

A Novel Variable Transformation Approach for Enhancing Conformational Sampling in Complex Systems

PETER MINARY
Department of Chemistry
and Courant Institute of Mathematical Sciences
New York University
New York, NY 10003, USA
pm432@nyu.edu

Abstract

One of the computational grand challenge problems is to develop methodology capable of sampling conformational equilibria in systems with rough energy landscapes. If met, many important problems, most notably protein folding, could be significantly impacted. In this work, a new approach for sampling the conformational space of complex systems will be presented. The new method builds on the variable transformation or REPSWA (Reference Potential Spatial Warping Algorithm) approach previously introduced by us [Z. Zhu, et al., *Phys. Rev. Lett.* **88**, 100201 (2002)], in which a change of variables in the canonical partition is made that effects a shrinking of barrier regions and an expansion of attractive basins in the phase space. The approach was shown to yield efficient sampling of very long alkane chains. However, in order to treat biological systems, several new developments are needed. In particular, new extensions for handling branching and strong short-range nonbonded interactions are discussed. The latter is achieved by the introduction of a dynamic transformation scheme that senses the presence of barriers due to the close proximity of neighboring atoms. The performance of these new developments is tested on branched alkanes, solvated polymers, and a poly-glycine chain.