



MDAnalysis User Group Meeting 2025

NUMFOCUS
[FISCALLY SPONSORED PROJECT]

ASU Center for
Biological Physics
Arizona State University



Arizona State University

Tempe, AZ

9-11 June 2025

Chan
Zuckerberg
Initiative



Organizing Team



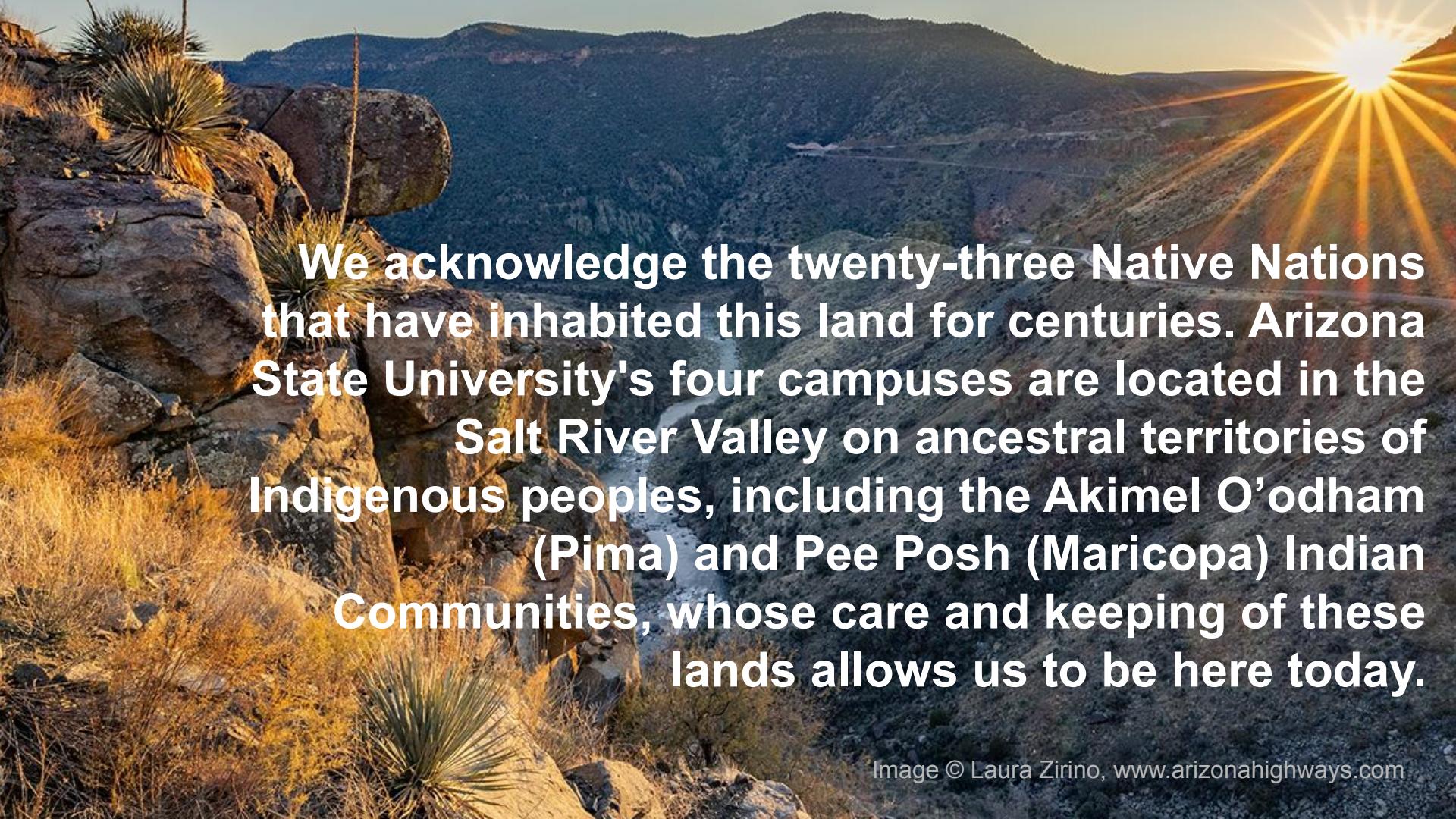
- Hugo Macdermott-Opeskin
- Jennifer Clark
- Irfan Alibay
- Oliver Beckstein
- Jenna Swarthout Goddard*



Local ASU Guides & Helpers

- Josh Uy
- Rekha Joshi
- Leah Repa
- Chenou Zhang

*online only

A scenic landscape at sunset, featuring a range of mountains in the background under a clear sky. In the foreground, there are large, light-colored rocks and a few yucca plants with long, thin leaves. The sun is low on the right side, casting bright rays of light across the scene.

**We acknowledge the twenty-three Native Nations
that have inhabited this land for centuries. Arizona
State University's four campuses are located in the
Salt River Valley on ancestral territories of
Indigenous peoples, including the Akimel O'odham
(Pima) and Pee Posh (Maricopa) Indian
Communities, whose care and keeping of these
lands allows us to be here today.**

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."



<https://www.mdanalysis.org/conduct/>

MDAnalysis Code of Conduct

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



Harassment or other CoC violations? Report!

Reporting and getting help



Need to talk to someone or something doesn't feel right?

Code of Conduct Committee members:



Yuxuan Zhuang (at conference)

- email: <yuxuan.zhuang@mdanalysis.org>
- MDAnalysis discord: @Yuxuan



Jenna Swarthout Goddard (online)

- email: <community@mdanalysis.org>
- MDAnalysis discord: @jennaswa

<https://www.mdanalysis.org/conduct/#how-to-report>



Emergencies

(can't get into building, lost on ASU campus, need help with anything else, ...)

MDAnalysis discord channel: UGM 2025

#contact-organizers

<https://discord.com/channels/807348386012987462/1436034423559557140>



Fire evacuation plan



ASSEMBLY POINTS

1 – Primary Assembly Point

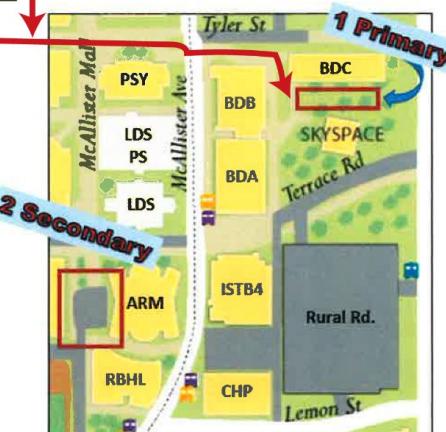
Exit the building and make your way towards the south side of BioDesign Building C (near BDC on map to the right)

2 – Secondary Assembly Point

Exit the building and make your way towards the parking lot area west of the ARM building (see map on right)

IMPORTANT REMINDERS

- Dial 911 to report the emergency
- Use **STAIRS**, do not use **ELEVATORS!**
- Assist those with special needs
- Go to *Primary Assembly Point* (if Primary is inaccessible, proceed to Secondary)
- Help floor wardens take roll
- Do not RE-ENTER building until instructed to do so!



Location

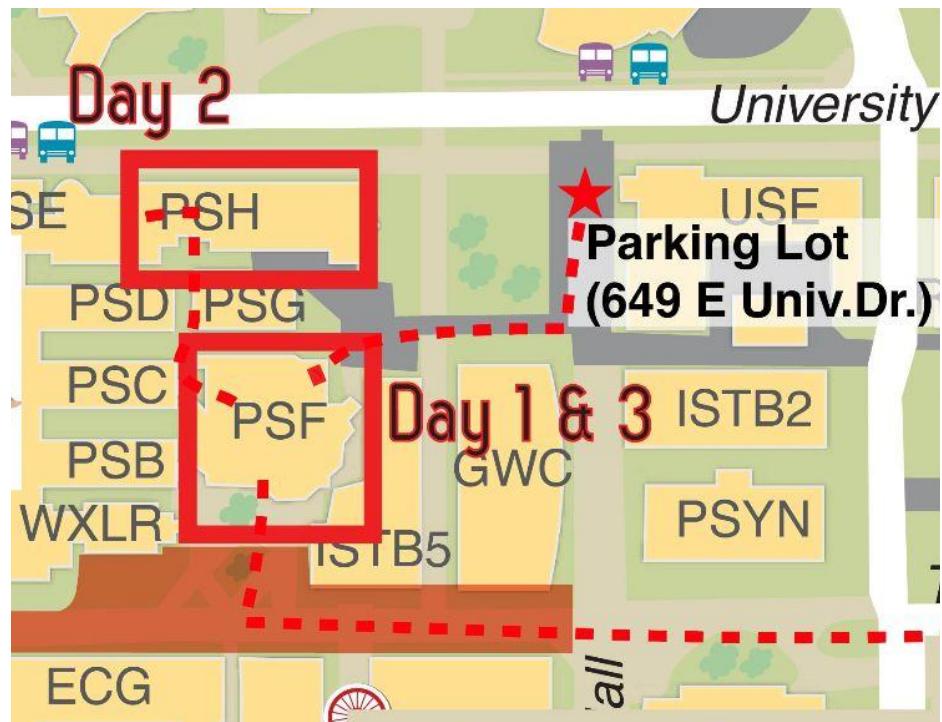
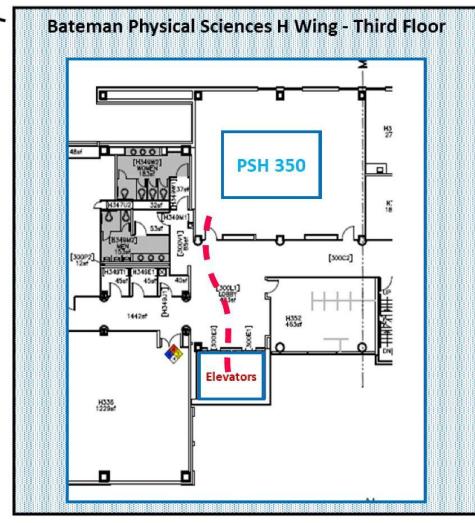


SUNDAY (Day 1) & TUESDAY (Day 3)

PSF 186

MONDAY (Day 2)

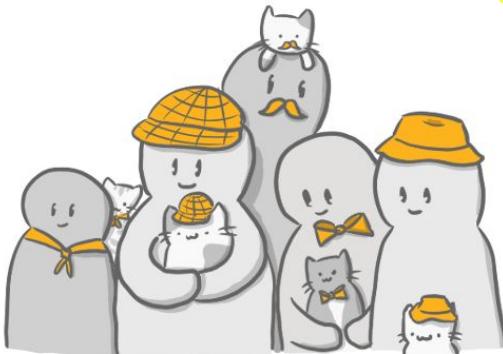
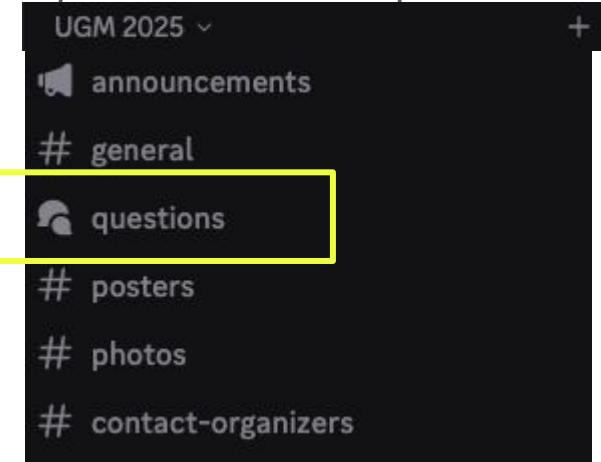
PSH 350





Talks and presentations

- Please do not take pictures of slides or posters without permission.
- Online: **captions** are available online by clicking *More → Captions → Show Captions*
- Ask **questions**
 - Online: Ask questions on **discord** in the relevant *questions* post
 - In-person: Raise your hand or
use the **sticky note system**
or on **discord**.



Join the MDAnalysis Discord
server <https://discord.gg/dMQWjNcZmh>

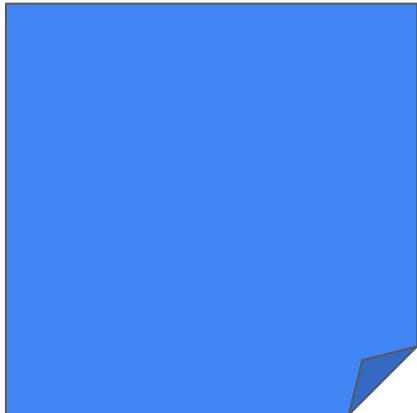
Cats by [@ExplainedByCats](#)
(Fiona Naughton)

Using the Sticky Notes



BLUE sticky note:

Ready to move on /
All good



RED sticky note:

Please stop! /
Ahh, I need help!



Lightning Talk preparations



MUST upload slides on DAY BEFORE TALK

- Upload to **presentation_materials** in <https://github.com/MDAnalysis/UGM2025>
- Create a **Pull Request** (follow instructions in README) or via **Add file** and *Upload Files*
- File formats: PDF, Powerpoint

The screenshot shows a GitHub repository page for 'MDAnalysis / UGM2025'. The 'Code' tab is selected. A red box highlights the 'UGM2025/presentation_materials/' folder path. An orange box highlights the 'Add file' dropdown menu, which includes options for 'Create new file' and 'Upload files'. Below the code area is a table of recent commits. At the bottom, there's a 'README.md' file and a 'Presentation Materials' section.

Name	Last commit message	Last commit date
...		
mdanalysis	Add MDAnalysis presentation folder	last month
posters	Add openff poster	15 hours ago
vasconez_noah	Add files via upload	10 hours ago
README.md	Add a readme and template readme	last month
Tyler_Reddy_MDA_UGM_2025.pptx	DOC: add Tyler talk information (#38)	15 hours ago
template-README.md	Add a readme and template readme	last month

README.md

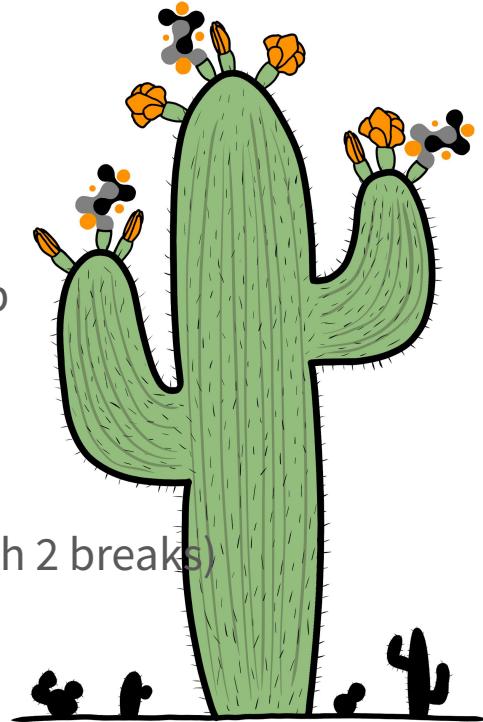
Presentation Materials

All presenters at the [MDAnalysis UGM](#) are encouraged (but not required) to make their presentations publicly available by depositing their presentation materials (e.g., slides, notebooks, data, etc.) in the [presentation_materials](#) directory.

Schedule - Day 1 (PSF 186)



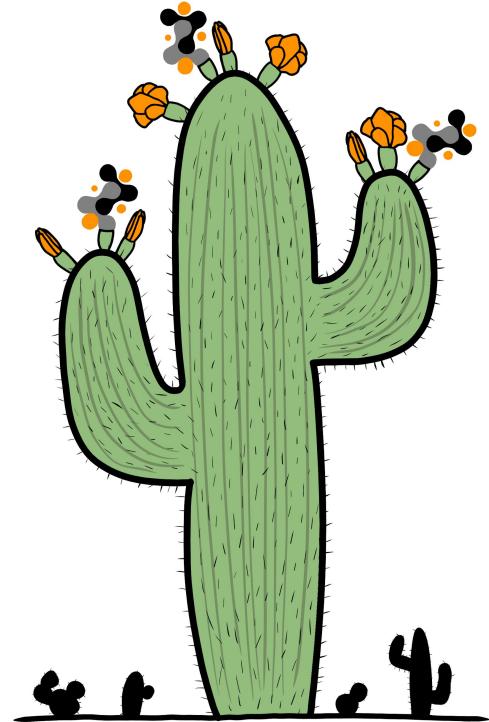
- **09:00am MST:** Introduction
- **09:15am MST:** MDAnalysis: Present and Future
- **9:45am MST:** **Keynote:** Matthias Heyden
- **10:45am MST:** *Break & GROUP PHOTO*, poster set-up
- **11:30am MST:** Contributed talks
- **12:30pm MST:** *lunch & POSTERS*
- **2:30pm MST:** **Focus:** Streaming with workshop (with 2 breaks)
- **6pm MST:** *end of day 1*



Schedule - Day 2 (PSH 350)



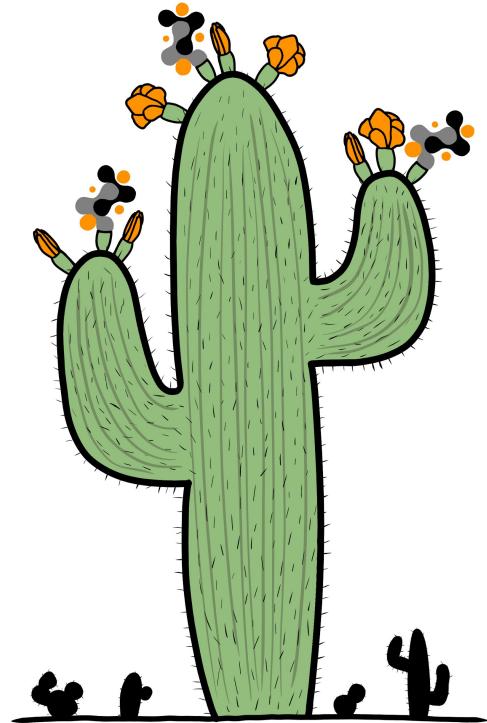
- **09:00am MST:** Opening remarks
- **9:10am MST:** **Keynote:** Lillian Chong
- **10:10am MST:** Contributed talks & 1 break
- **12:20pm MST:** *lunch*
- **1:35pm MST:** Lightning & Contributed Talks, breaks
- **4:35pm MST:** Master Classes
- **6pm MST:** *end of Day 2*
- **>7:30pm MST:** SOCIAL at 4 peaks brewing
1340 E 8th St Ste 104, Tempe, AZ 85281



Schedule - Day 3 (PSF 186)



- **08:30am MST:** Workshop installation clinic
- **8:55am MST:** Opening remarks
- **9am MST:** Visualization **workshop** & break
- **11:20am MST:** Lightning Talks
- **11:45am MST:** Introduction to OMSF
- **12pm MST:** Open Force Field **workshop**
- **1:05pm MST:** *lunch*
- **2:20pm MST:** Open Free Energy **workshop** & break
- **3:35pm MST:** OpenADMET **workshop**
- **4:35pm MST:** closing remarks
- **4:50pm MST:** *end of conference*



And now...



...on to the first session!

Day 2 - be social



Meet up at Four Peaks 8th St
Pub ≥ 7:30pm

Casual dining with

- Speciality beers
- Pub food
- And MDAnalysis folks!

1340 E 8th St Ste 104,
Tempe, AZ 85281

