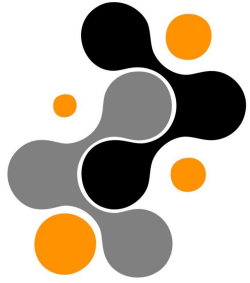
Introduction to Molecular Dynamics Trajectory Analysis using MDAnalysis

10 May 2024



MD ANALYSIS

Hybrid Workshop

CECAM-UK-JCMAXWELL

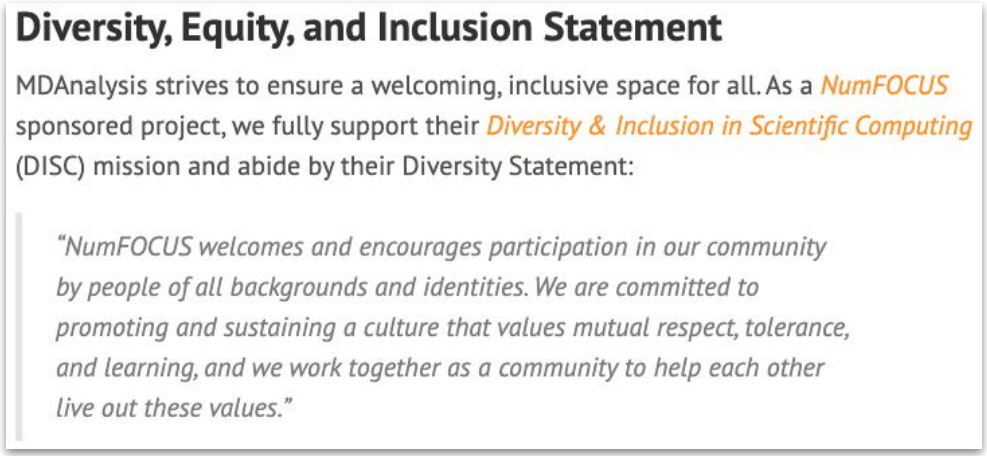
cecam

Centre Européen de Calcul Atomique et Moléculaire

CCPBioSim

Chan Zuckerberg Initiative

Code of Conduct



Diversity, Equity, and Inclusion Statement

MDAnalysis strives to ensure a welcoming, inclusive space for all. As a *NumFOCUS* sponsored project, we fully support their *Diversity & Inclusion in Scientific Computing* (DISC) mission and abide by their Diversity Statement:

> *"NumFOCUS welcomes and encourages participation in our community by people of all backgrounds and identities. We are committed to promoting and sustaining a culture that values mutual respect, tolerance, and learning, and we work together as a community to help each other live out these values."*

Code of Conduct

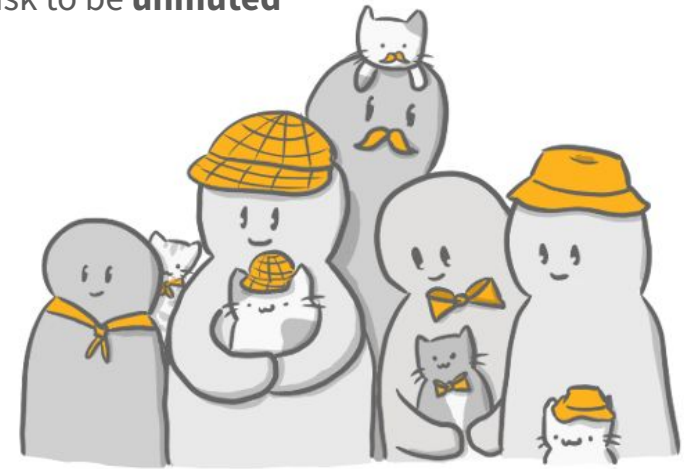
1. Be friendly and patient
2. Be welcoming
3. Be considerate
4. Be respectful
5. Be careful in the words that you choose
6. Moderate your expectations
7. When we disagree, try to understand why
8. A simple apology can go a long way

https://www.mdanalysis.org/pages/conduct/

Housekeeping

- Advanced sessions will be **recorded** and posted on https://www.youtube.com/@mdanalysis3040
- **Captions** are available online by clicking *More* → *Captions* → *Show Captions*
- Ask **questions**
  - Online: Use Q&A or 'Raise Hand' (in *Reactions*) to ask to be **unmuted**
  - In-person: Raise your hand or

    use the **sticky note system**



Cats by @ExplainedByCats
(Fiona Naughton)

Using the Sticky Notes

Pink sticky note:

I need help / more time

Yellow sticky note:

I’m ready to move on / all good

Setting up Your Environment

- **Materials** on ‘may24-ws’ branch in https://github.com/MDAnalysis/MDAnalysisWorkshop-Intro1Day repo
- Full **installation** instructions can be found in INSTALL.md
- Make sure to **pull the repo** again to ensure all materials are up-to-date!

GitHub repository

Schedule

- **09:15 - 09:25 BST:** Introduction
- **09:25 - 10:45 BST:** **Session 1:** MDAnalysis Basics and System Manipulation
- **10:45 - 11:10 BST:** Coffee Break
- **11:10 - 12:30 BST:** **Session 2:** Distances and Trajectories
- **12:30 - 13:45 BST:** 

Lunch
- **13:45 - 15:05 BST:** **Session 3:** Analysis Tools
- **15:05 - 15:30 BST:** Coffee Break
- **15:30 - 16:50 BST:** **Session 4:** Advanced Tips and Requests
- **16:50 - 17:00 BST:** Closing Remarks

What is MDAnalysis?

- A Python library for analysis of simulation data - built *by* scientists, *for* scientists
- Supports over 40 file formats from a variety of simulation software
- Flexible *and* fast
- More information at https://www.mdanalysis.org/

Mission

The MDAnalysis Community is interested in all facets of **working with data in the computational molecular sciences**. We welcome everyone. **We all follow our Code of Conduct and strive to create an environment that is welcoming to all.** Our primary purpose is to produce software that scientists in academia and industry will trust to use in their research.

We develop and maintain projects related to the broader goal of processing and analyzing data in the computational molecular sciences. We aim to empower users/developers to work with our packages following FAIR principles. Our central package is the MDAnalysis library for the analysis of computer simulations of many-body systems at the molecular scale.

We believe that scientific software should be open to all while using best practices to maintain high standards of correctness and reproducibility. We emphasize educating our users to make best use of the tools that we produce, to enable them to become contributors to our community and code bases.

And now…

…on to the first session!

Final Announcements

- Advanced sessions will be **recorded** and posted on https://www.youtube.com/@mdanalysis3040
- We will send a follow-up email with all relevant **resources** and the recording link
- We want to hear **your feedback**! Please complete the survey.
- More workshops to come! For updates follow our:
- ***Discord:*** https://discord.gg/t3bx25zd7v
- ***GitHub Discussions:*** https://github.com/MDAnalysis/mdanalysis/discussions
- ***Blog:*** https://www.mdanalysis.org/blog/
- ***LinkedIn:*** https://linkedin.com/company/mdanalysis

https://forms.gle/pfTX7PH2DTfwFaL29

Post-workshop survey

Discord invite