1P049**A new backbone-torsion-energy term represented by a double Fourier series**○Yoshitake Sakae¹, Yuko Okamoto²¹QuLiS, Hiroshima Univ., ²Dept. of Physics, Nagoya Univ.

A force field for protein systems is necessary to perform molecular simulations. Recently, we have carried out detailed comparisons of some force fields [1]. It was shown there that these force fields yield quite different secondary-structure-forming tendencies. We need to refine and improve the existing force-field parameters. Among the force-field terms, the torsion-energy term is the most problematic.

Therefore, we proposed a new backbone-torsion-energy term in the force field for protein systems [2]. This torsion-energy term is represented by a double Fourier series in two variables, the backbone dihedral angles ϕ and φ . This expression gives a natural representation of the torsion energy in the Ramachandran space. We can then easily control secondary-structure-forming tendencies by modifying the backbone-torsion-energy surface. We tested whether our modifications of the backbone-torsion-energy term resulted in the expected change of secondary-structure-forming tendencies. Moreover, we performed the optimization of the Fourier-coefficient parameters using our optimization method [3]. We then performed folding simulations of some peptides using the optimized Fourier-coefficient parameters.

References:

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1P051**Free Energy Landscape Picture and Correlation of Multiple Time Scale Conformational Fluctuations in Protein Allostery**

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Elucidation of the allosteric mechanism, by which protein conformation largely changes in functioning through cooperative communication between spatially distant sites, is a fascinating problem. Recent single-molecule experiments revealed an anomalous correlation in distance fluctuation in proteins, which provided evidence for the broad distribution of time scales and the memory effect in protein conformational dynamics [1]. These features should be generic to other proteins as multi-dimensional systems and suggest that the rare and intermittent large-amplitude fluctuations within a local region have an effect on the much slower global fluctuations. Sequence of intermittent large-amplitude fluctuations may lead to the large conformational changes, which should be described by a diffusive motion over the free energy surface. In the previous paper on the photo-signal transduction we have proposed a mechanism that the global collective fluctuation induced by the local and thermal structural changes mediates the communication between spatially distant sites in a protein [2]. In the present study, we generalize the method developed in [2] to explain coupling and correlation among multiple-time-scale fluctuations accompanying the diffusive motion on the free energy surface and discuss the dynamics of collective fluctuation mediating allostery. [1] H. Yang et al., Science 302, 262 (2003). [2] K. Itoh and M. Sasai, PNAS 101, 14736 (2004).

1P050**Extracting dynamical regularity during structural transition**

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It has been pointed out that during structural transition of molecules several systems undergo regularity in dynamics. But it hasn't confirmed whether this is also the case for larger systems. Moreover it is not clear either whether there are any relations between the regularity around saddle region of the potential energy surface and that in the basin structure. We think that clarifying these questions should be vital to the control of structural transition of molecules via vibrational excitation. To challenge these problems, we devised a new methodology to extract the regularity in a manner that is applicable to systems that have large degree of freedom such as proteins. This regularity is deeply related to stability of trajectories, so first we focus on stability matrix that gives us information about stability of trajectories, then we decompose them into stable directions and rotational directions. By monitoring the modes of these stable directions, we capture the regularity very clearly. In this presentation, first we verify our methodology in small degrees of freedom system, which the existence of such regularity has already been confirmed. Then, we apply our methodology to larger degrees of freedom system such as rare gas cluster and toy model of protein.

1P052**Development of a Technique to Dynamically Predict Protein Structures for the Reproduction of Protein Folding Process**

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The research field of protein structure prediction has shown a remarkable progress in recent years as witnessed in the biannual contest of Critical Assessment of Techniques for Protein Structure Prediction (CASP). However, most of the techniques thus developed have been specialized for the prediction of the native structure, but lacked the ability to describe dynamical folding processes. Though many researchers have enthusiastically carried out molecular simulations to reproduce the native structure of proteins in the computer, it has remained impossible to simulate the folding process of milliseconds or longer even with the power of recent computers. Thus, there have been no successful models that are useful to calculate the dynamical folding process with a high enough ability to predict the native structure. Here, we have developed a technique to predict the native structure through the simulation of the dynamical folding process. In this work, each of amino-acid residues is expressed as one particle, and newly constructed empirical potentials are used to represent interactions between amino-acid residues. Using this coarse-grained model, the Langevin molecular dynamics simulation was carried out for target proteins starting from a linear conformation. The results of the benchmark test for small proteins with several tens of residues showed that the lowest energy structures generated by this method resemble the native ones.