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aims PAX: Automated, Parallel Active Learning for Machine Learning Force Fields

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We present ab initio molecular simulation Parallel Active eXploration (aims PAX), an automated framework for constructing diverse and high-quality datasets for training machine learning force fields (MLFFs) [1] through active learning (AL). This software combines the electronic structure code FHI-aims [2] with the MACE MLFF [3, 4], offering a user-friendly approach for efficient dataset creation. Through a parallelized, automated AL algorithm that leverages continual learning and simultaneous sampling across multiple trajectories, our approach minimizes user intervention and optimizes computational resource use.

We showcase the framework by applying it to a peptide with 100 atoms, generating a balanced dataset with under a thousand DFT reference calculations. The resulting MLFF enables stable, nanosecond-scale molecular dynamics simulations, reducing the computational time needed for dataset creation by up to three orders of magnitude.

Additionally, we investigate an organic molecule adsorbed to an inorganic surface where the dynamics are dominated by weak interactions between the surface and molecule. These often pose a challenge for standard MLFF training procedures. To address this, we use an intermolecular force uncertainty measure and dynamics loss function inside aims PAX to improve a model's description of intermolecular interactions. This highlights the software's flexible nature, facilitating quick implementation of new tools for specific systems and problems.

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