LATENT EWALD SUMMATION FOR MACHINE LEARNING OF LONG-RANGE INTERACTIONS

Tech ID: 33715 / UC Case 2025-023-0

PATENT STATUS

Country	Type	Number	Dated	Case
United States Of America	Published Application	20260057250	02/26/2026	2025-023

BRIEF DESCRIPTION

Molecular dynamics (MD) is a computational materials science modality widely used in academic and industrial settings for materials discovery and more. A critical aspect of modern MD calculations are machine learning interatomic potentials (MLIPs), which learn from reference quantum mechanical calculations and predict the energy and forces of atomic configurations quickly. MLIPs allow for more accurate and comprehensive exploration of material/molecular properties at-scale. However, state-of-the-art MLIP methods mostly use a short-range approximation, which may be sufficient for describing properties of homogeneous bulk systems but fail for liquid-vapor interfaces, dielectric response, dilute ionic solutions with Debye-Huckel screening, and interactions between gas phase molecules. Short-range MLIPs neglect all long-range interactions, such as Coulomb and dispersion interactions.

To address the current shortcoming, UC Berkeley researchers have developed a straightforward and efficient algorithm to account for long-range interactions in MLIPs. The algorithm can predict system properties including those with charged, polar or apolar molecular dimers, bulk water, and water-vapor interfaces. In these cases standard short-range MLIPs lead to unphysical predictions, even when utilizing message passing algorithms. The present method eliminates artifacts while only about doubling the computational cost. Furthermore, it can be incorporated into most existing MLIP architectures, including potentials based on local atomic environments such as HDNNP, Gaussian Approximation Potentials (GAP), Moment Tensor Potentials (MTPs), atomic cluster expansion (ACE), and MPNN (e.g., NequIP, MACE).

SUGGESTED USES

» Molecular dynamics calculations

» Systems including Coloumb and/or dispersion interactions, e.g., liquid-vapor interfaces, dielectric response, systems with charged polar or apolar dimers, etc.

ADVANTAGES

» Computationally efficient accounting of long-range interactions to state-of-the-art Machine Learning Interatomic Potentials (MLIPs)

» Compatible with most existing MLIP architectures

RELATED MATERIALS

» Cheng, B. Latent Ewald summation for machine learning of long-range interactions. npj Comput Mater 11, 80 (2025). https://doi.org/10.1038/s41524-025-01577-7 - 03/26/2025

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OTHER INFORMATION

CATEGORIZED AS

» **Computer**
» Other
» Software
» **Materials & Chemicals**
» Chemicals
» Nanomaterials
» Other
» Polymers
» **Nanotechnology**
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