MD ANALYSIS

MDAnalysis is a Python library for the analysis of computer simulations of many-body systems at the molecular scale, spanning use cases from interactions of drugs with proteins to novel materials. It is widely used in the scientific community and is written by scientists for scientists.

The goal of MDAnalysis is to make it easy for users to analyze data that are produced by simulations (primarily molecular dynamics simulations) that run on some of the largest supercomputers in the world. MDAnalysis accomplishes this goal by providing a toolkit of programming building blocks that provide an abstract Python interface to the simulation data — agnostic of the specific simulation package that produced it — that lends itself to interactive data exploration and rapid prototyping but is also a robust foundational library that can form the basis for new computational tools.

USE CASES

In the last year (2020) alone, MDAnalysis has been cited approximately 424 times[1]. These publications cover a wide range of molecular simulation topics and have been authored by members of research institutions across the world. In total, MDAnalysis has been cited 1328 times.   MDAnalysis has been used as a foundation for the development of many other libraries, with some listed at https://www.mdanalysis.org/pages/used-by/.

taurenmd: A command-line interface for analysis of Molecular Dynamics simulations. From https://taurenmd.readthedocs.io/: Taurenmd provides an easy, flexible and extensible, command-line interface for the most common (and not so common) routines of analysis and representation of Molecular Dynamics (MD) data. It bridges the gap between the highly complex (and powerful) Python libraries available for analysis of MD data and the non-developer users that lack the programming skills to perform a thorough and proficient use those libraries.

Swarm-CG: A tool to automatically optimize coarse-grained MD forcefields. http://www.github.com/GMPavanLab/SwarmCG From the abstract of the paper (DOI 10.1021/acsomega.0c05469):   By coupling fuzzy self-tuning particle swarm optimization to Boltzmann inversion, Swarm-CG performs accurate bottom-up parametrization of bonded terms in CG models composed of up to 200 pseudo atoms within 4–24 h on standard desktop machines, using default settings. The software benefits from a user-friendly interface.

PLANNED FEATURES

+ Interoperability: One of the main priorities for MDAnalysis post version 1.0, is a focus on improving interoperability between software packages in the molecular modelling community.

+ High performance distance calculations: As part of ongoing efforts to accelerate the performance of MDAnalysis, work is currently ongoing on developing a robust high performance distance calculation library.

+ Developing training material: With the goal of improving usability and furthering the growth of our user and developer base, the MDAnalysis organisation aims to produce new online training and education materials. These will likely be provided through a mix of online worked examples (as currently done in the MDAnalysis userguide), video presentations, and workshops.

PROJECT NEEDS

C++ developer time for high performance distance calculations.	2 months of dev time
Interoperability lead developer	6 months of dev time
Developing teaching materials	6 months of dev time

MDAnalysis is a Sponsored Project of NumFOCUS, a US 501(c)(3) public charity.

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For more information on MDAnalysis!, including our governance structure and project roadmap, please visit

http://www.mathjax.org/

For more information:
info@numfocus.org | +1 (512) 831-2870.