LAGRANGIAN AND HAMILTONIAN GRAPH NEURAL NETWORKS FOR ROBUST MOLECULAR SIMULATIONS

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Simulating atomic systems require accurate knowledge of the interatomic potentials that are either empirical in nature. Here, we present a framework using Graph neural network which allows learning the interatomic potential directly the trajectory of atomic systems. The framework termed as Lagrangian and Hamiltonian graph neural networks exhibits a generic architecture that allows the incorporation of different types of interactions and charges. In addition, it allows incorporation thermostat as a natural framework. Some of the specialities of the Lagrangian GNN includes the ability to learn very few data points, ability to generalize to arbitrary system size, and ability to conserve momentum and energy. Altogether, the framework presents a robust scheme to learn the interactions trajecotry.

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