Enhanced MD-GAN for Stable Prediction of Molecular Dynamics Simulation Data

Kota Sakaki[1, S, C], Katsuhiro Endo[1] and Kenji Yasuoka[1]

[1]*Mechanical Engineering, Keio University, Yokohama, Japan*
ks.12630@keio.jp

Molecular Dynamics (MD) simulation is a valuable tool for predicting particle motion within a system by numerically solving the momentum equation step by step. However, the computational demands for large-scale and long-time simulations are substantial, making capturing molecular behavior on a realistic time scale challenging. Addressing this issue, MD-GAN emerges as a solution, employing machine learning to simulate with lower computational costs. MD-GAN achieves this by learning the transition probability that dictates how simulation data from the M-time step transitions to the next M-time step. Through deep neural network training, it can predict long-time trajectories based on short-time trajectories obtained from MD simulations. Previous research has demonstrated that MD-GAN can match the accuracy of conventional MD simulations while significantly reducing computation time in specific molecular systems.

Nevertheless, MD-GAN's predictions do not consistently exhibit high accuracy, displaying variability across iterations. The average accuracy of predictions over iterations also tends to be lower, limiting its practicality. To address these limitations, we implemented a new MD-GAN utilizing an advanced architecture, specifically the Self-Attention GAN, deviating from the basic GAN structure in previous MD-GAN models. This updated MD-GAN exhibits reduced variability in accuracy and achieves a higher average accuracy of predictions over multiple iterations. Consequently, this improvement positions MD-GAN as a more realistic and reliable method for predicting molecular dynamics, showcasing the potential of deep neural network models in advancing simulation techniques.