ACCELERATING PROTEIN CONFORMATIONAL SAMPLING USING MULTISCALE APPROACH

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Abstract
Searching conformational ensembles of proteins remains a challenge in atomistic simulation of biomolecules. One approach to accelerate the protein sampling is to take advantage of rough energy surface from the coarse-grained model and, at the same time, to persist atomistic details from the all-atom model. Multiscale enhanced sampling (MSES) of all atoms and topology-based coarse-grained replica exchange simulation has been implemented in CHARMM and shown success of protein folding with few small peptides in our previous study. Our present object is to perform MSES simulation with the explicit solvent. We currently have implemented a version of MSES in NAMD, which is recognized to have better parallel scaling and is suitable for explicit solvent simulation in parallel computing. Our preliminary results show that once the atomistic and coarse-grained models are coupled in MSES the protein sampling is accelerated. However, it requires more sampling to archive thermodynamic properties for the lowest condition.