Dynamic training enhances machine learning potentials for long-lasting molecular dynamics

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Molecular Dynamics (MD) simulations are vital for exploring complex systems in computational physics and chemistry. While machine learning methods dramatically reduce computational costs relative to ab initio methods, their accuracy in long-lasting simulations remain limited [1]. Here we propose Dynamic Training (DT), a method designed to enhance model performance over extended MD simulations. Applying DT to Equivariant Graph Neural Network (EGNN) [2] on the challenging system of a hydrogen molecule interacting with a palladium cluster anchored in a graphene vacancy [3] demonstrates a superior prediction accuracy compared to conventional approaches. Crucially, the architecture-independent design of DT ensures its applicability across diverse machine learning potentials, making it a practical tool for advancing MD simulations.

References

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[3] Alducin, Maite, et al. "Dynamics of cluster isomerization induced by hydrogen adsorption." *The Journal of Physical Chemistry C* 123.24 (2019): 15236-15243.

Figures

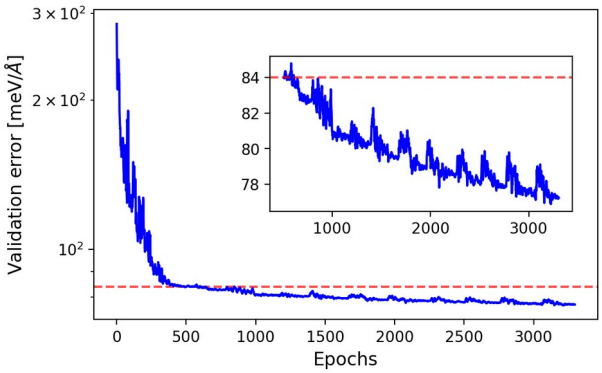

Figure 1. Blue line represents the validation error during training process, while the red dashed line indicates the value of validation error at first convergence (epoch number 549). Inset: Detailed view of the validation error behaviour after the first convergence.

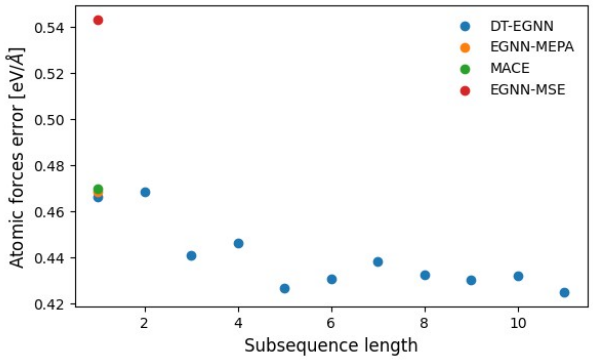

Figure 2. Mean error of atomic forces per atom type and per simulation step calculated on 300-timestep simulation between MLPs and DFT.