Computational elucidations for biomolecules

QM/MM and MD simulations using supercomputers

In biology, there still remain numerous questions regarding to the actual structures, functions and reaction mechanisms for biomolecules, though these are critically important for all living organisms. In order to elucidate such challenging issues, we have been performed highly accurate physical simulations based on quantum mechanics / molecular mechanics (QM/MM) and molecular dynamics (MD), in which fundamental physical principles are only used.

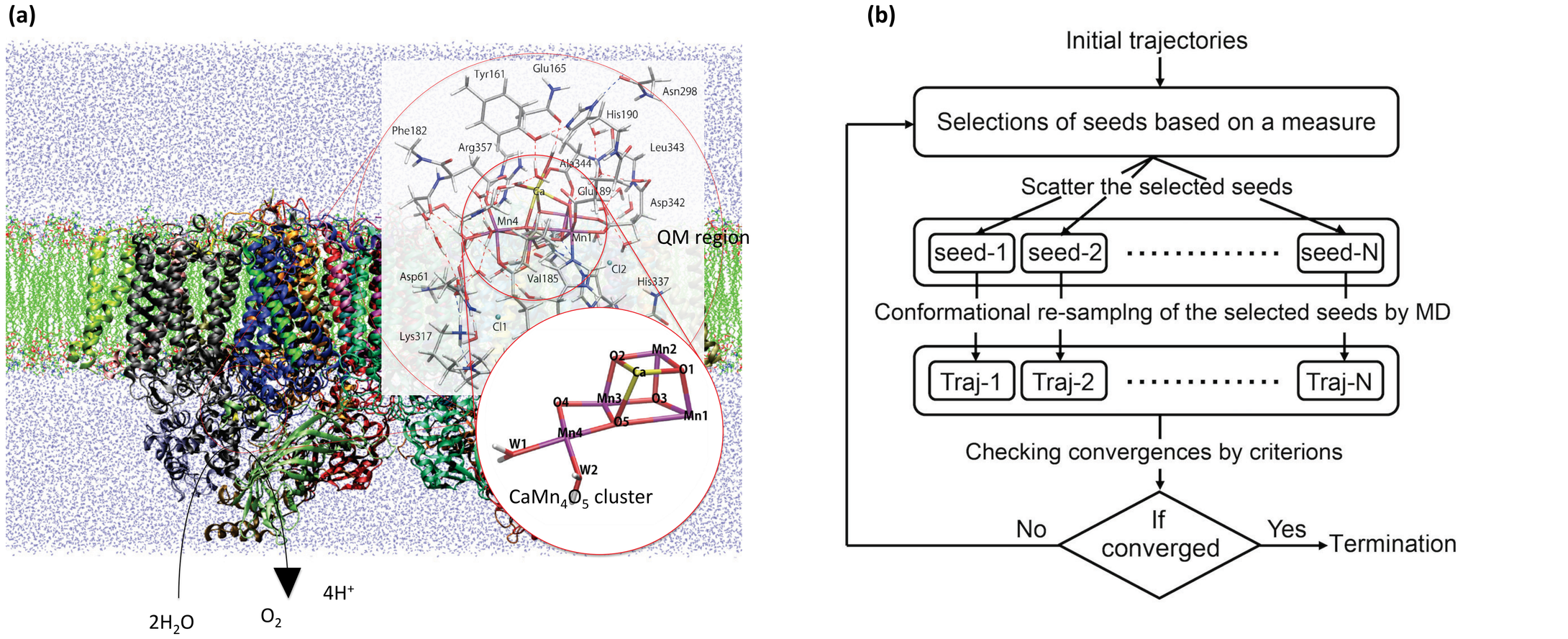
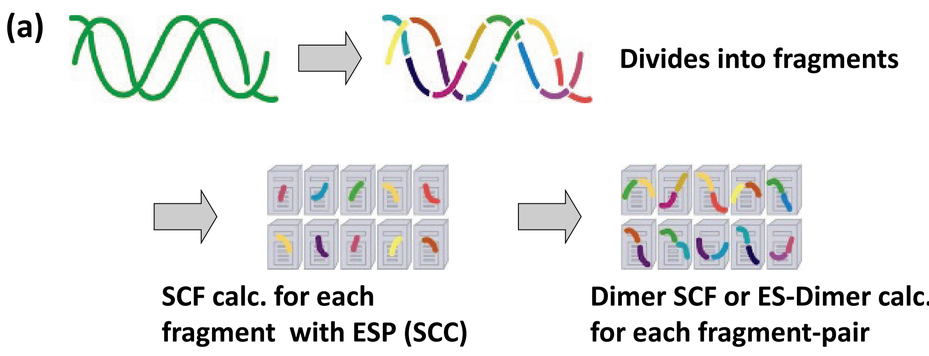


Fig. 1: (a) QM/MM model of oxygen evolving complex in photosystem II. Key intermediate states in the catalytic reaction "$2H_2O$ + 4hv -> $4H^+$+$4e^-$+O_2" has been investigated using the large model. [M. Shoji et al., Catal. Soc. Technol., 3, 1831 (2013).]
(b) Effective conformational sampling of MD 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. [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 FMO (fragment molecular orbital) 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.
[Umeda, H., et al., IPSJ Transactions on Advanced Computing Systems 6, 4, (2013) 26-37. Umeda, H., et al., SC15 poster (2015).]



(b)

Application	Lysozyme			HA3
#Atoms	1,961			23,460
#Nodes (#GPU)	8 (32)	8 (0)		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

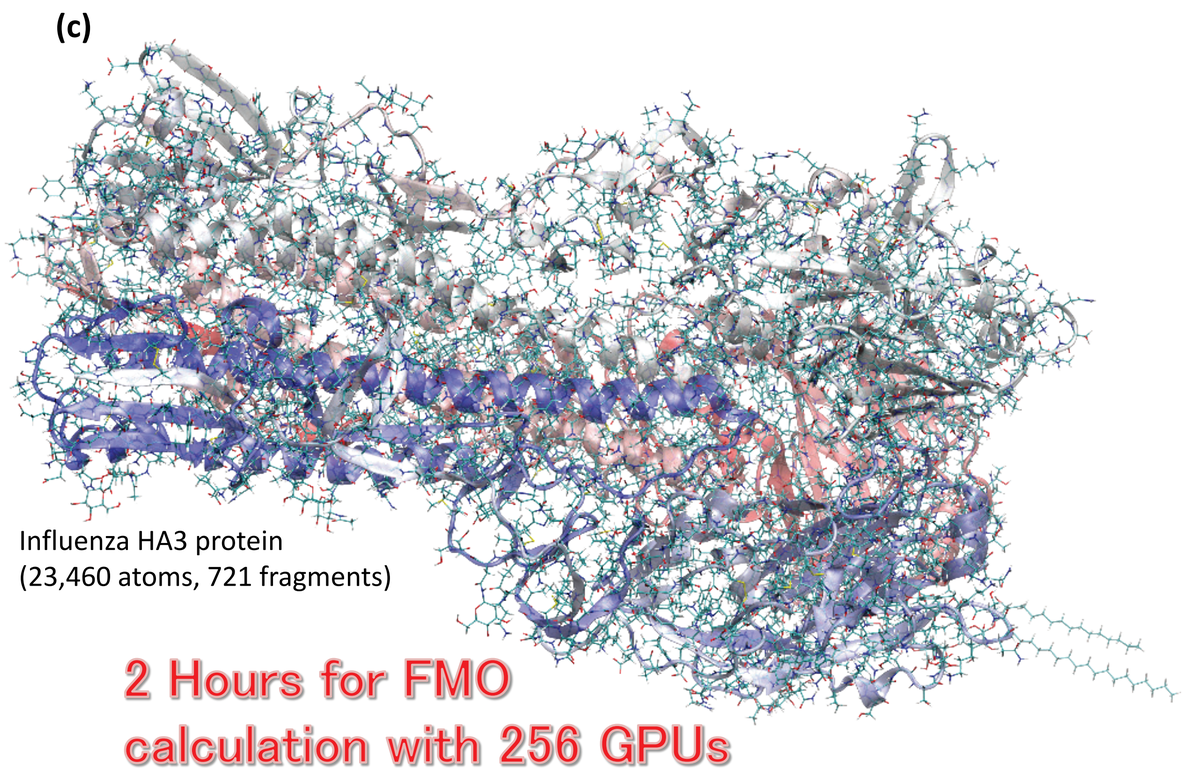


Fig. 2: (a) FMO calculation scheme, where large molecule is divided into many small fragments. Total molecular properties are reconstructed from MO calculation of fragments and fragment-pairs with SCC (self-consistent-charge)-condition-satisfied electrostatic potential (ESP).
(b) Performance of GPU-accelerated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