The Algorithm of Automatic Umbrella Sampling with Umbrella Integration

Yuki Mitsuta[1], Shusuke Yamanaka[1], Takashi Kawakami[1], Mitsutaka Okumura[1]

[1]Osaka University, Graduate School of Science, Osaka, Japan, 560-0043

Computation of free energy profiles along reaction coordinates, which are called potential of mean force (PMF), is essential to understand chemical reactions. The umbrella sampling is a typical method, which however requires specific parameters that depend on the systems. In our study, we proposed a new algorithm based on the umbrella integration method [1] towards an "automated" umbrella sampling. To exemplify effectiveness of our algorithm, we examined two-dimensional PMF (2D-PMF) of alanine dipeptide (Fig. 1). In Fig. 2, we showed a computational process of 2D-PMF for increasing the number of windows. These figures show that our algorithm is useful for effectively sampling important regions of the PMF.

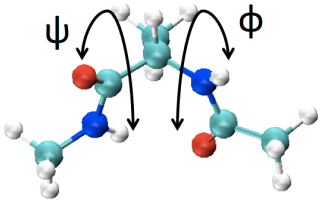

Fig. 1 The figure of alanine dipeptide and two dihedrals that were reaction coordinates for calculations of 2D-PMFs.

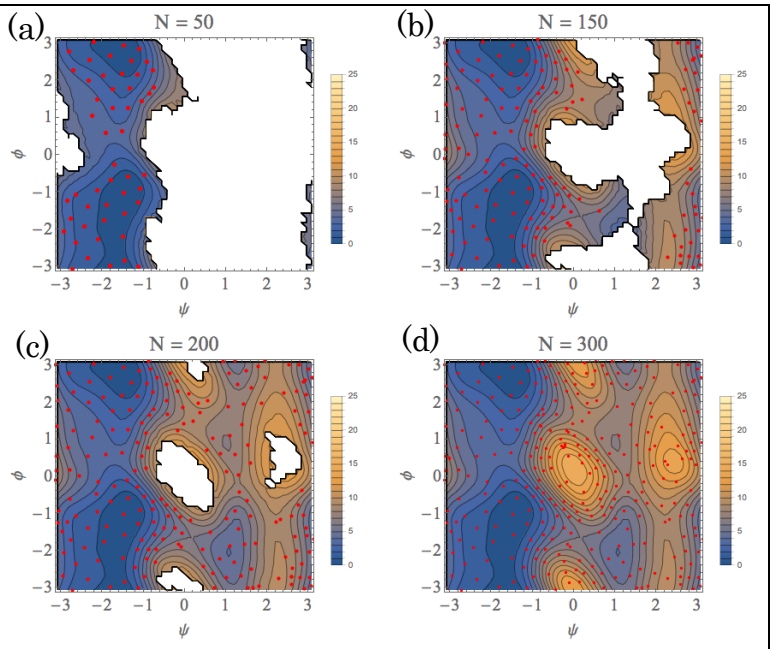

Fig. 2 The graphs of 2D-PMFs of alanine dipeptide in water. These red points are average points of windows. The numbers of windows (N) are (a) N=50, (b) N=150, (c) N=200, (d) N=300

[1] Kästner, Johannes. "Umbrella sampling." Wiley Interdisciplinary Reviews: Computational Molecular Science 1.6 (2011): 932-942.