The zero-dipole summation method and its application to molecular simulation with homogenous and inhomogeneous systems

Ikuo Fukuda, Narutoshi Kamiya, Kota Kasahara, Haruki Nakamura

Institute for Protein Research, Osaka University, 3-2 Yamadaoka, Suita, Osaka 565-0871, Japan

ifukuda@protein.osaka-u.ac.jp

Appropriate treatment of the electrostatic interaction of classical charged particles is critical for computational study of materials in a realistic manner. We introduced a novel idea, zero-dipole summation [1], which is based on the cut-off based approach to calculate the electrostatic interactions. This summation prevents the nonzero-charge and nonzero-dipole states artificially generated by a simple cutoff truncation, which often generates large energetic noises and several significant artifacts. In the presentation, we discuss the theoretical details, including the assumption and derivation, of our method. We also discuss the computational timing of the method to show that the simple pairwise formulation enables us to actually realize high-performance parallel computation. We will also exhibit the numerical results of molecular dynamics simulations with applying our method. The accuracies, stabilities, and static and dynamic properties of molecular systems were investigated. We obtained very accurate results, including for the electrostatic energy and the distance-dependent Kirkwood factor for a water system [2]. In particular, the latter quantity is highly sensitive to the treatment of the electrostatic interaction, leading to failures for many cut-off based approaches. Accurate descriptions were obtained in a membrane protein system [3], composed from explicit ions and membrane and water molecules, and also in a DNA system. The relationships and differences between the current method and the other promising cut-off based methods [4] will be discussed.