MDAnalysis: A Python Package for the Rapid Analysis of Molecular Dynamics Simulations

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Abstract—MDAnalysis (http://mdanalysis.org) is an library for structural and temporal analysis of molecular dynamics (MD) simulation trajectories and individual protein structures. MD simulations of biological molecules have become an important tool to elucidate the relationship between molecular structure and physiological function. Simulations are performed with highly optimized software packages on HPC resources but most codes generate output trajectories in their own formats so that the development of new trajectory analysis algorithms is confined to specific user communities and widespread adoption and further development is delayed. The MDAnalysis library addresses this problem by abstracting access to the raw simulation data and presenting a uniform object-oriented Python interface to the user. It thus enables users to rapidly write code that is portable and immediately usable in virtually all biomolecular simulation communities. The user interface and modular design work equally well in complex scripted workflows, as foundations for other packages, and for interactive and rapid prototyping work in IPython [PG07] / Jupyter notebooks, especially together with molecular visualization provided by nglview and time series analysis with pandas [McK10]. MDAnalysis is written in Python and Cython and uses NumPy [VCV11] arrays for easy interoperability with the wider scientific Python ecosystem. It is widely used and forms the foundation for more specialized biomolecular simulation tools. MDAnalysis is available under the GNU General Public License v2.

Index Terms—molecular dynamics simulations, science, chemistry, physics, biology

Introduction

Molecular dynamics (MD) simulations of biological molecules have become an important tool to elucidate the relationship between molecular structure and physiological function. Simulations are performed with highly optimized software packages on HPC resources but most codes generate output trajectories in their own formats so that the development of new trajectory analysis algorithms is confined to specific user communities and widespread adoption and further development is delayed. Typical trajectory sizes range from gigabytes to terabytes so it is typically not feasible to convert trajectories into a range of different formats just to use a tool that requires this specific form. Instead, a framework is required that provides a common interface to raw simulation data. The MDAnalysis library [MADWB11] addresses this problem by abstracting access to the raw simulation data and presenting a uniform object-oriented Python interface to the user. Here we report on the general philosophy of MDAnalysis, its capabilities, and recent improvements.

Overview

MDAnalysis is written in Python and Cython and uses NumPy arrays [VCV11] for easy interoperability with the wider scientific Python ecosystem. Although the primary dependency is NumPy, other Python packages such as netcdf4 (http://unidata.github.io/netcdf4-python/) and BioPython [HM03] also provide specialized functionality to the core of the library (Figure 1).

MDAnalysis currently supports more than 25 different file formats and covers the vast majority of data formats that are used in the biomolecular simulation community, including the formats required and produced by the most popular packages NAMD, Amber, Gromacs, CHARMM, LAMMPS, DL_POLY, HOOMD. The user interface provides "physics-based" abstractions (e.g. "atoms", "bonds", "molecules") of the data that can be easily manipulated by the user. It hides the complexity of accessing data and frees the user from having to implement the details of different trajectory and topology file formats (which by themselves are often only poorly documented and just adhere to certain "community expectations" that can be difficult to understand for outsiders).

The user interface and modular design work equally well in complex scripted workflows, as foundations for other packages like ENCORE [TPB+15] and ProtoMD *Somogyi:2016aa*, and for interactive and rapid prototyping work in IPython/Jupyter notebooks, especially together with molecular visualization provided by nglview and time series analysis with pandas. Since the original publication [MADWB11], improvements in speed and data structures make it now possible to work with terabyte-sized trajectories containing up to ~10 million particles. MDAnalysis also comes with specialized analysis classes in the MDAnalysis.analysis module that are unique to MDAnalysis such as the LeafletFinder graph-based algorithm for the analysis of lipid bilayers [MADWB11] or the Path Similarity Analysis for the quantitative comparison of macromolecular conformational changes [SKTB15].

MDAnalysis is available in source form under the GNU General Public License v2 from GitHub as MDAnalysis/mdanalysis,

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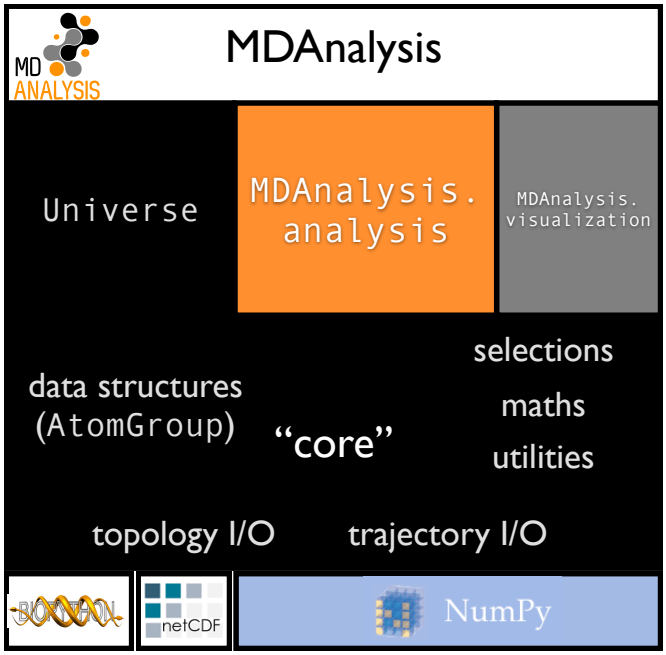

Fig. 1: *Structure of the MDAnalysis package. MDAnalysis consists of the "core" with the* Universe *class as the primary entry point for users. The* MDAnalysis.analysis *package contains independent modules that make use of the core to implement a wide range of algorithms to analyze MD simulations. The* MDAnalysis.visualization *package contains a growing number of tools that are specifically geared towards calculating visual representations such as, for instance, streamlines of molecules.*

and as PyPi and conda packages. The documentation is extensive and includes an introductory tutorial. The develoment community is very active with more than five active core developers and many community contributions in every release. We use modern software development practices [WAB+14], [SM14] with continous integration (provided by *Travis CI*) and an extensive automated testsuite (containing over 3500 tests with >92% coverage for our core modules). Development occurs on *GitHub* through pull requests that are reviewed by core developers and other contributors, supported by the results from the automated tests, test coverage reports provided by *Coveralls*, and *QuantifiedCode* code quality reports. Users and developers communicate extensively on the community mailing list (*Google* groups) and the GitHub issue tracker; new users and developers are very welcome.

Analysis Module

In the MDAnalysis.analysis module we provide a large variety of standard analysis algorithms, like RMSD, alignment [LAT10], native contacts [BHE13], [FKDD07], as well as unique algorithms, like the LeaftleftFinder [MADWB11] and Path Similarity Analysis [SKTB15]. Historically these algorithms were contributed by various researchers as individual moduldes to satisfy their own needs but this lead to some fragmentation in the user interface of these modules. We have recently started to unify the interface to the different algorithms with an *AnalysisBase* class. Currently PersistenceLength, InterRDF, LinearDensity and Contacts analysis have been ported. PersistenceLength calculates the persistence length of a polymer, InterRDF calculates the pairwise radial distribution function inside of a molecule, LinearDensity generates a density along a given exis and Contacts analysis native contacts, as desribed in more detail below. If applicable we also strive to make the API's to the algorithms generic. Most other tools hand the user analysis algorithms as black boxes. We want to avoid that and give the users all he needs to adapt an analysis to his/her needs.

The new Contacts class is a good example a generic API that allows easy adaptations of algorithms while still offering an easy setup for standard analysis types. The Contacts class is calculating a contact map for atoms in a frame and compares it with a reference map using different metrics. The used metric then decides which quantity is measued. A common quantity of interest is the fraction of native contacts, native contacts are all atoms that are nearby in the reference. For native contacts there exists two metrics [BHE13], [FKDD07] and we default to the later. We have designed the API to choose between the two metrics and pass user defined functions to develop new metrics or measure other quantities. This generic interface allowed us to implement a q1q2 analysis [FKDD07] on top of the Contacts class. Below is incomplete code example that shows how to implement a q1q2 analysis, the default value for the *method* kwarg is overwriten with a user defined method *radius_cut_q*. A more detailed explanatain can be found in the docs.

```
def radius_cut_q(r, r0, radius):
    y = r <= radius
    return y.sum() / r.size

contacts = Contacts(u, selection,
                    (first_frame_refs, last_frame_refs),
                    radius=radius, method=radius_cut_q,
                    start=start, stop=stop, step=step,
                    kwargs={'radius': radius})
```

This type of flexible analysis algorithms paired with a collection of base classes allow quick and easy analysis of simulations as well as development of new algorithms.

New data Structures

Originally MDAnalysis followed a strict object oriented approach with a separate instance of an Atom object for each particle in the simulation data. The AtomGroup then simply stored its contents as a list of these Atom instances. With simulation data commonly containing 10^6 particles this solution did not scale well and so recently this design was overhauled to improve the scalability of MDAnalysis.

Because all Atoms have the same property fields (i.e. mass, position) it is possible to store this information as a single NumPy array for each property. Now an AtomGroup can keep track of its contents as a simple integer array, which can be used to slice to property arrays to yield the relevant data.

Overall this approach means that the same number of Python objects are created for each Universe, with the number of particles only changing the size of the arrays. This translates into a much smaller memory footprint (BENCHMARK HERE) highlighting the memory cost of millions of simple Python objects.

This transformation of the data structures from an Array of Structs to a Struct of Arrays also better suits the typical access patterns within MDAnalysis. It is quite common to compare a single property across many Atoms, but rarely are different properties within a single Atom compared. Additionally, it is possible to utilise NumPy's faster indexing rather than using a list comprehension. Overall this meant that accessing the data from a

subset of Atoms is much faster than previously. (BENCHMARK HERE)

Conclusions

MDAnalysis provides a uniform interface to simulation data, which comes in a bewildering array of formats. It enables users to rapidly write code that is portable and immediately usable in virtually all biomolecular simulation communities. It has a very active international developer community with researchers that are expert developers and users of a wide range of simulation codes. MDAnalysis is widely used (the original paper [MADWB11] has been cited more than 180 times) and forms the foundation for more specialized biomolecular simulation tools. Ongoing and future developments will improve performance further, introduce transparent parallelisation schemes to utilize multi-core systems efficiently, and interface with the SPIDAL library for high performance data analytics algorithms.

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