

Introduction to Molecular Dynamics Trajectory Analysis using MDAnalysis



CECAM-UK-JCMAXWELL

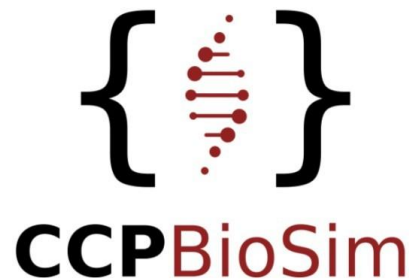


10 May 2024



MD
ANALYSIS

Hybrid Workshop





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

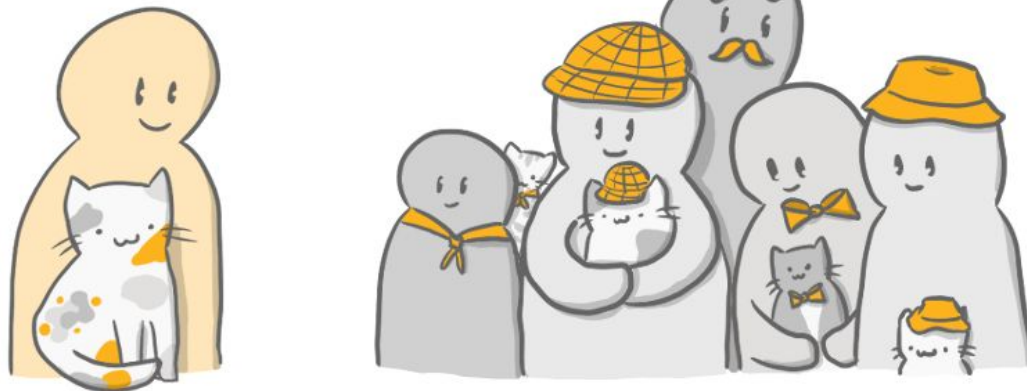
1. Be friendly and patient
2. Be welcoming
3. Be considerate
4. Be respectful
5. Be careful in the words that you choose
6. Moderate your expectations
7. When we disagree, try to understand why
8. A simple apology can go a long way



Housekeeping



- Session 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**



Setting up Your Environment



- **Materials** on 'may24-ws' branch in <https://github.com/MDAnalysis/MDAnalysisWorkshop-UCL24> 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

Using The Sticky Notes



Pink sticky note:

I need help/ more time






Yellow sticky note:

I'm ready to move on/ all good



Schedule



- **09:30 - 09:40 GMT:** Introduction
- **09:40 - 10:45 GMT:** Lecture 1 / Tutorial 1
- **10:45 - 11:10 GMT:**  Break
- **11:10 - 12:15 GMT:** Lecture 2 / Tutorial 2
- **12:15 - 13:30 GMT:**  Lunch
- **13:30 - 14:45 GMT:** Lecture 3 / Tutorial 3
- **14:45 - 15:10 GMT:**  Break
- **15:10 - 16:15 GMT:** Lecture 4 / Tutorial 4
- **16:15 - 16:50 GMT:** Code Clinic / Office Hours
- **16:50 - 17:00 GMT:** Closing Remarks

Final Announcements



- Session 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>
- *Blog:* <https://www.mdanalysis.org/blog/>
- *LinkedIn:* <https://linkedin.com/company/mdanalysis>



<https://forms.gle/pfTX7PH2DTfwFaL29>

Post-workshop survey



Discord invite