MDcraft: a modern framework for accurate and scalable molecular dynamics simulations

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Molecular dynamics has become a cornerstone of computational materials science, enabling the study of complex phenomena ranging from atomic diffusion to extreme-condition response. As simulation demands grow, so does the need for frameworks that combine physical fidelity, algorithmic efficiency, and scalability. Here we present our noval code Mdcraft which addresses this need by integrating quantum-accurate, machine-learned interatomic potentials into a modern, high-performance architecture. The code features a high-level Python interface for usability and rapid prototyping, while its core algorithms—implemented in modern C++—ensure computational efficiency. Designed for contemporary high-performance computing environments, MDcraft supports MPI-based distributed parallelism with dynamic load balancing and leverages shared-memory parallelism within nodes. This combination of accuracy, flexibility, and scalability makes MDcraft a powerful tool for researchers across materials science, condensed matter physics, and computational chemistry.
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