

Introduction to MDAnalysis and Molecular Nodes

February 28, 2024





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 by clicking *More* → *Captions* → *Show Captions*
- Ask **questions** in Q&A
- ‘Raise Hand’ (in *Reactions*) to ask to be **unmuted**
- **Materials** on ‘feb24-ws’ branch in <https://github.com/MDAnalysis/MDAnalysisWorkshop-Intro0.5Day> repo



GitHub repository



Cats by [@ExplainedByCats](#)
(Fiona Naughton)

Schedule



- **03:00 - 03:05 UTC:** Introduction
- **03:05 - 04:15 UTC:** MDAAnalysis Lecture 1 / Tutorial 1
- **04:15 - 04:20 UTC:** Q&A / Break
- **04:20 - 05:30 UTC:** MDAAnalysis Lecture 2 / Tutorial 2
- **05:30 - 05:35 UTC:** Q&A / Break
- **05:35 - 06:45 UTC:** Molecular Nodes Lecture / Tutorial
- **06:45 - 06:50 UTC:** Final Announcements
- **06:50 - 07:00 UTC:** Final Q&A

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:
 - Blog: <https://www.mdanalysis.org/blog/>
 - Discord: <https://discord.com/channels/807348386012987462/807712221769367622> (join link: <https://discord.gg/dprFy4RqCH>)
 - LinkedIn: <https://linkedin.com/company/mdanalysis>



Post-workshop survey