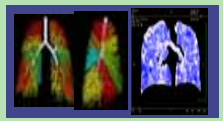
Multi-Scale Computing Grid

Organ and Tissue Simulation



Physiome; Simulations of surface muscle electric potential and lung ventilation

Cell Simulation

Cellome; Simulation to study the drug inhibitions to ion channels in human cardiac muscle cells.

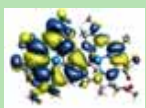
Protein Folding Simulation

Proteome; Prediction of ab initio protein folds from amino acid sequence information

Simulation for Protein Complexes

***In silico* Drug screening;**
prestoX-basic
The molecular dynamics program

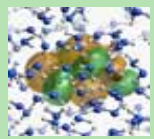
Electron level Simulation

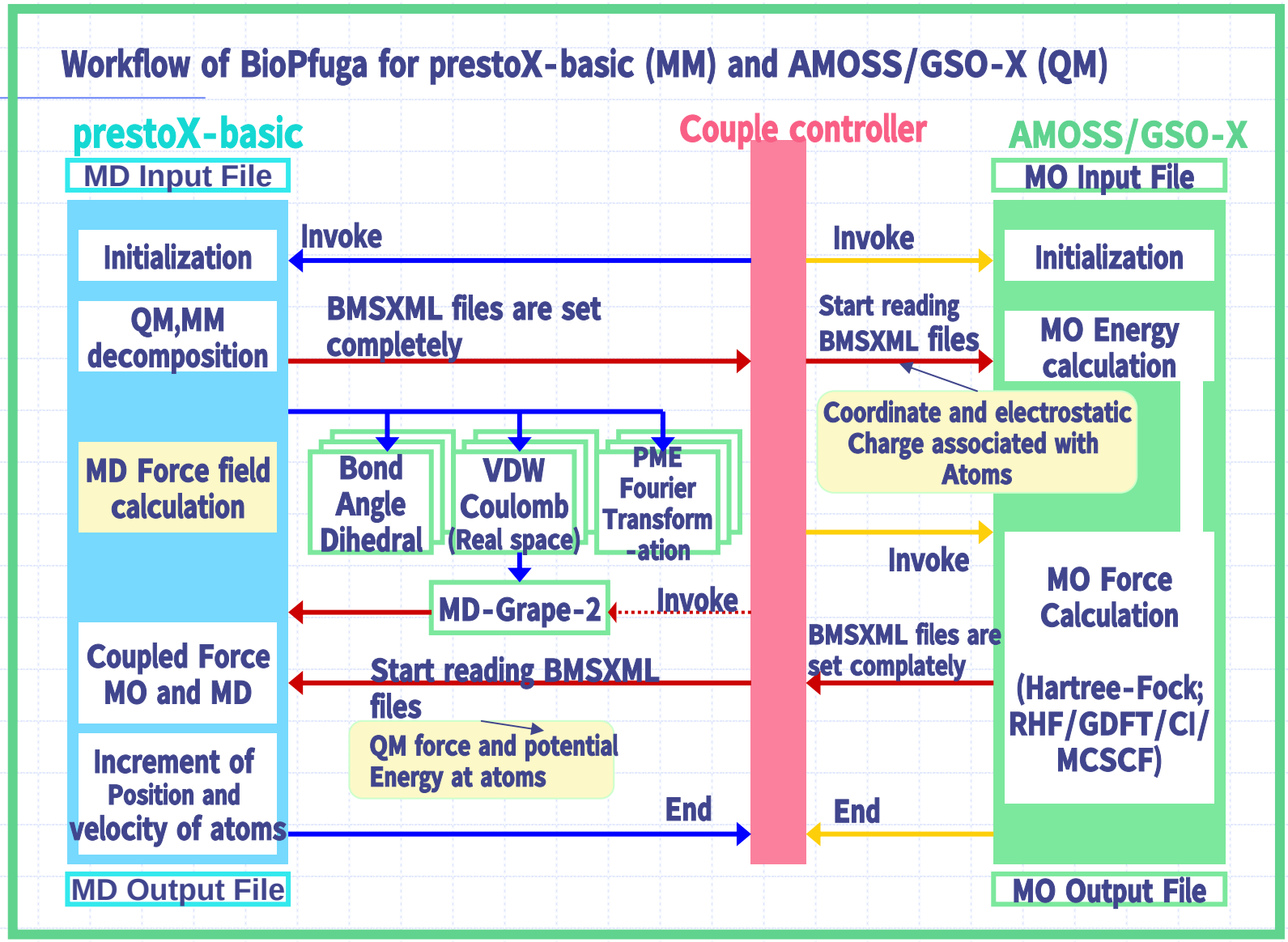


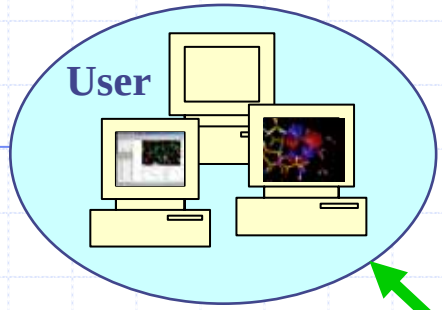
Biochemical Reactions; AMOSS and GSO-X
The quantum chemical program for computing
ab initio molecular orbital.

ownian Dynamics Simulation

BioPfuga;
Hybrid QM/MM Simulation




Workflow of BioPfuga for prestoX-basic (MM) and AMOSS/GSO-X (QM)
prestoX-basic
Couple controller
AMOSS/GSO-X
MD Input File
MO Input File
Initialization
Invoke
Invoke
Initialization
QM,MM decomposition
BMSXML files are set completely
Start reading BMSXML files
MO Energy calculation
Coordinate and electrostatic Charge associated with Atoms
MD Force field calculation
Bond Angle Dihedral
VDW Coulomb (Real space)
PME Fourier Transform -ation
Invoke
MO Force Calculation
(Hartree-Fock; RHF/GDFT/CI/ MCSCF)
MD-Grape-2
Invoke
BMSXML files are set complately
Coupled Force MO and MD
Start reading BMSXML files
QM force and potential Energy at atoms
Increment of Position and velocity of atoms
End
End
MD Output File
MO Output File



http

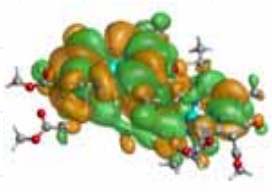
SOAP

Portal

Molecular Dynamics
-Service

prestoX

MDGrape2

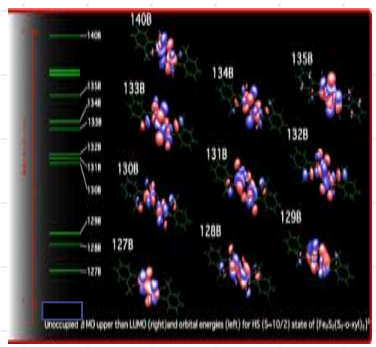


Notification:
BMSML

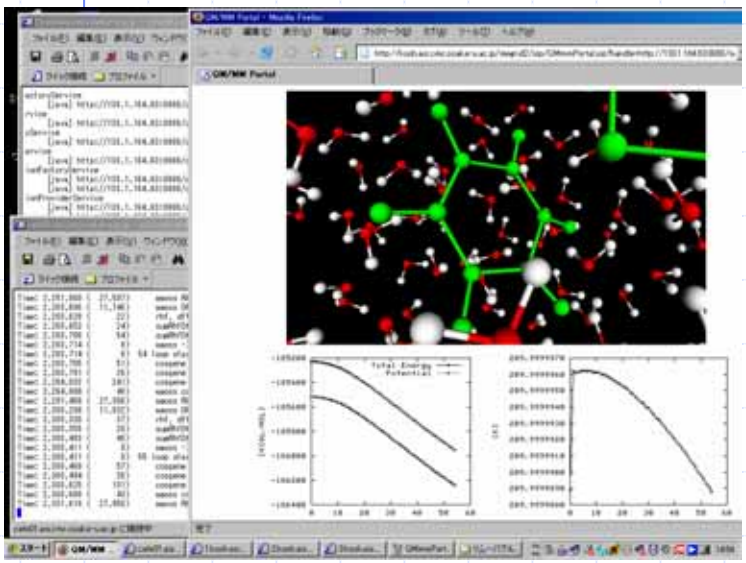
Hybrid Quantum
Mechanics-Service

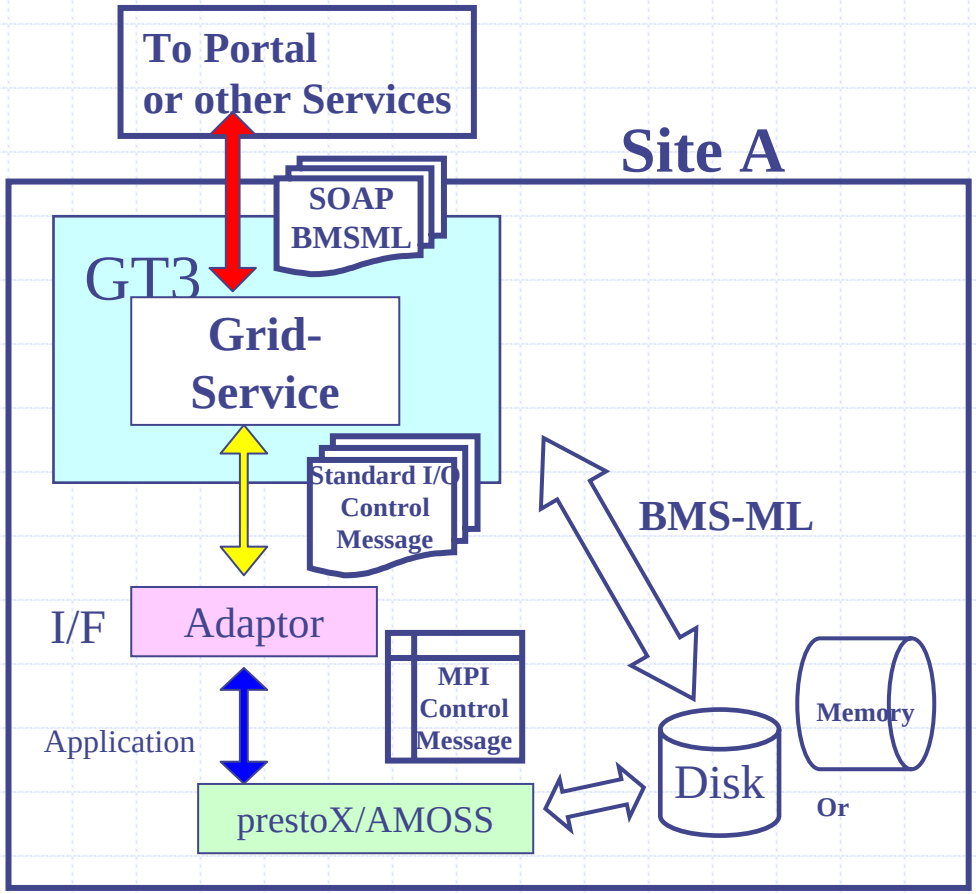
AMOSS
Hartree Fock
calculation

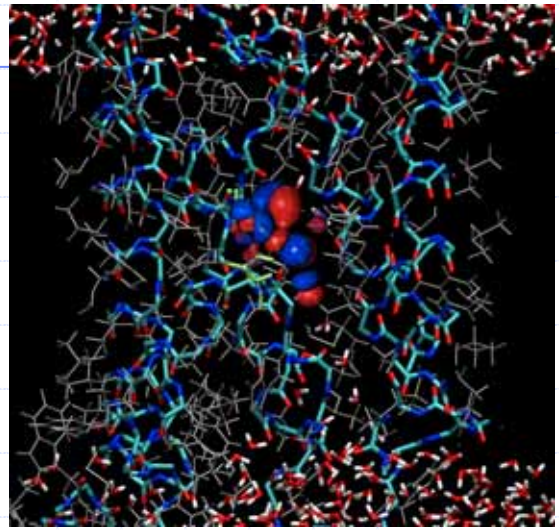
GSO-X
DFT spin
calculation

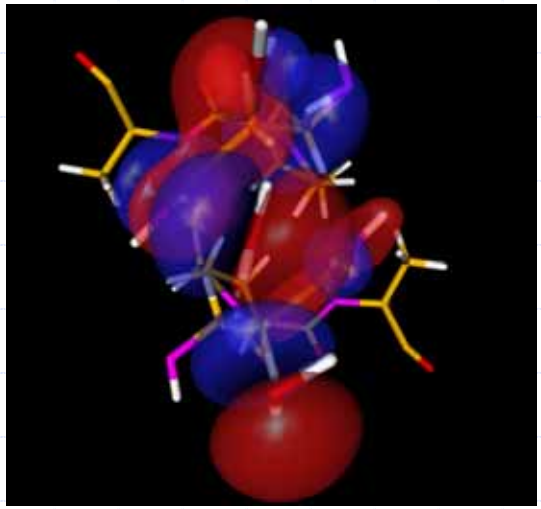


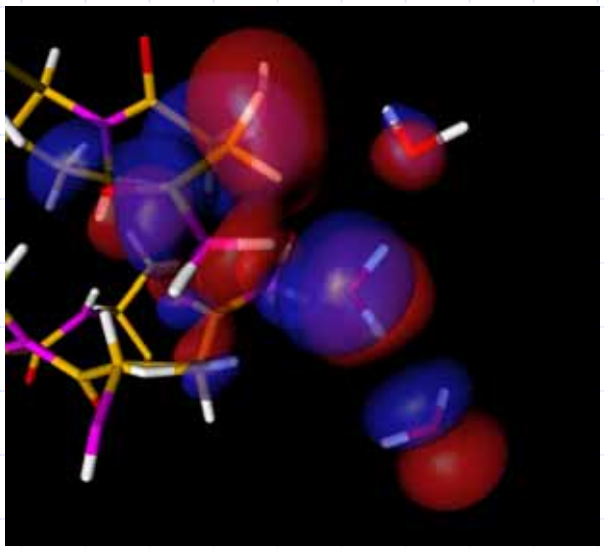
Data transfer of Grid-Service for QM/MM Calculation on *BioPfuga*











This work Supported by

HITACHI NEC