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Abstract of FSPIP2013

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Protein folding into a unique native structure is a major subject in the bioscience and biotechnology. Recently in a kinetic point of view for the protein folding, a kinetic hub model is proposed [1]. The key point in this model is the hypothesis that the native structure is a hub in the network whose nodes represent protein structures. By assuming that the protein structure exhibits a stochastic motion with a weight defined on this network, this model explains rapid protein folding into the native structure from any unfolded states by the property of the hub. Furthermore, a model protein folding dynamics on the similar weighted network of structures in the free energy has been analyzed based on an ergodic Markov state model. The analysis clarifies an ultrametricity of transition states [2]. These network picture based on the free energy landscape will provide a novel kinetic point of view for the folding beyond the funnel energy landscape picture [3].

In these kinetic analyses, the first step is to prepare the weighted network describing the folding dynamics. In the present work, we propose a method to construct the weighted network of structures on the free energy landscape based on the Wang-Landau Monte Carlo method [4]. We attempt to apply this method to a simple Ising like model [5] of a multidomain protein fragment and will discuss the network of structures in a kinetic point of view.

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