lammpsio: Transparent and reproducible handling of LAMMPS particle data in Python

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Summary

lammpsio provides a Python interface for reading and writing particle data in LAMMPS (A. P. Thompson et al., 2022) data and dump files. It aims to simplify the creation and parsing of these LAMMPS inputs and outputs, enabling LAMMPS users to more easily set up their simulations and to analyze their results with other Python tools. lammpsio also interconverts LAMMPS data and dump files with the GSD file used by HOOMD-blue (Anderson et al., 2020), another simulation package with an overlapping user base.

Statement of need

LAMMPS is a popular particle-based simulation package used across many scientific fields. Two of its important file formats are the data file, which defines the simulation state, and the dump file, which records particle trajectories. These files are text-based and can be tedious to parse or manipulate. Python tools such as Atomman and Pizza.py support reading and writing LAMMPS particle-data files, but their interfaces can be complex. Moltemplate (Jewett et al., 2021) can perform a variety of configuration tasks for LAMMPS simulations and includes Python tools for some file format conversions, but its Python interface is limited. Other established simulation analysis software such as MDAnalysis (Gowers et al., 2016; Michaud-Agrawal et al., 2011), MDTraj (McGibbon et al., 2015), and OVITO (Stukowski, 2009) also may only provide a subset of required features. As a result, researchers may rely on their own codes, but private codes are vulnerable to unnoticed errors and hinder reproducibility.

lammpsio addresses this need by providing an object-oriented Python interface for reading and writing LAMMPS data and dump files while adhering to the TRUE (transparent, reproducible, usable by others, and extensible) principles of scientific software development (M. W. Thompson et al., 2020). It allows users to create a particle configuration (simulation input) and parse a trajectory (simulation output) in a consistent manner. lammpsio additionally supports interconversion with the GSD file used by HOOMD-blue, enabling sharing of particle configurations between simulation packages. This functionality is leveraged, for example, in our relative-entropy minimization software (Sreenivasan et al., 2024) to support runtime selection of LAMMPS or HOOMD-blue as a simulation engine. Taken together, the features of lammpsio help meet needs for creating reproducible, interoperable, and maintainable simulation workflows for LAMMPS.

Design and implementation

lammpsio is organized around a central `Snapshot` object representing a single configuration of particles. `DataFile` and `DumpFile` objects provide read–write functionality for Snapshots in the corresponding LAMMPS file formats.

The `Snapshot` stores information about particles at a given time in a volume prescribed using the LAMMPS restricted-triclinic convention. Each `Snapshot` stores per-particle data, such as position or velocity, in NumPy (Harris et al., 2020) arrays. Topology data, defining the connectivity between subsets of particles (Allen & Tildesley, 2017), is also stored in the `Snapshot` as NumPy arrays. Importantly, lammpsio allocates its per-particle and per-connection arrays with the correct shape and type only when they are first accessed. This design prevents mismatches in array attributes and can reduce memory requirements.

The `DataFile` reads and writes LAMMPS data files, which are text-based files that store a single particle configuration. A data file contains a header with high-level simulation information and a body with sections defining per-particle and per-connection data. Sections have standardized formats, but the Atoms section may have a different format depending on the atom style in the simulation. The `DataFile`'s read method parses a data file into a `Snapshot` by tokenizing the headers and sections. The `DataFile`'s create method writes a data file containing only explicitly set information in the `Snapshot` and documented defaults for any data that is required but not explicitly set.

The `DumpFile` reads and writes LAMMPS dump files, which are text-based files that store a trajectory (sequence of particle configurations). A dump file has a significantly more flexible format than a data file. It is organized into a sequence of items, including timestep, number of atoms (particles), box bounds, and atoms. The atoms item contains one or more columns representing per-particle properties and can be configured in a variety of ways. The `DumpFile`'s read method loads one `Snapshot` at a time; users may provide a `Snapshot` to copy information not stored in the dump file (e.g., topology or omitted static properties). The `DumpFile`'s create method generates a dump file from a sequence of `Snapshots` according to a user-defined schema for the atoms item. Dump files may have binary or compressed formats; gzip and Zstandard compression are currently supported.

Discussion

By providing a lightweight and intuitive object-oriented interface, lammpsio streamlines workflows on LAMMPS input and output particle data. With only a few lines of code, users are able to feed their simulation data to tools that do not natively support LAMMPS files but do use NumPy arrays. For example, lammpsio enables users to directly interface their data with freud (Ramasubramani et al., 2020), a simulation analysis tool that makes minimal assumptions about its input format, as demonstrated in an example in our documentation. In a similar way, lammpsio data can also be passed to popular machine-learning toolkits with Python interfaces. Additionally, lammpsio can be used as a file converter for LAMMPS dump files, both from other formats such as HOOMD-blue's GSD file and between LAMMPS dump files with different schemas. This functionality can be particularly useful when working with legacy analysis tools that assume a LAMMPS dump file with a specific schema. Future development of lammpsio is planned to add support for reading restart files, working with molecule templates, and general triclinic boxes.

Availability

lammpsio is freely available under the BSD 3-Clause License on GitHub and is publicly distributed on PyPI and conda-forge. lammpsio has continuous integration testing using GitHub Actions for all currently supported combinations of Python and stable LAMMPS releases. We test both the core Python functionality of lammpsio and round-trip file compatibility with LAMMPS. For installation instructions and Python API documentation, please visit the publicly hosted documentation. For examples of how to use lammpsio, please visit the tutorials.

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Conflict of interest statement

The authors declare the absence of any conflicts of interest: No author has any financial, personal, professional, or other relationship that affect our objectivity toward this work.

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