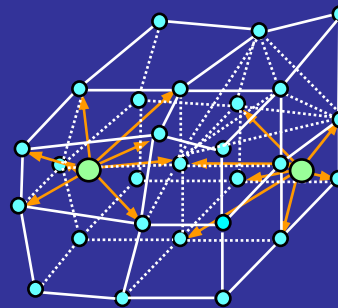
# Mediator: Grid middleware for Coupled Simulations

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.

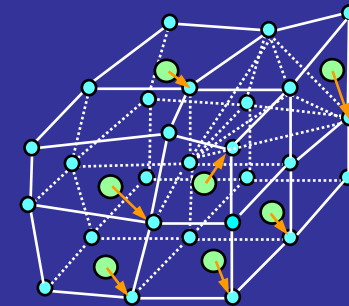
## *Correlative specification( examples )*



**In-sphere**



**First nearest neighbors**



**Nearest points**

# Mediator

-version released in march 2005

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## Discretization methods

*Particle method, Finite difference method,  
Finite element method*

## Parallel programming style

*SPMD or MPMD in static or dynamic invoke*

## High-level semantic transformation

*In-sphere, In-rectangle, 1st nearest neighbors,  
Nearest points*

## Communication paradigm

*One-way, Variable, two-way communication*

## Interconnection

*MPICH-G2, MPICH, GridMPI( developed by WP2-NAREGI )*

## Hardware architecture

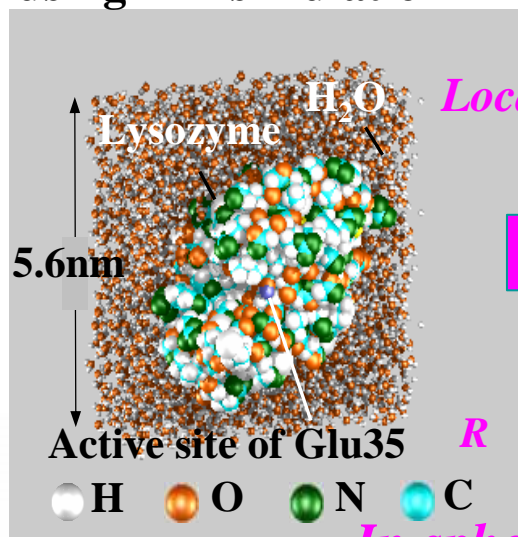
*Linux clusters, AIX, Solaris, etc.*



# Mediator assisted Molecular dynamics(MD) and Poisson-Boltzmann(PB) coupled simulation(1)

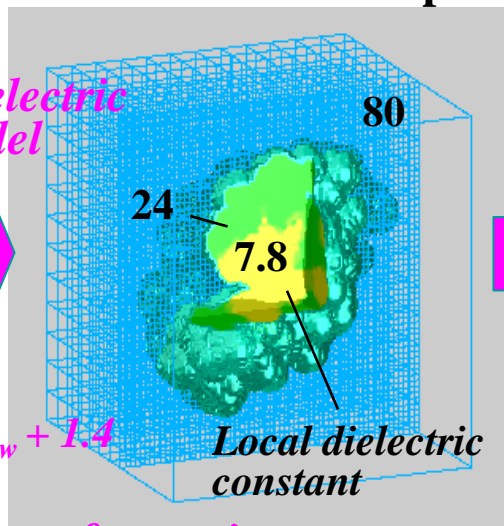
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Hydrate structure using MD simulation



*Local dielectric model*

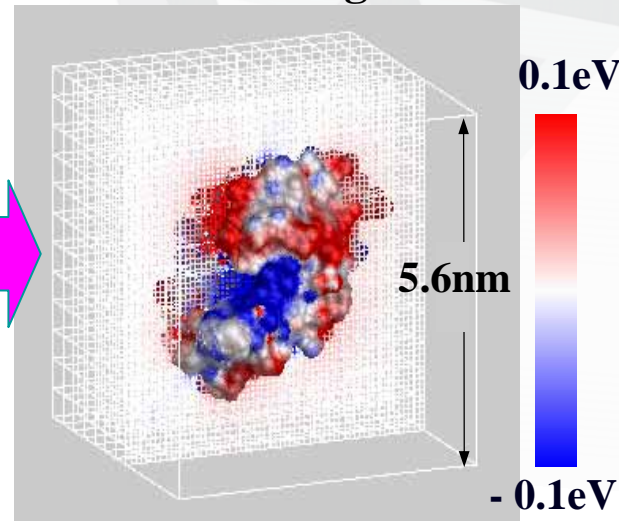
Distribution of dielectric constant over mesh point



$$R = R_{vdw} + 1.4$$

*In-sphere transformation used*

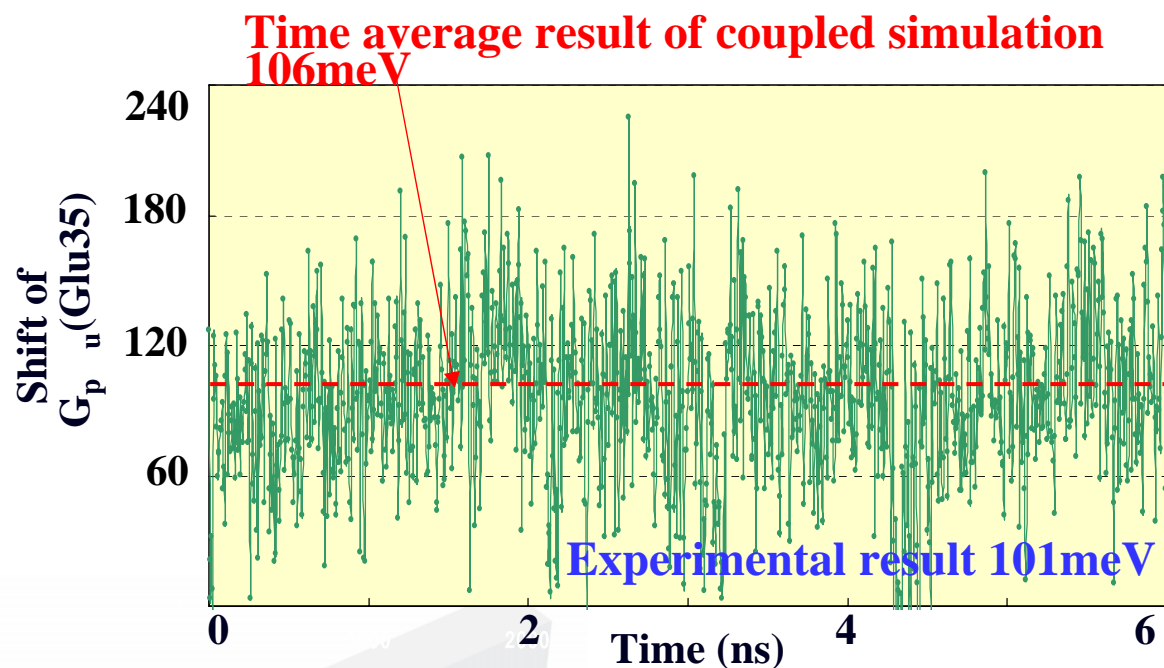
Electrostatic potential simulation using PB



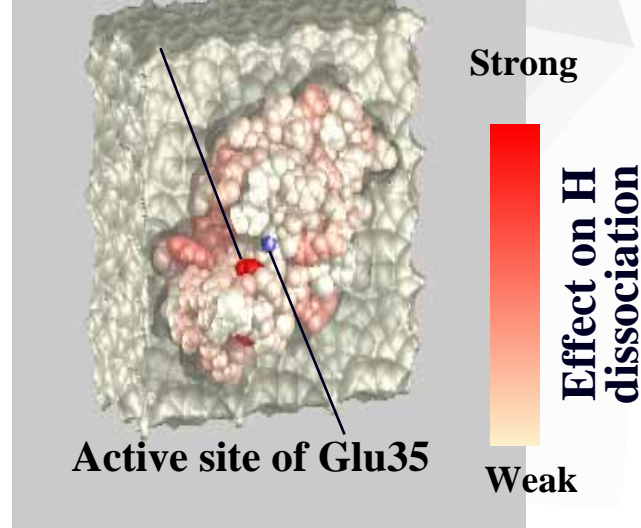
Roughly estimate “Active Site” of lysozyme and H-Dissociation energy at Glu35.

# Mediator assisted Molecular dynamics(MD) and Poisson-Boltzmann(PB) coupled simulation(2)

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Amino site that leads to H dissociation at Glu35



$$\text{pKa} = G_{p_u}(\text{protein}) / 2.303 k_B T - \text{pKa}(\text{Glu}) (=4.4)$$

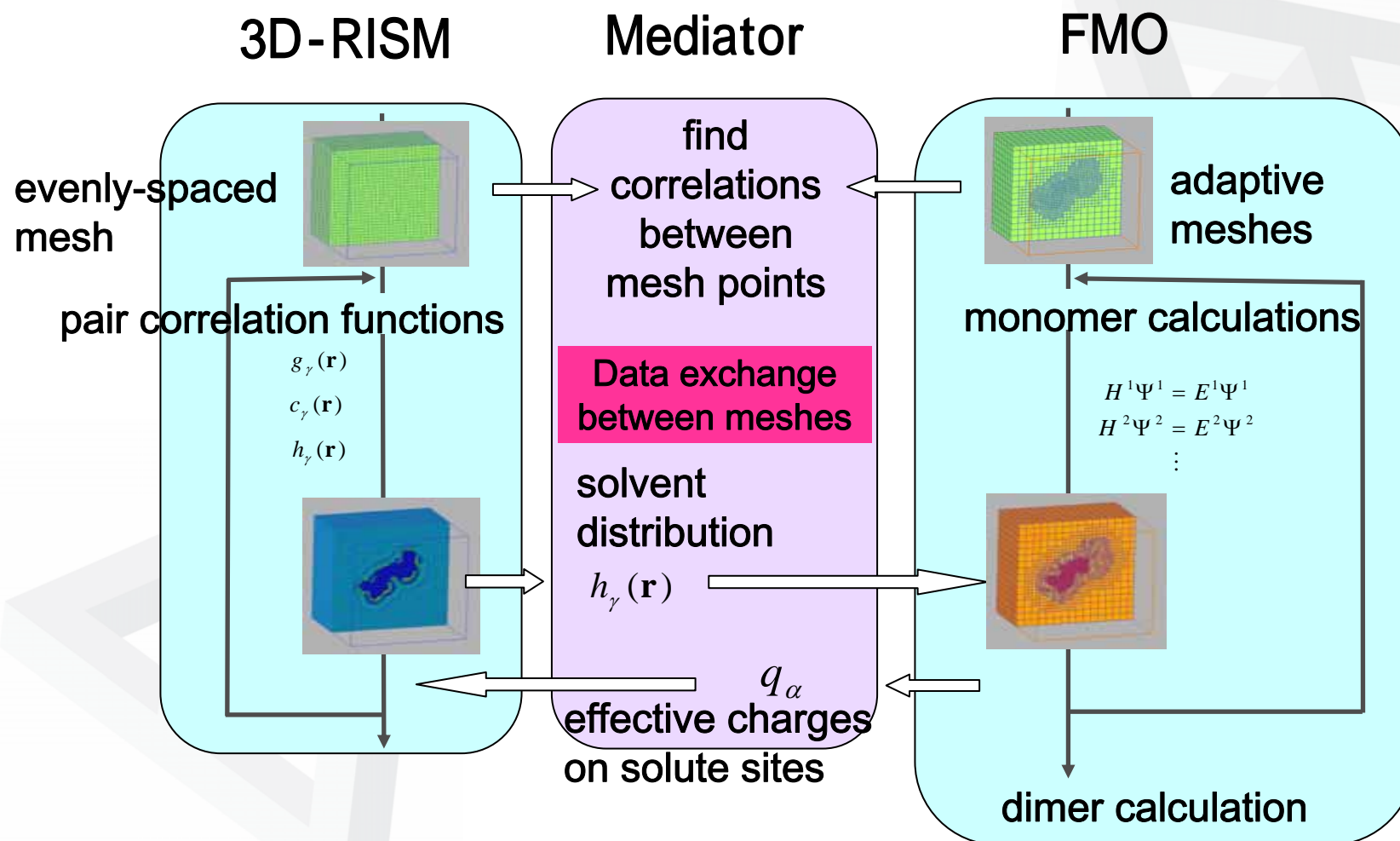
**pKa value( ~ 6) at COOH in Glu35  
roughly 50 times larger probability  
compared with amino sites around**



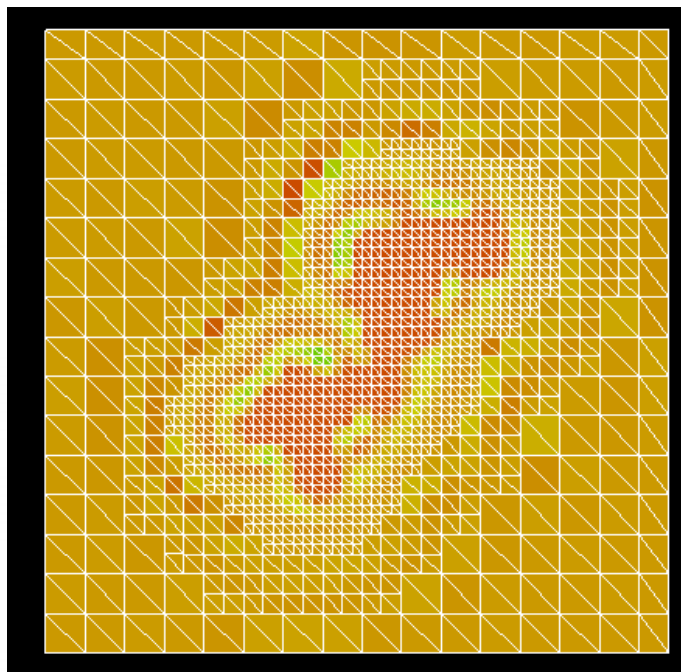
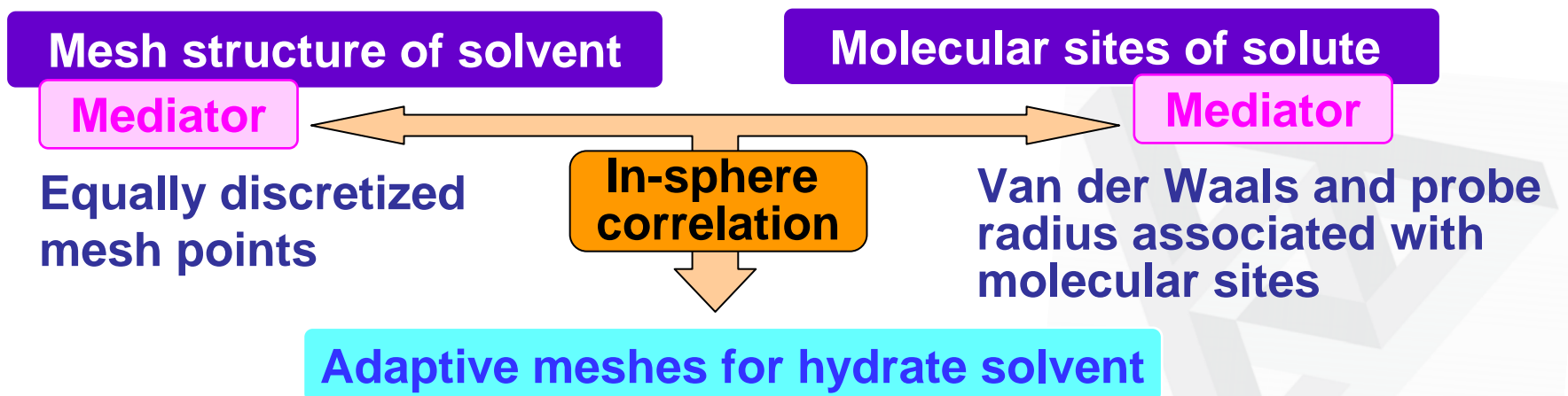
# 2<sup>nd</sup> Example: RISM-FMO coupled Simulation

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## Simulation Scheme



# Data Exchanges in RISM-FMO



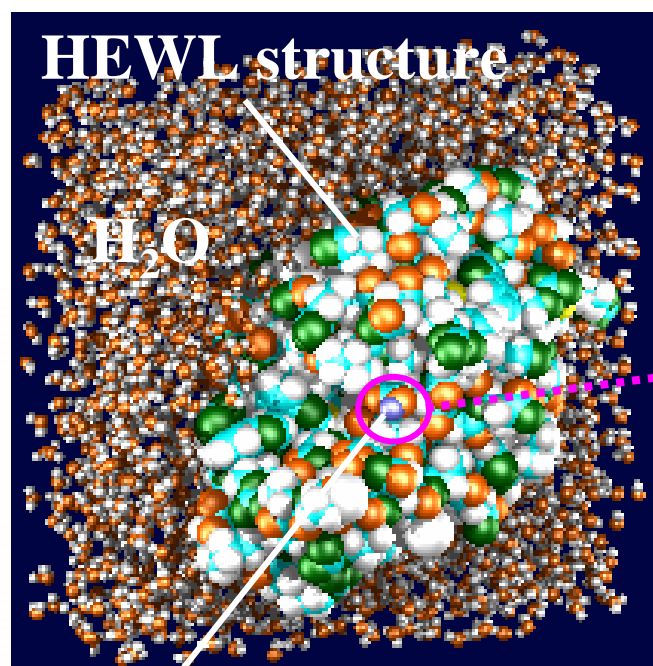
# Summary of Coupled simulation model

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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

# Solvent interactions of hydrolysis in Lysozyme

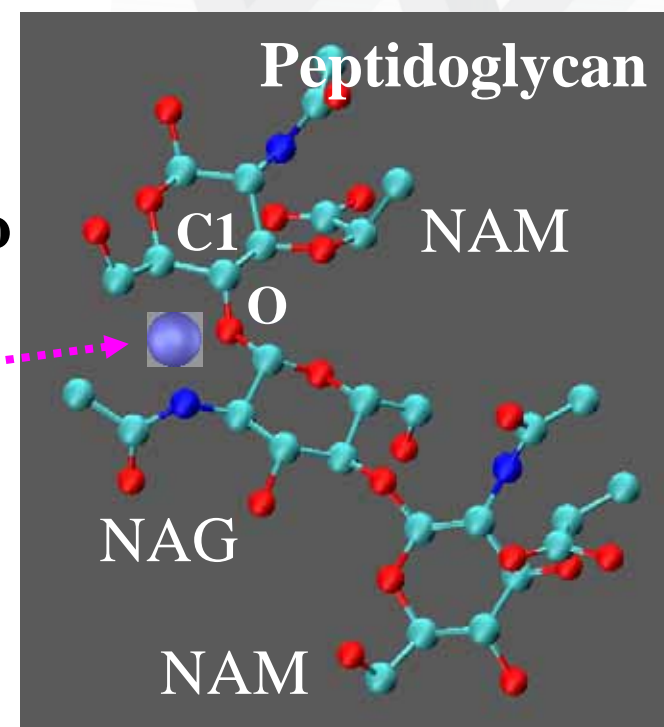
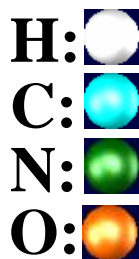
A catalytic mechanism of hydrolysis in Lysozyme is Analyzed by RISM-FMO, in which proton transfer leads to bacteriolysis in peptidoglycan of bacterial cell wall.



Active site of Glu35

Bacteriolysis by hydrolysis due to H dissociation

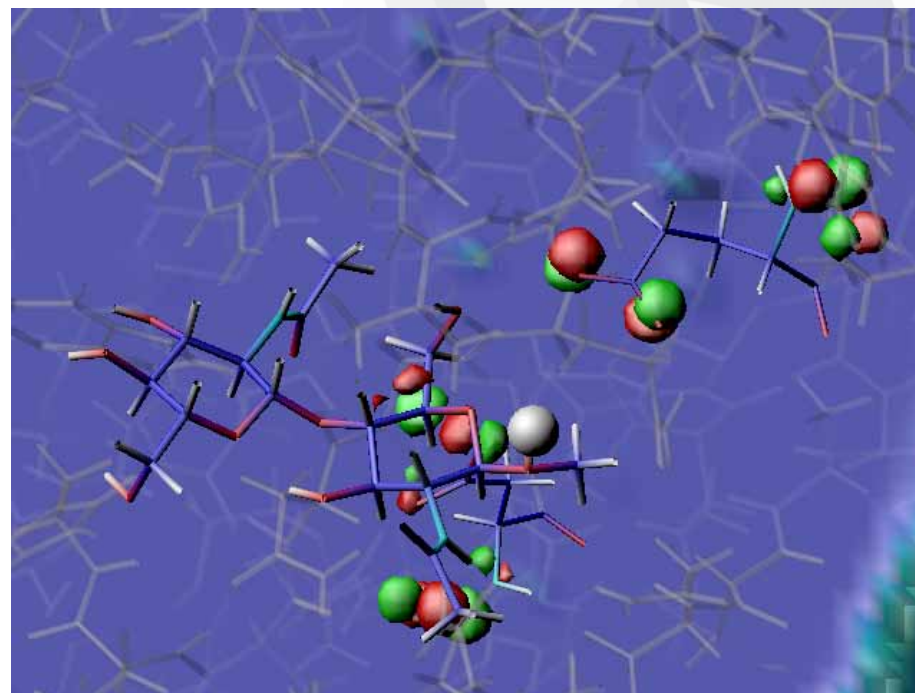
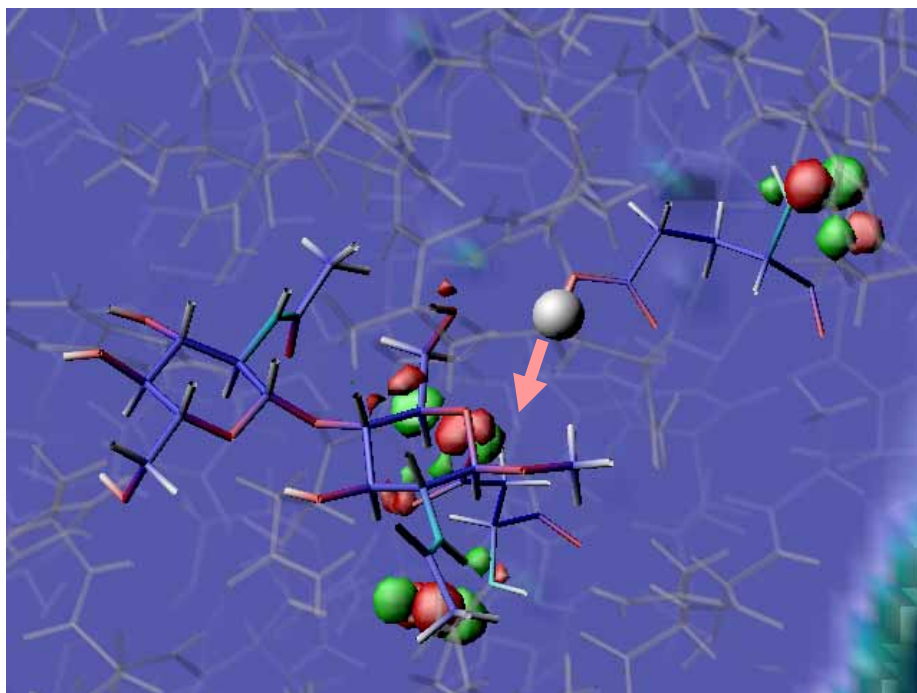
$H^+$



NAM: N-Acetylmuramin  
 NAG: N-Acetylglucosamin

# Electronic structure analysis on Proton transfer in Lysozyme (in solution)

## Proton transfer from active site of Glu35 to peptidoglycan



RISM-FMO coupled simulations reveal realistic microscopic picture  
of proton transfer in Lysozyme

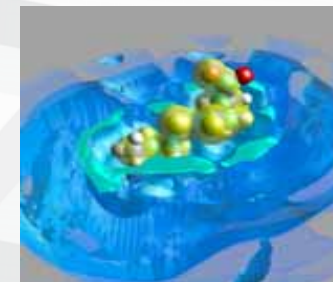


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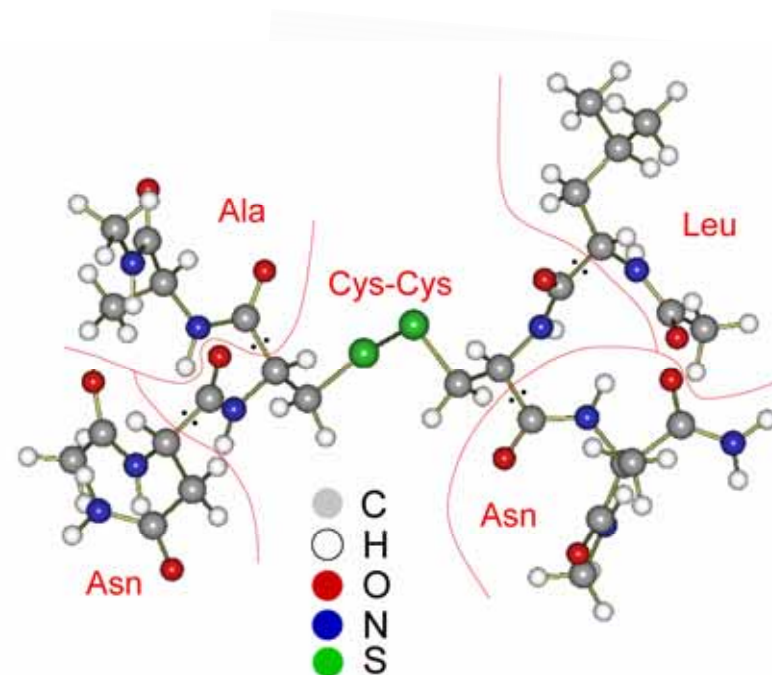
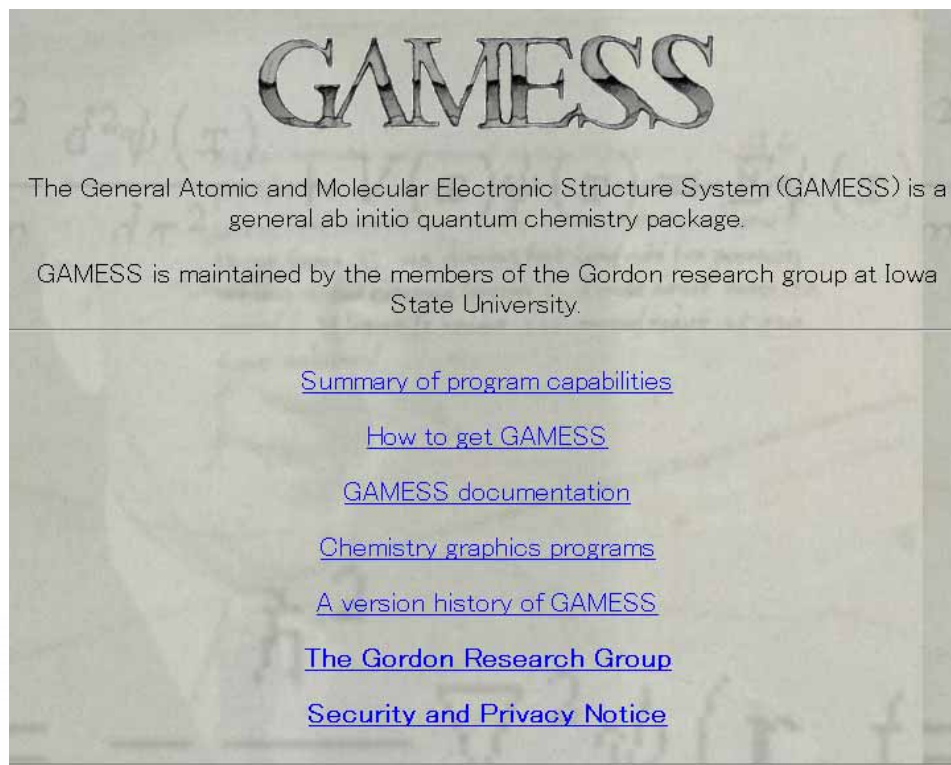
## 2. Grid-Enabling by NAREGI middlewares

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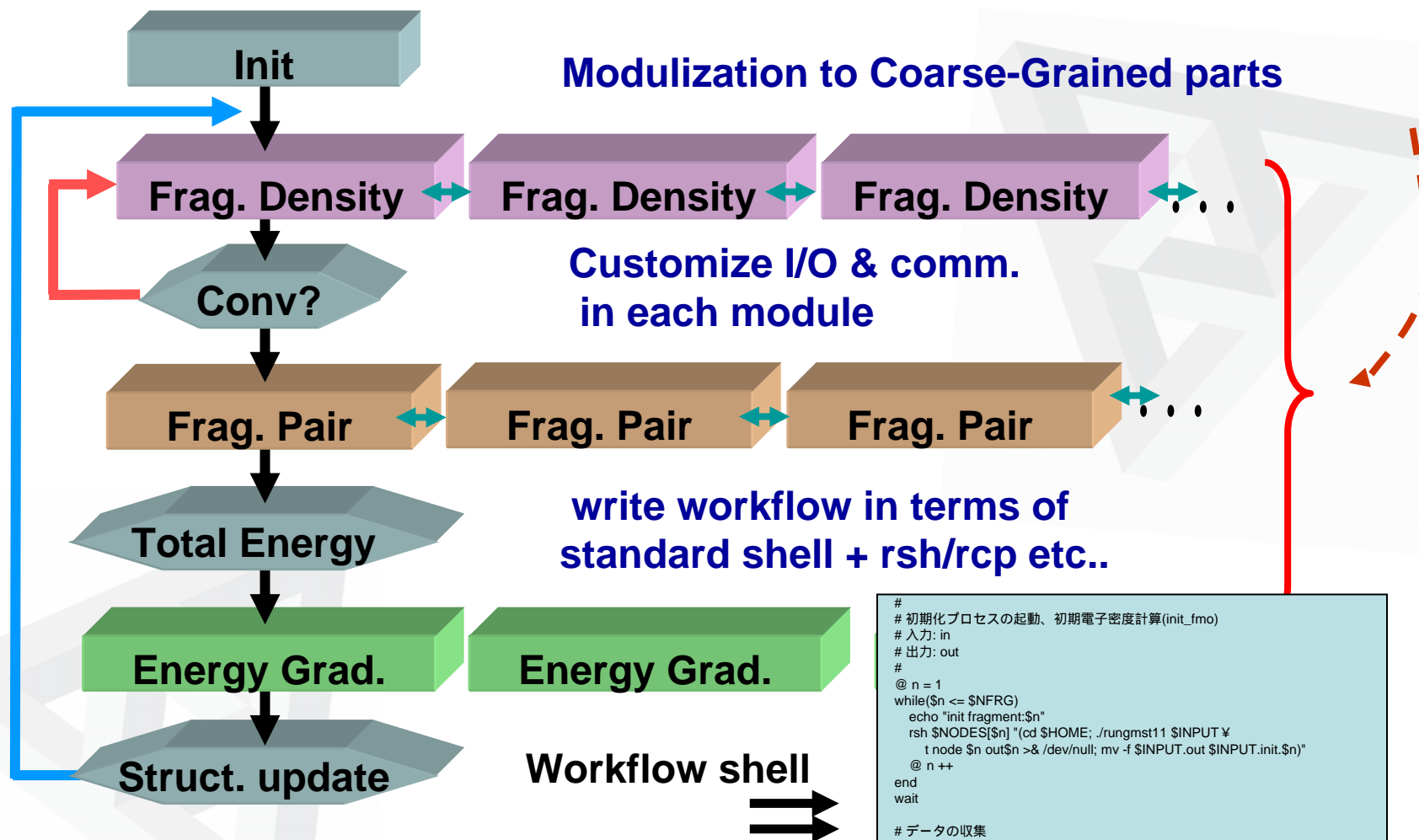


# Grid enabling of the GAMESS FMO prog.



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

# Grid enabling of the GAMESS FMO prog.



deploy each module and translate  
shell scripts into UNICORE NAREGI workflow

Science Gateways in GGF14 Chicago

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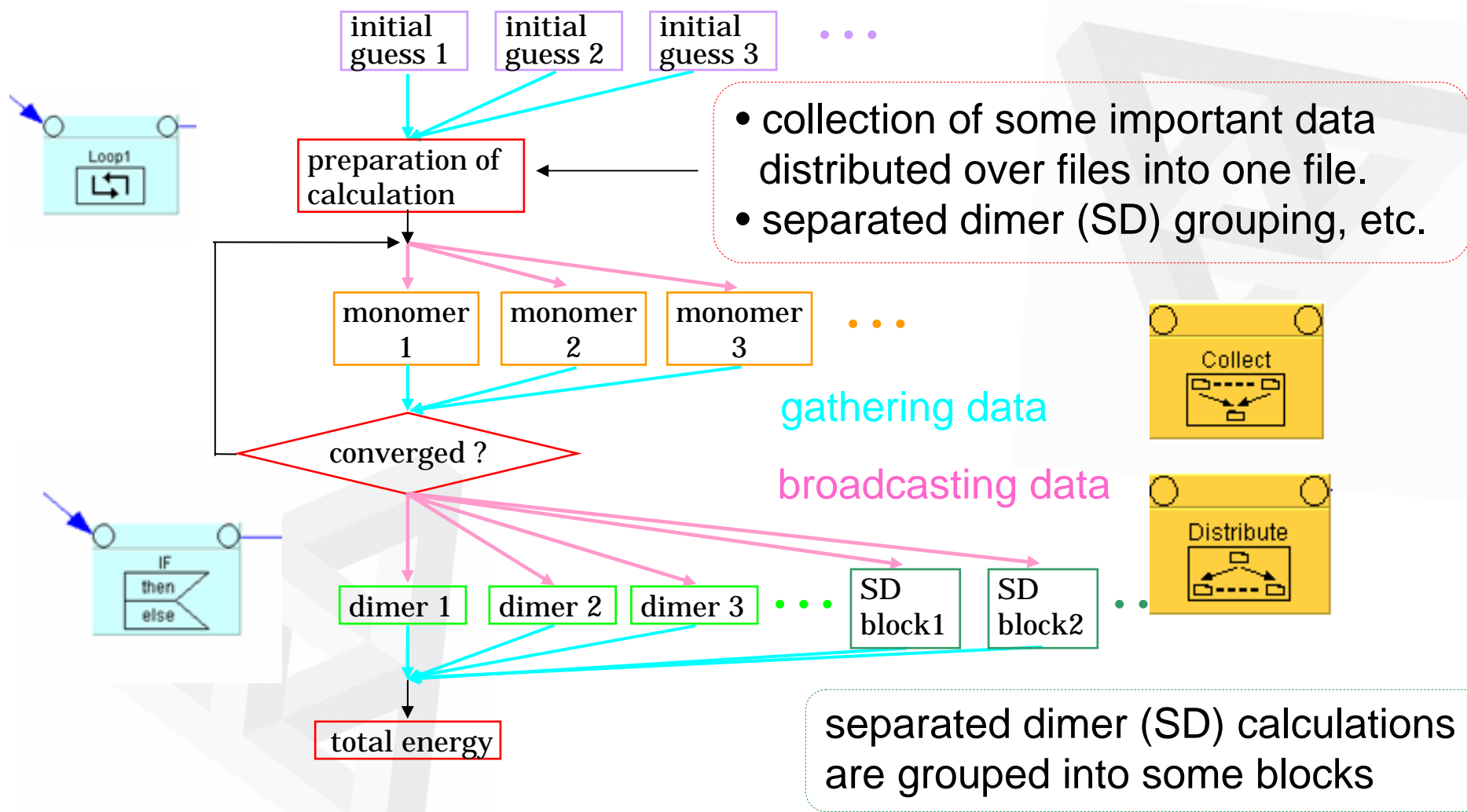
#
# 初期化プロセスの起動、初期電子密度計算(init_fmo)
# 入力: in
# 出力: out
#
@ n = 1
while($n <= $NFRG)
  echo "init fragment:$n"
  rsh $NODES[$n] "(cd $HOME; ./rungmst11 $INPUT ¥
    t node $n out$n >& /dev/null; mv -f $INPUT.out $INPUT.init.$n)"
  @ n ++
end
wait

# データの収集
@ n = 1
while($n <= $NFRG)
  if($MY != $NODES[$n]) then
    rcp $NODES[$n]:$HOME/out$n out$n >& /dev/null
  endif
  @ n ++
end
wait
  
```

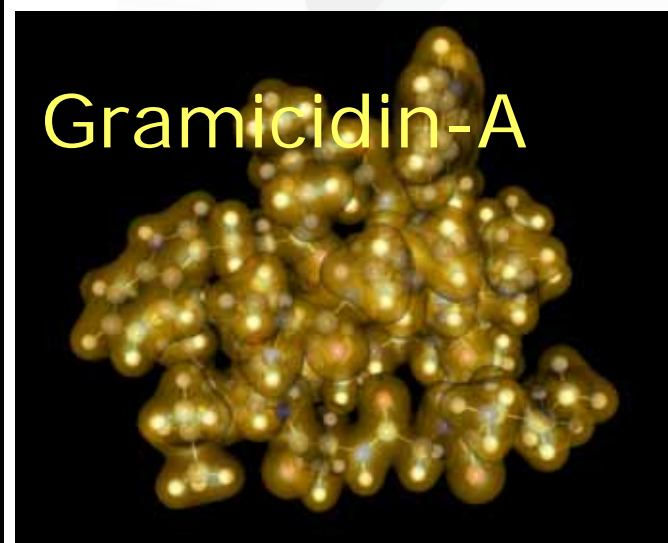
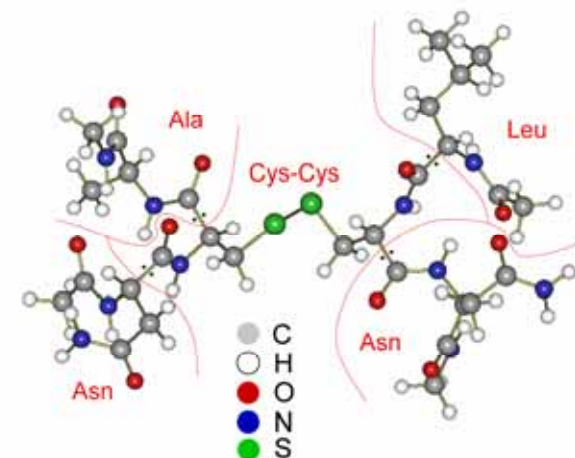
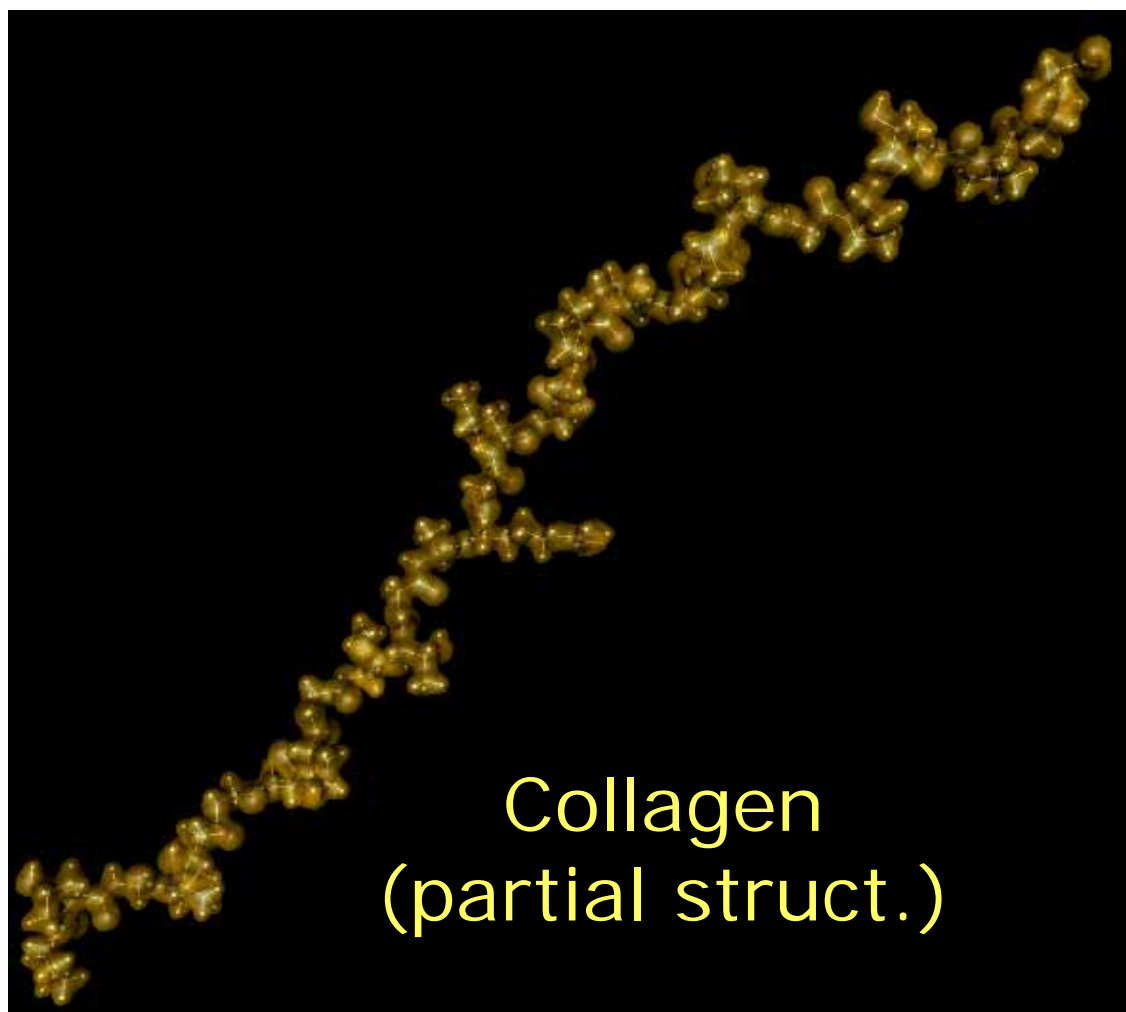
Shell scripts

ative

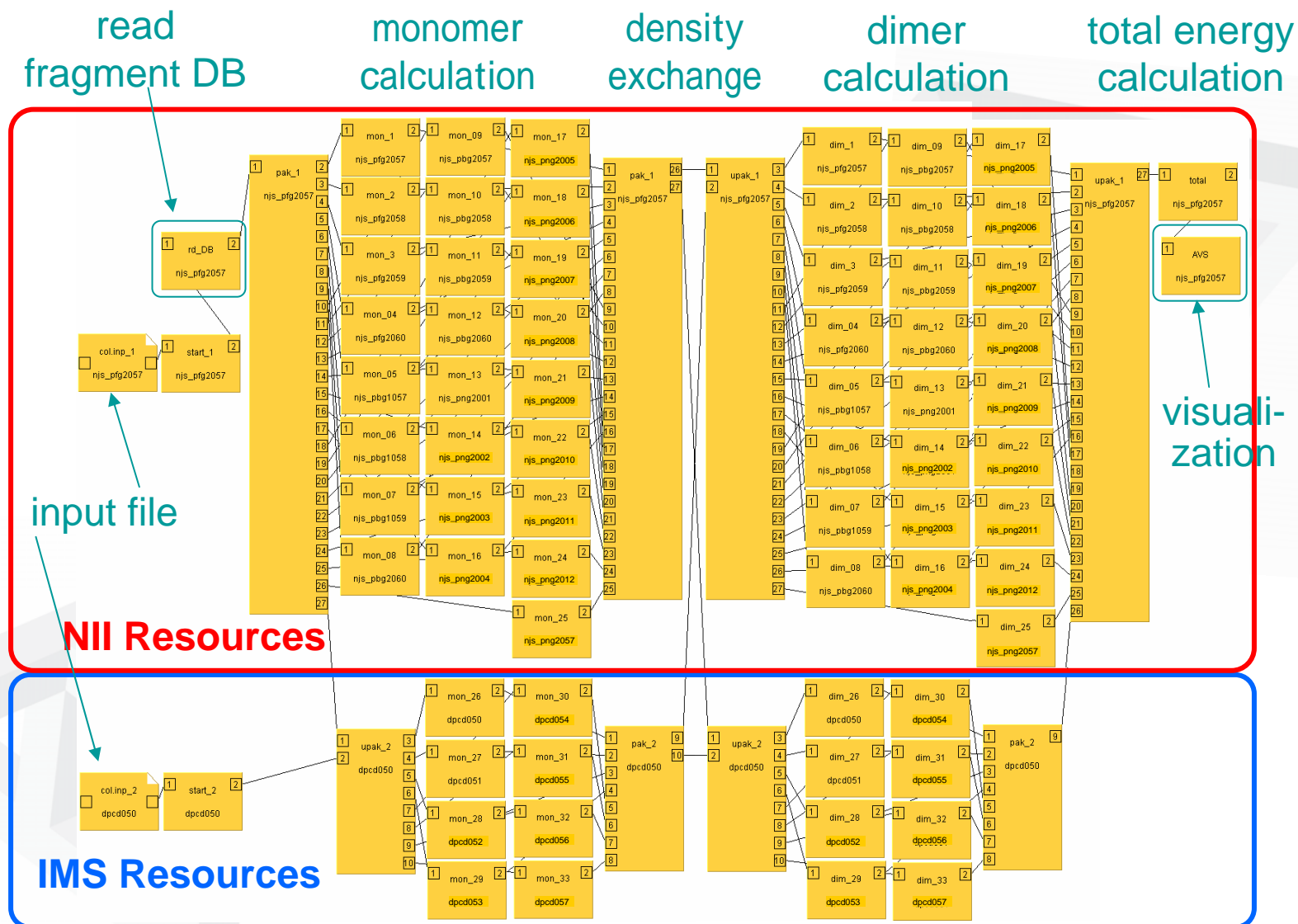
# NAREGI WorkFlow Tool



# Protein Molecules examined by Loosely coupled FMO on Computational Grid

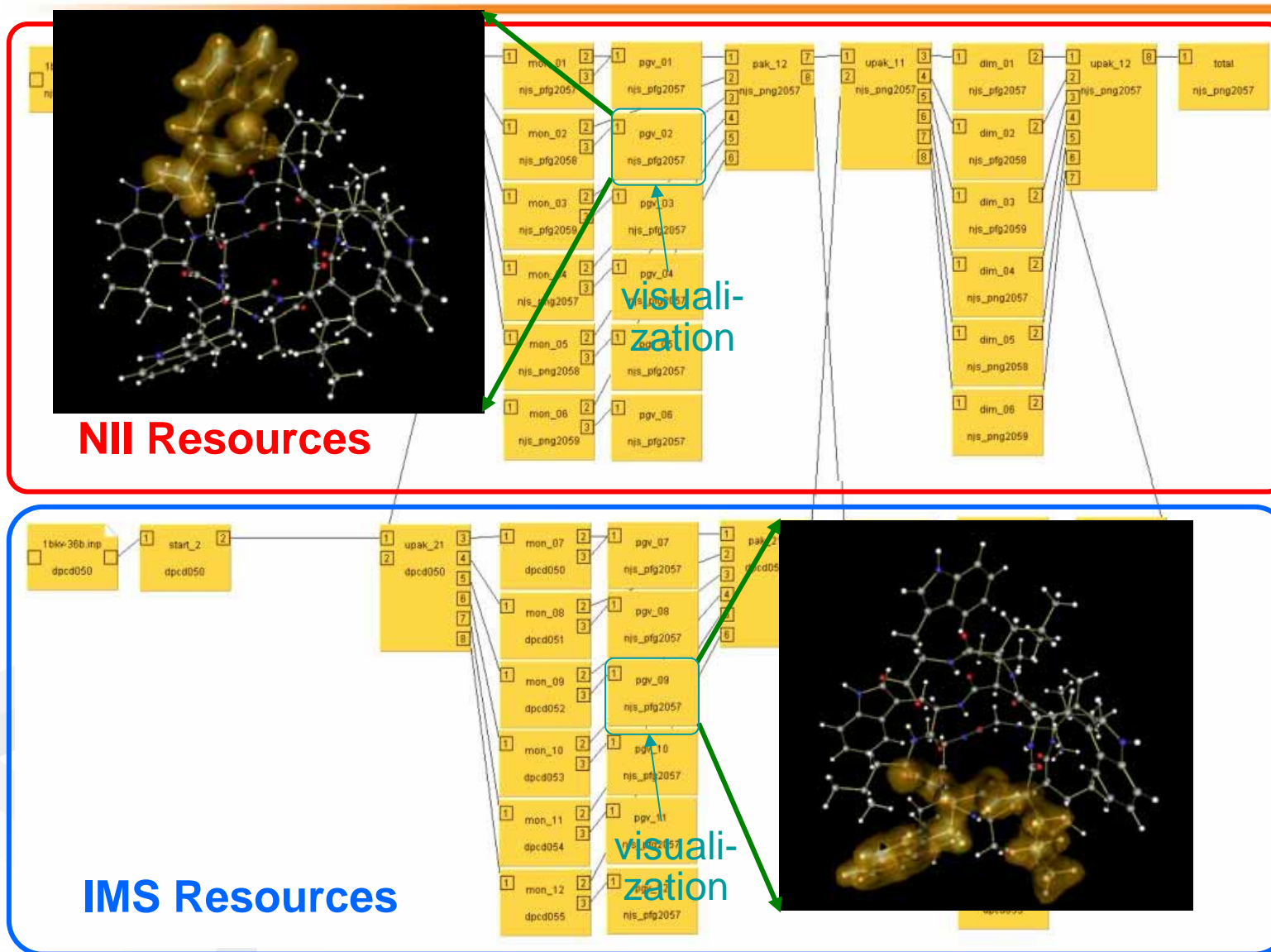


# Workflow based Grid FMO Simulations of protein





# Fragment Electron Density in Grid FMO

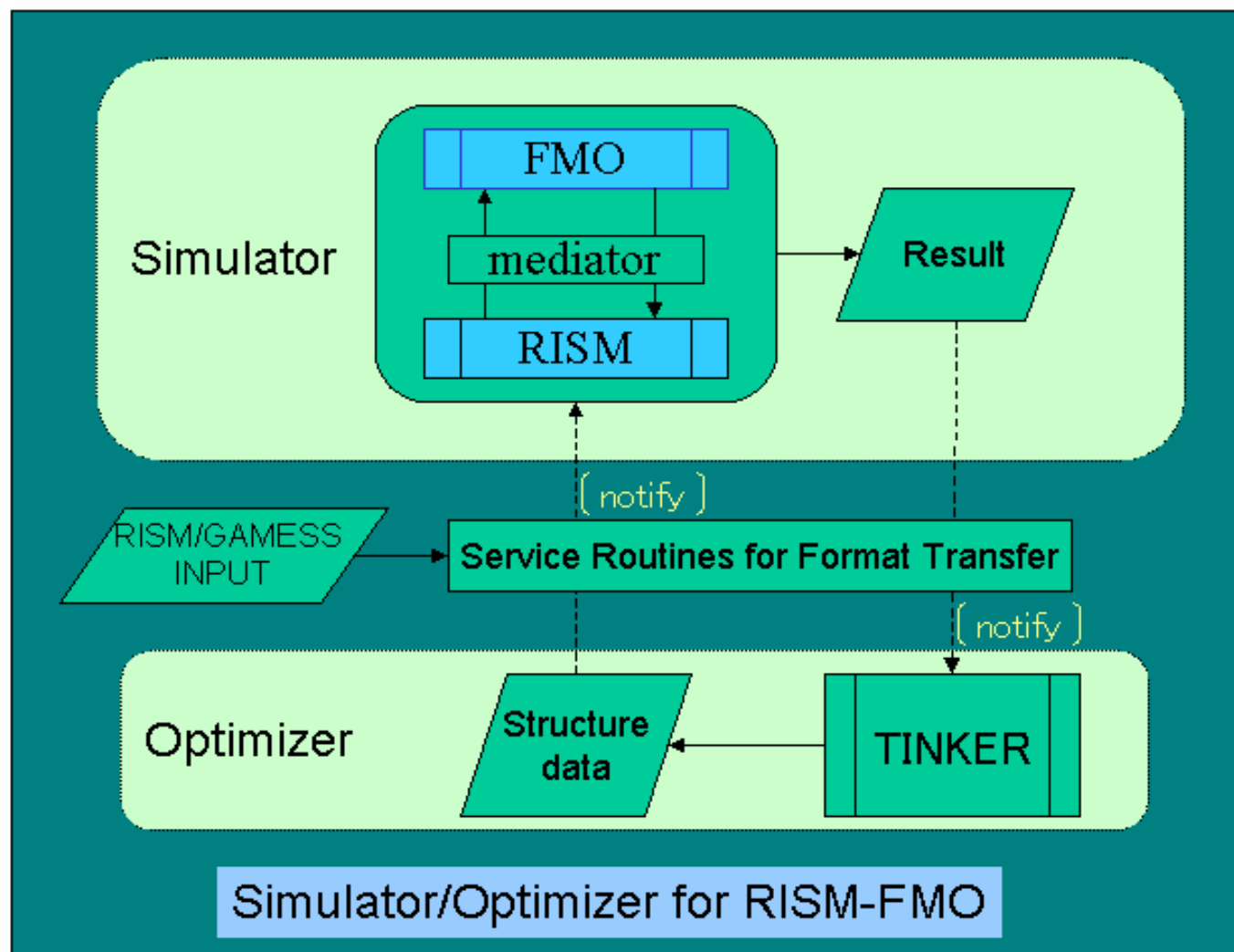




# Full Geometry Optimization of Protein in water

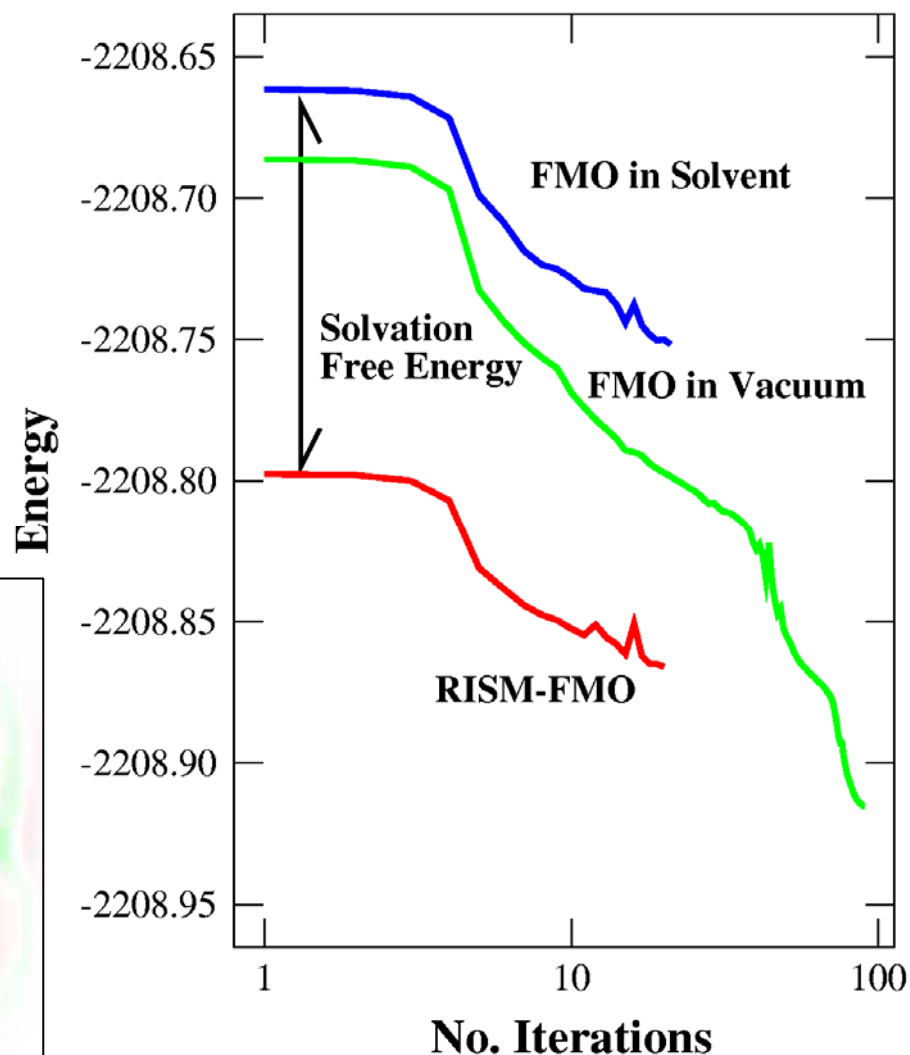
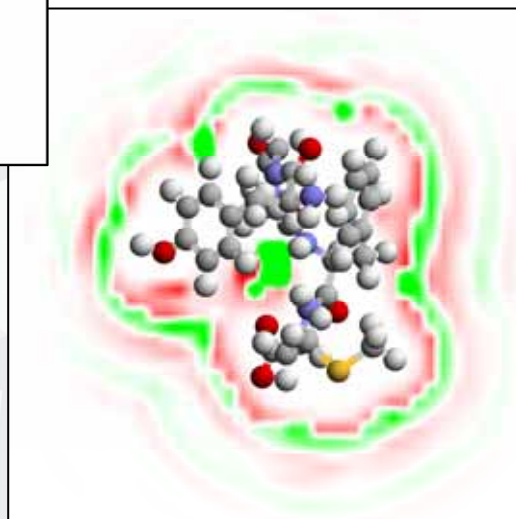
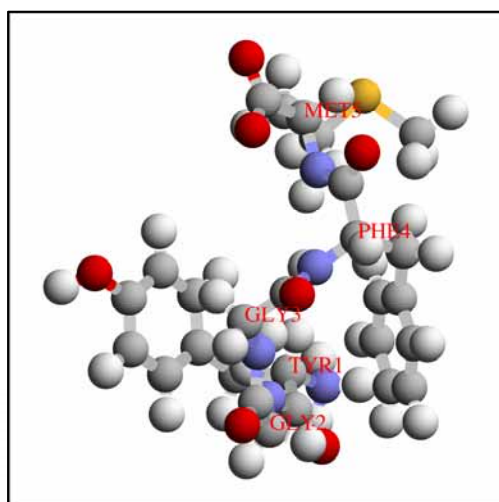
## 3D-RISM/FMO with loosely coupled TINKER

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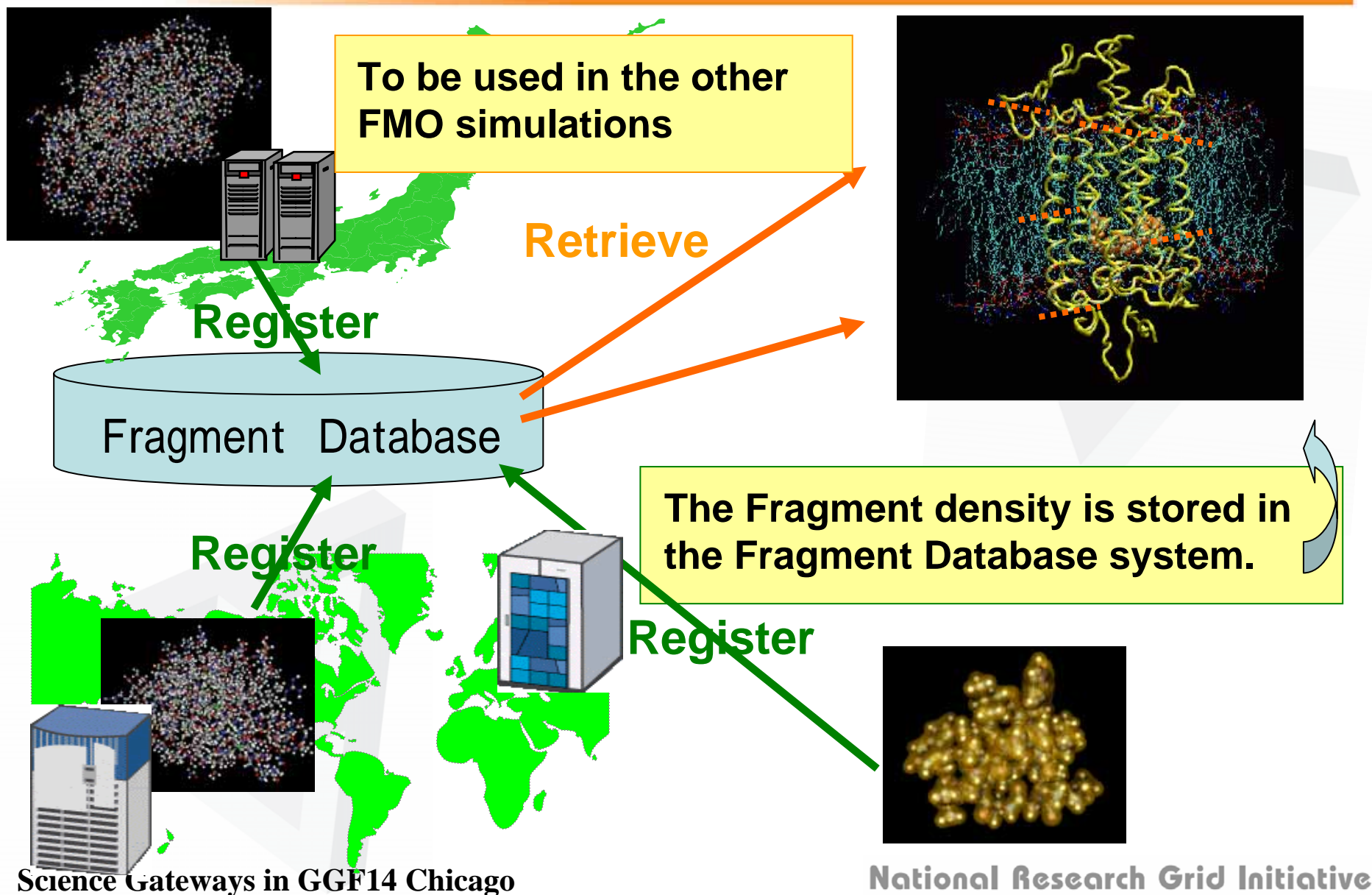


# Full Geometry OPT. of Met-enkephalin

The amino-acid sequence is 'TYR-GLY-GLY-PHE-MET'. We start the optimization process from the Model 1 of PDB data "1plw".

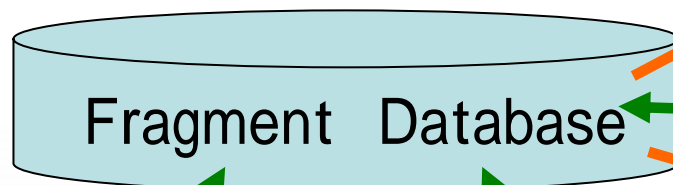
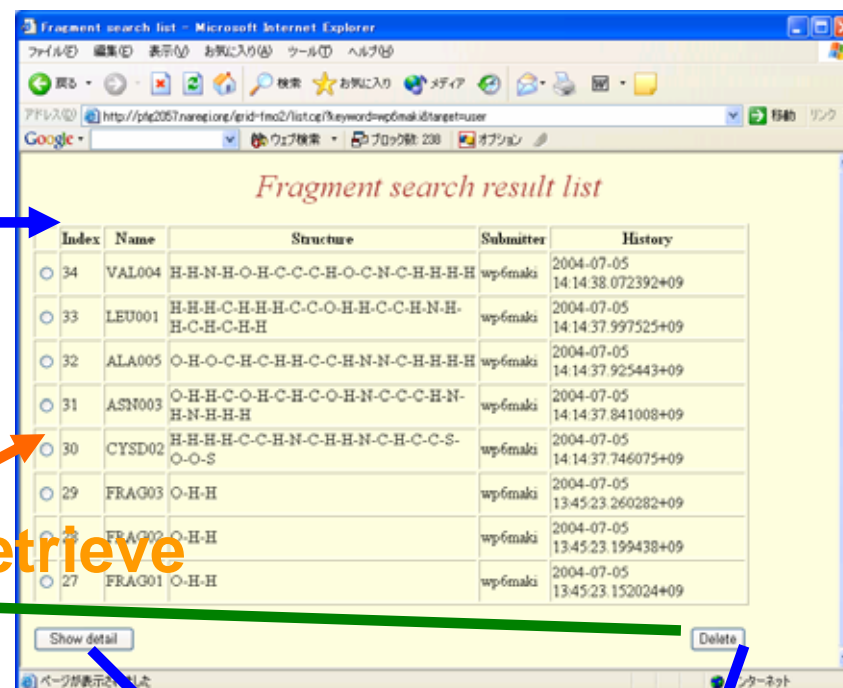
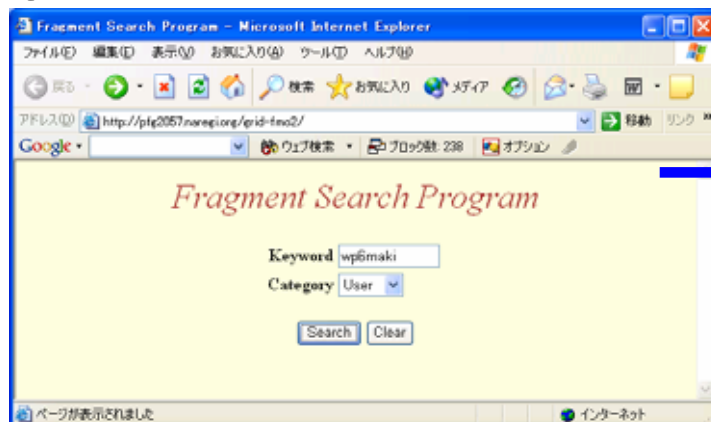


# Grid Database tool for Optimized Protein Structures and Fragment density



# Fragment Database Tools

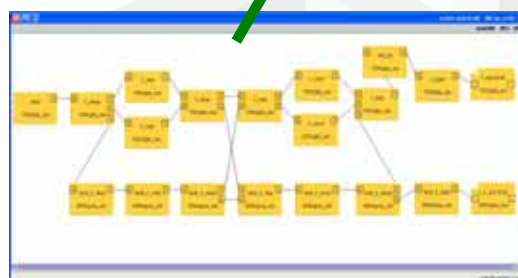
## Search



Retrieve

more information...

Register



# Concluding remarks

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**A solution based on Research Grid will have significant advantages for customizing interdisciplinary simulations,**

**and**

**Grid will make a big chance for the Collaboration between Computational Scientists and Computer/Information Scientists in HPC field.**

# Acknowledgement

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Dr. S. Sekiguchi and Prof. S. Matsuoka

## NAREGI

- Workflow Team
- SuperScheduler Team
- Dr. Ho, Dr. Kubo (Hitachi)
- Mr. Miura, Mr. Takano (Fujitsu Kyushu)