Computational Elucidations for Biomolecules

QM/MM and MD simulations using supercomputers

In biology, there still remain numerous unsolved issues regarding to the actual structures, functions and reaction mechanisms for biomolecules, though they are critically important for all living organisms. In order to answer such challenging questions, we have been using highly accurate physical simulations based on quantum mechanics / molecular mechanics (QM/MM) and molecular dynamics (MD). In both methods, fundamental physical equations are numerically solved by computers.

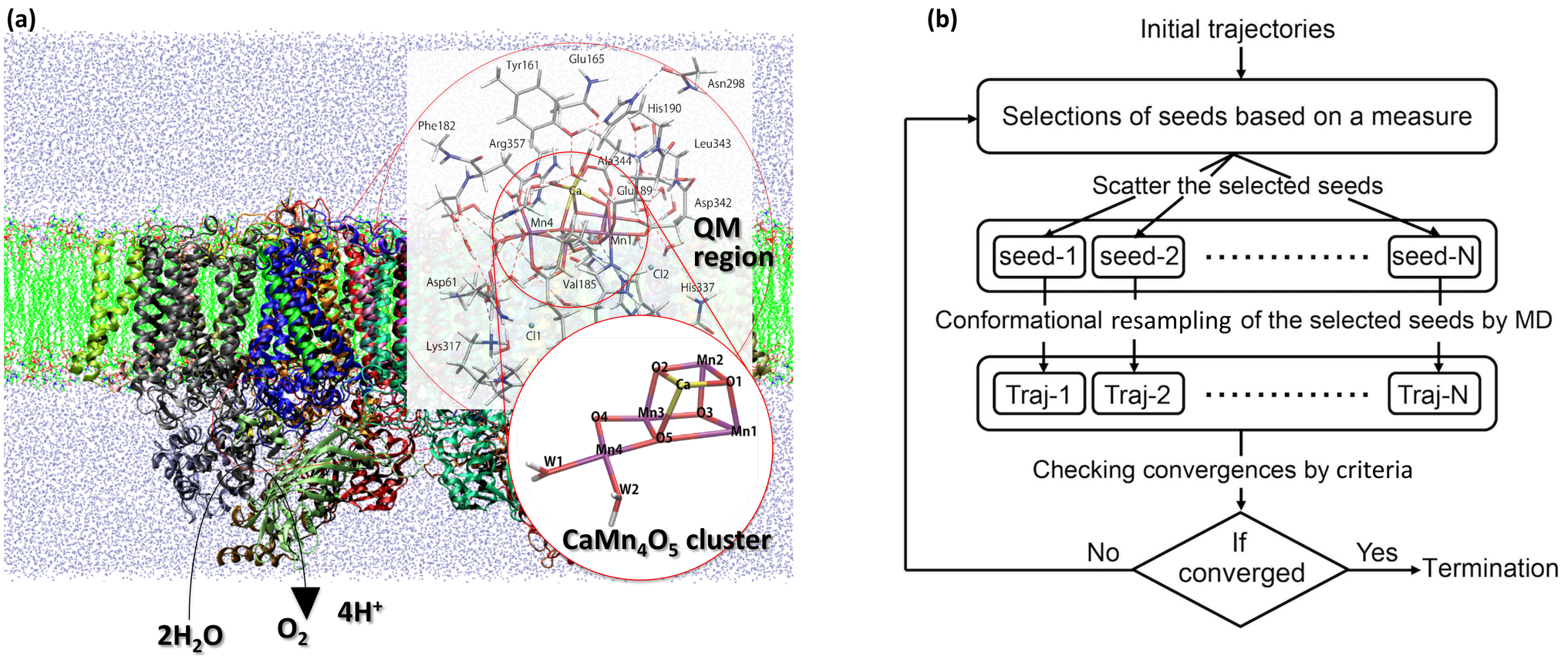
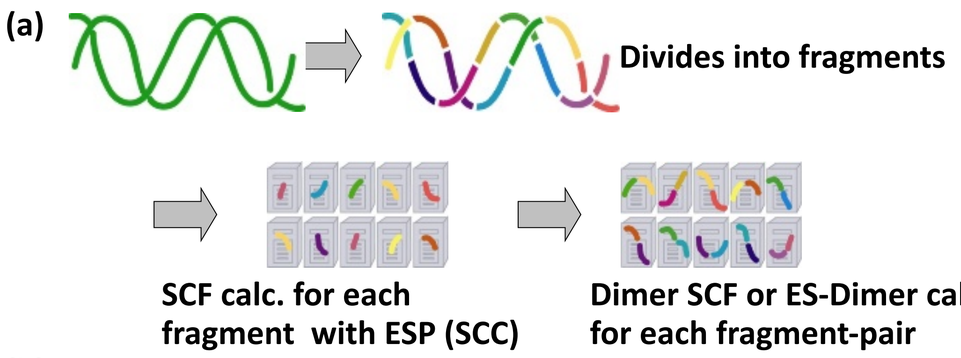


Fig. 1: (a) QM/MM model of oxygen evolving complex in photosystem II. Key intermediate states in the catalytic reaction "$2H_2O$ + 4hv -> $4H^+$+$4e^-$+O_2" have been investigated using the large model. [M. Shoji et al., Catal. Soc. Technol., 3, 1831 (2013).]
(b) Effective conformational sampling of MD simulations: Parallel Cascade Selection MD (PaCS-MD). To promote the conformational transition, the following cycle is repeated in PaCS-MD; (I) Selections of initial seeds (structures) that have high potential to transit. (II) The conformational resampling through restarting multiple MD simulations from the selected initial seeds. [R. Harada et al., J. Chem. Phys. 139 035103 (2013)]

GPU-accelerated Molecular Orbital Calculation

Large-scale *ab initio* molecular orbital calculation is a target application in quantum chemistry for HPC computer systems, and the fragment molecular orbital (FMO) method is one of such application because it is designed for parallel computer. We have developed GPU-accelerated FMO calculation program with CUDA, and obtained 3.8x speedups from CPU on-the-fly FMO calculation of 1,961 atomic protein. [H. Umeda et al., IPSJ Transactions on Advanced Computing Systems 6, 4, (2013) 26-37. H. Umeda et al., SC15 poster (2015).]



(b)

Application	Lysozyme			HA3
#Atoms	1,961			23,460
#Nodes (#GPU)	8 (0)	8 (32)		64 (256)
SCC	3,071 s	828 s	3.7x	0.52 hr
Dimer SCF	6,246 s	1,675 s	3.7x	0.90 hr
ES Dimer	407 s	78 s	5.2x	0.45 hr
Total	9,770 s	2,597 s	3.8x	1.97 hr

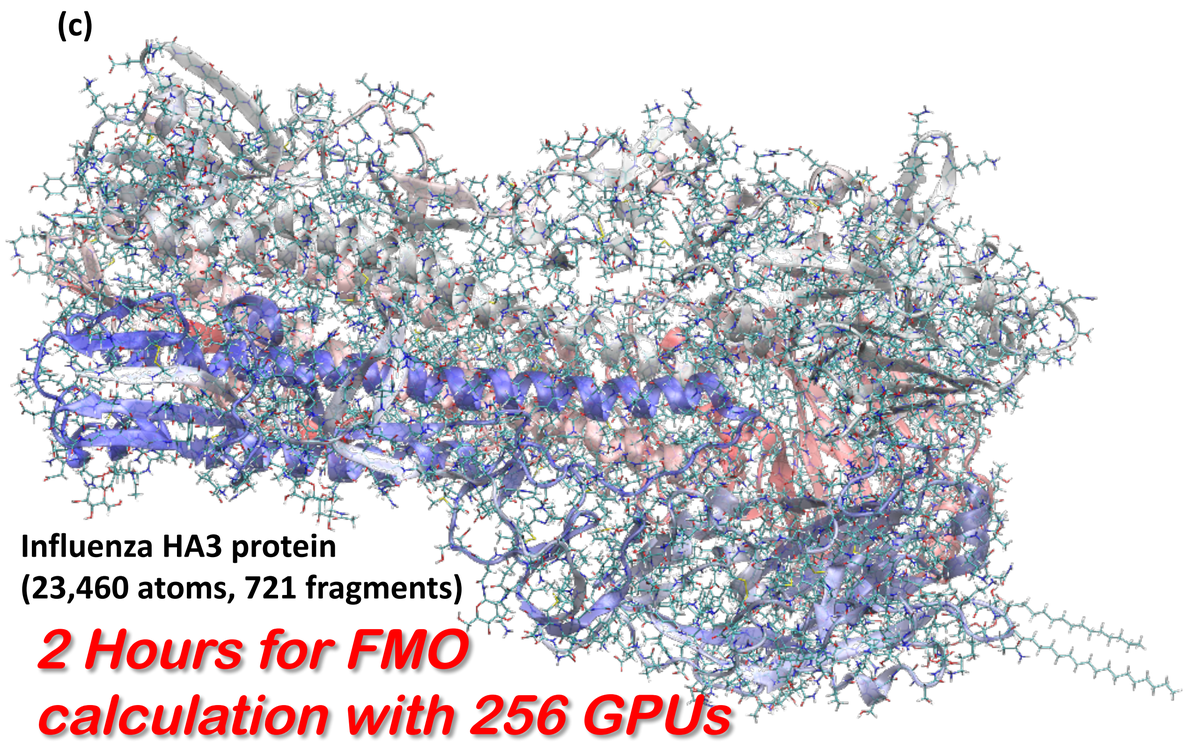


Fig. 2: (a) FMO calculation scheme, where large molecule is divided into many small fragments. Total molecular properties are reconstructed from the self consistent field (SCF) calculations of fragments and fragment-pairs with SCC (self-consistent-charge)-condition-satisfied electrostatic potential (ESP).
(b) Performance of GPU-accelerated FMO calculations. GPU-accelerated FMO-HF/6-31G(d) calculation of lysozyme with HA-PACS base cluster shows 3.8x speedups.
(c) As large-scale MO application, FMO-HF/6-31G(d) calculation of Influenza HA3 protein is successfully performed with 256 GPUs within two hours.

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