Parallel algorithm for graph neural network interatomic potential

Message-passing graph neural network interatomic potentials (GNN-IPs), particularly those with equivariant representations, are attracting significant attention due to their high accuracy. However, parallelizing GNN-IPs in molecular dynamics simulations poses challenges due to their multiple message-passing layers. In this article, we propose an efficient parallelization GNN-IPs and develop a package, SevenNet (Scalable EquiVariance-Enabled Neural NETwork). Through benchmark tests, SevenNet achieves over 80% parallel efficiency in weak-scaling and exhibits nearly ideal strong-scaling performance as long as GPUs are fully utilized. We also develop a general-purpose GNN-IP, SevenNet-0, which is trained on a vast data set from the Materials Project. By parallelizing GNN-IPs, this work aims to bridge the gap between advanced machine-learning models and large-scale MD simulations. This study was published in Journal of Chemical Theory and Computation 2024, **20**, 4857.