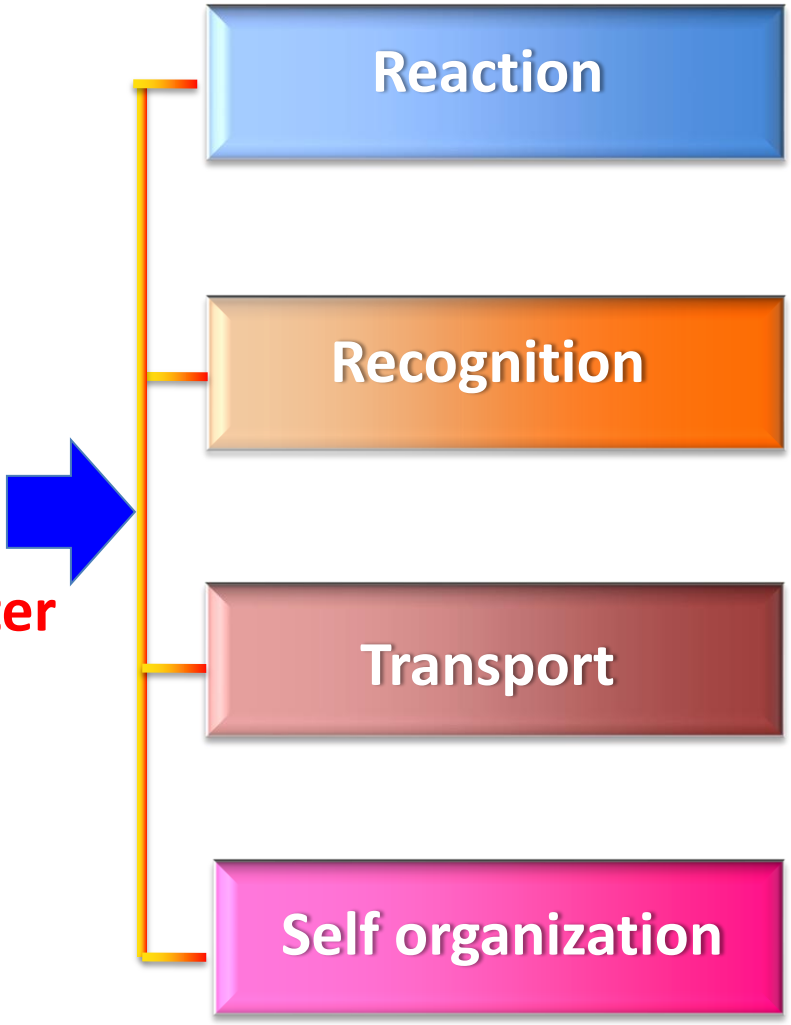
Future plans: biological function and information

Insight from Physics, Chemistry, Biology with Computer Simulations



Origin of Biomolecules, Detecting Life
Many Enzymatic Reactions :
Synthetase, Ligase, Hydrase, Peptitase, Lyase, and so on.

Enzyme-Substrate interaction, Substrate and Environment selectivity, Signal transport

Proton transfer, Electron transfer, Ion transport, Molecule transport, Protein transport, Signal transport

Entropy-driven effects (some cases), Dynamic order/disorder transition, Non-equilibrium phenomena

All topics are of great importance to know bio-functions

Our Goal is to treat with these phenomena at Atomic-level

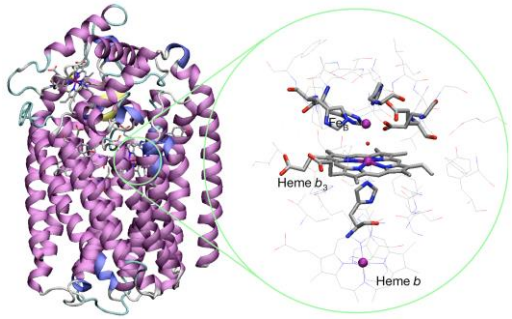
Total Design of Our Group

Accuracy

Theory , Algorithms, Code developments and Its Applications

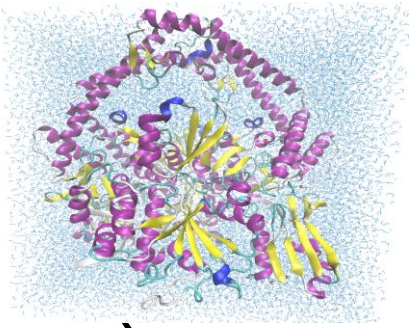
Fragment MO

Analyses on Interaction energy



RSCPMD/PWCPMD

Dynamics on Enzymatic reactions

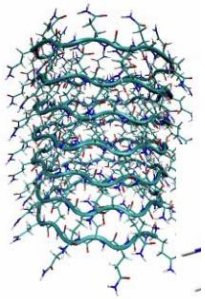


QM/MM

Static Enzymatic Reaction Analyses

Classical MD

Analyses on structures, large amplitude motion, etc.



Coarse-grained/ Accelerated MD

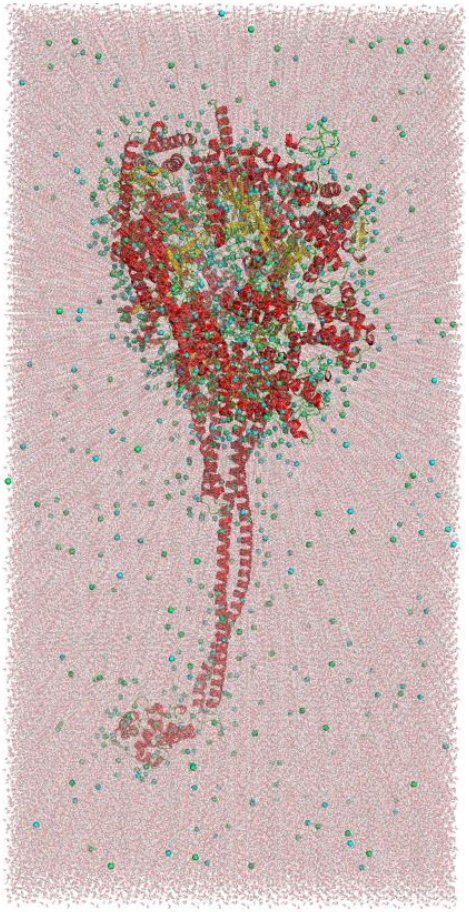
Protein-Protein, Protein-Enzyme complex formation

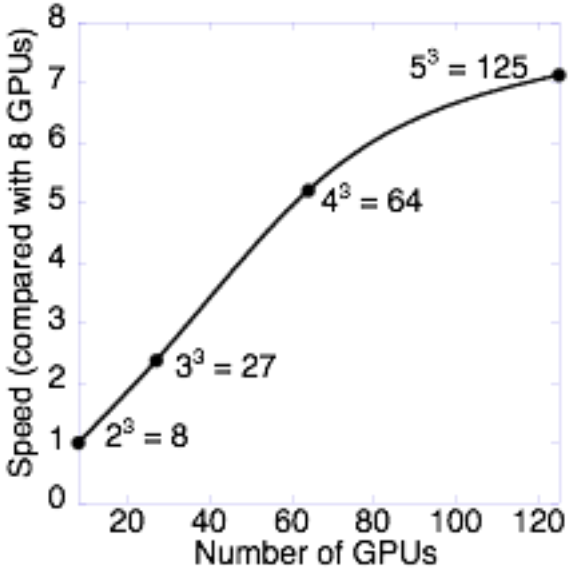
Fluid Mech., Continuum Models, Bio informatics (we need in future)

MD of Dynein using a GPGPU-based program

dynein(3,322 residues) + 4ADP (ADP form) + 1Mg^{2+} + 309,689 TIP3P water + 574Na^{+} + 528 Cl^{-} (cygene) MD

Totally one million atoms by platypus





Collaboration with Dr. Takano @ Nakamura Group IPR Osaka Univ.

It scales well until 64 GPUs

Even with 125GPUs, we can still retain high parallel efficiency

2^3GPU→5^3GPU: 7 times faster

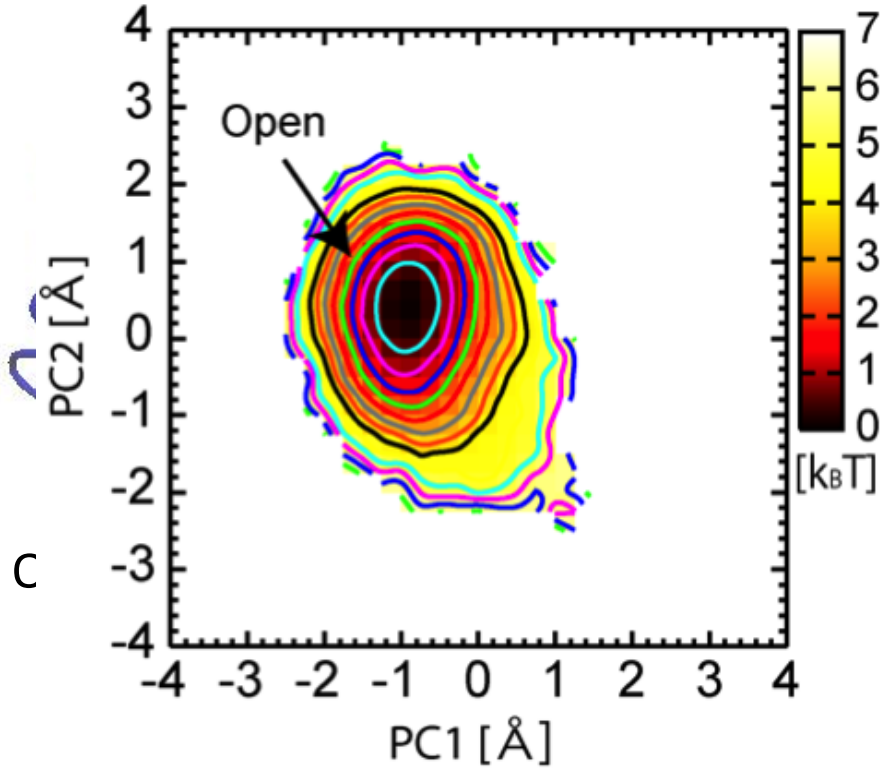
◆CPU time for 1,000 step MD (sec)

cluster		Total	calc	comm
HA-PACS	8(2^3)GPU	**278.1**	**203.8**	**44.8**
	27(3^3)GPU	**131.1**	**85.9**	**15.6**
	64(4^3)GPU	**75.7**	**39.2**	**6.7**
	125(5^3)GPU	**64.7**	**28.6**	**4.5**

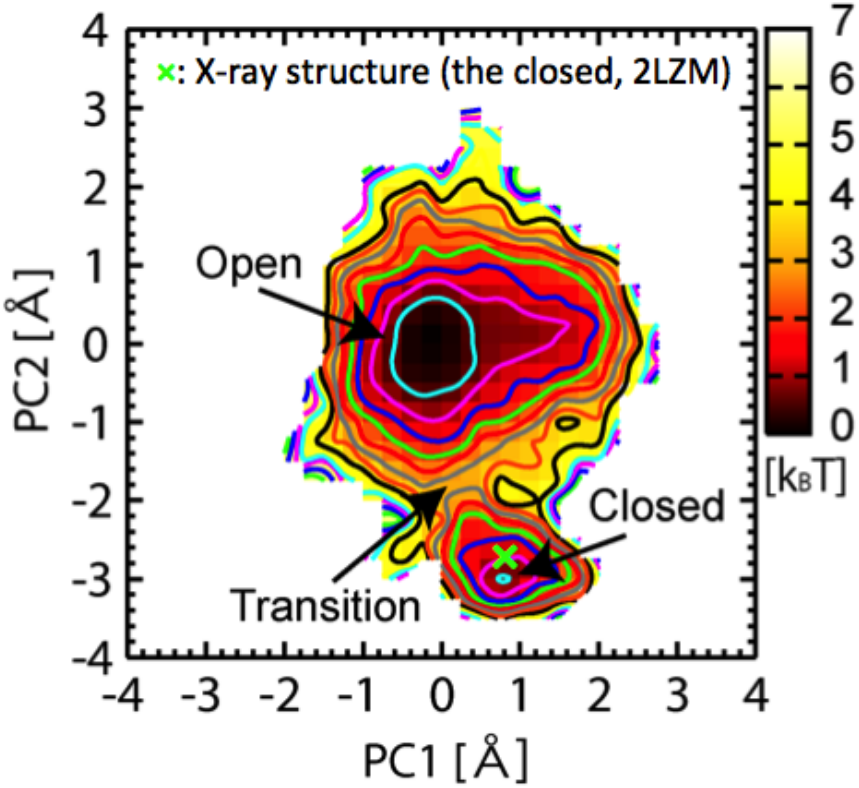
Open-Closed Transition (Protein Folding)

Collaboration with Dr. Harada

◆Canonical long time (**1 μs**)
MD started from the open



◆FEL calculated by FFM and MIUS
(**1 ns × 100 runs**)



◆**FFM could find the closed state as a local energy minimum, although 1μs long-time CMD failed to find the closed structure!**

Summary for future plans

Analyses on various functions that are carried by proteins will be analyzed with Multi-scale Modelings

1. Interaction Analyses（FMO）

2. Enzymatic Reaction Analyses（QM･MM-CPMD）

3. Structural Stability & Change Analyses（MD）

4. Induced-fit proesses, Protein Folding, Complex Formation Analyses（PaCS-MD, FMM, OFLOOD)

5. Cell, Organ, and etc.（Coarse-graining MD, Macrscopic Models）