Poster E-3

Analysis of Prion Protein: deeper understanding of protein motion from the molecular dynamics simulation

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Short Abstract: We will present classification of local minim structures by molecular dynamics simulation. In our simulation, huge molecular dynamics trajectory data were obtained by Tera FLOPS computer (like Blue Gene and Earth Simulator). Our presentation will suggest that huge data are different from classical short range molecular dynamics simulation.

Long Abstract:
Molecular dynamics (MD) simulations are widely used for simulating the motion of molecules in order to gain a deeper understanding of the chemical reactions, fluid flow, phase transitions, and other physical phenomena due to molecular interactions. Unfolding simulation by using MD is effective procedure to analyze dynamics and properties of protein. Prion protein (PrP) has very similar 3D structures among many species in C-terminal region: they have an intramolecular disulfide bridge, three α-helices, and a short double-stranded β-sheet. PrP is related to transmissible spongiform encephalopathies (TSEs). A central theme in PrP researches is revealing the process of conformational transition from the normal cellular form (PrPC) to pathologic isoform (PrPSc). Previous studies have shown that the sequence of the PrPs from cat and dog differ only by four residues (within Res 121-230). But there is no report of TSE-infected dogs whereas TSE-infected cats have not been reported. Recently the structures of PrP in many species have been determined by NMR. In this study, we performed molecular dynamics simulation at 300K and 500K of the PrPs from mouse, dog, cat, pig, sheep, cattle, and human. We discuss the differences in dynamics and sequence of the PrP between these species, especially dog and cat.