XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

Implementation of Configurational Bias Monte Carlo Method to Sample Flexible Solute in Solvent Media

Henrique M. Cezar, Sylvio Canuto, Kaline Coutinho

Institute of Physics, University of São Paulo, São Paulo, Brazil

Abstract: The molecular structure has an important role in several processes in chemistry, physics and biology. In computer simulations, structures are usually sampled through either Monte Carlo (MC) or Molecular Dynamics (MD). The method of choice, usually depends on the system and the properties one is interested in investigating. To study flexible molecules usually MD is applied, since several efficient implementations are available and MC lacks a standard and established method to sample the molecular internal degrees of freedom of a molecule. This problem arises since the standard atomic displacements usually applied within MC are very inefficient to generate new configurations with large conformational changes. In this work we implemented and improved a Configurational Bias Monte Carlo (CBMC) method used to sample molecular conformations in solvent. Based on the work of Shah and Maginn [1,2] we implemented in the DICE package [3] a CBMC strategy that separates hard and soft degrees of freedom within a fragment scheme. By enforcing the detailed balance while obtaining the acceptance criterion, we guarantee that the correct ensemble is sampled. We checked and benchmarked our implementation [4] by using it to sample octane and 1,2-dicholoroethane in different solvents. The trans and gauche populations were compared with experimental data and results from MD simulations. In both cases the results had an excellent agreement. We observe that at least for those systems, the correct population is achieved faster with our CBMC implementation than with MD. The CBMC also has a lower autocorrelation time, and is less likely to get trapped in local minima.

Key-words: Sampling, Configurational Bias, Monte Carlo, solute, solvent.
Support: This work has been supported by the National Council for Scientific and Technological Development (CNPq)

References:

[1] J. K. Shah, E. J. Maginn J. Chem. Phys. 2011, 135(13), 134121.
[2] J. K. Shah, E. Marin-Rimoldi, R. G. Mullen, B. P. Keene, S. Khan, A. S. Paluch, N. Rai, L. L. Romanielo, T. W. Rosch, B. Yoo, E. J. Maginn. J. Comput. Chem. 2017, 38(19), 1727.
[3] K. Coutinho, S. Canuto, *DICE: A Monte Carlo Program for Molecular Liquid Simulation*, v: 2.9; University of São Paulo: Brazil, 2011.
[4] H. M. Cezar, S. Canuto, K. Coutinho (manuscript in preparation)