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Bio

Yutaka Maruyama is a postdoctoral fellow of institute for molecular science. He engages in The Grand Challenge to Next-Generation Integrated Nanoscience, Development & Application of Advanced High-Performance Supercomputer Project, MEXT. He graduated as a Ph. D from the Graduate University for Advanced Studies in 1998 with a Ph. D. thesis on "Gaussian-Markovian quantum Fokker-Planck approach to nonlinear spectroscopy and wavepacket dynamics for a dissipative molecular system". His current research interests are classified into two problems: 1) thermodynamics stability of bio-molecules and molecular recognition, 2) high performance computing for scientific calculation.

Abstract

The molecular recognition by protein is the most fundamental process in a living system to maintain its life. It is regarded as a process in which a host molecule makes a complex with a guest molecule through non-covalent chemical bonds. Especially, the ion binding is essential in a variety of physiological processes including information transmission through ion channels. Such processes are characterized by highly selective ion recognition by a protein. It is of great importance, therefore, for the life science to clarify the origin of the ion selectivity in molecular detail.

A theoretical prediction of the ion binding by protein, however, is nontrivial for any type of theories in chemical physics. The reason why it is so is because the problem involves stability or the free energy of ions in extremely inhomogeneous environments of protein immersed in an electrolyte solution, which extends over an infinite range or in the thermodynamic limit.

Recently, a new theoretical methodology has been introduced to tackle the problem, which is based on the three-dimensional reference interaction site model (3D-RISM) theory. It is a statistical mechanics which samples essentially the entire configuration space of the solvent, including that of guest molecules inside cavities or clefts of a host molecule. We have demonstrated the ability of the 3D-RISM theory to probe Na+ and Ca2+ ions bound inside a cavity of human lysozyme. The ions are detected only for the mutated protein produced from the wild type by changing particular amino acids.

Now we try to search optimized structures of wild and mutated proteins in several electrolyte solutions by a structure optimizer combined with the 3D-RISM theory. We need to perform 3D-RISM calculation many times for the optimization, and have to make 3D-RISM faster to reduce the calculation time. Then parallelization of the 3D-RISM program is required. Parallel 3D-FFT routine is an essential for massive parallelization of the 3D-RISM program.