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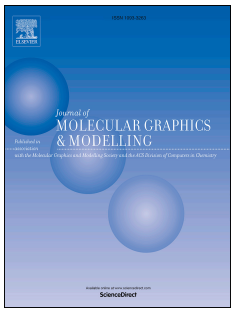

Faster Protein Folding Using Enhanced Conformational Sampling of Molecular Dynamics Simulation

Hiqmet Kamberaj

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Faster Protein Folding Using Enhanced Conformational Sampling of Molecular Dynamics Simulation

Hiqmet Kamberaj*

Department of Computer Engineering, Faculty of Engineering, International Balkan University, Tashko Karadza 11A, Skopje, Republic of Macedonia

Abstract

In this study, we applied swarm particle-like molecular dynamics (SPMD) approach to enhance conformational sampling of replica exchange simulations. In particular, the approach showed significant improvement in sampling efficiency of conformational phase space when combined with replica exchange method (REM) in computer simulation of peptide/protein folding. First we introduce the augmented dynamical system of equations, and demonstrate the stability of the algorithm. Then, we illustrate the approach by using different fully atomistic and coarse-grained model systems, comparing them with the standard replica exchange method. In addition, we applied SPMD simulation to calculate the time correlation functions of the transitions in a two dimensional surface to demonstrate the enhancement of transition path sampling. Our results showed that folded structure can be obtained in a shorter simulation time using the new method when compared with non-augmented dynamical system. Typically, in less than 0.5 ns using replica exchange runs assuming that native folded structure is known and within simulation time scale of 40 ns in the case of blind structure prediction. Furthermore, the root mean square deviations from the reference structures were less than 2 Å. To demonstrate the performance of

*Corresponding author
Email address: kamberaj@gmail.com (Hiqmet Kamberaj)