MD ANALYSIS
UGM 2023
Lisbon, Portugal

Welcome
2023-09-27

Oliver Beckstein
Jenna Swarthout-Goddard

NUMF⚬CUS
OPEN CODE = BETTER SCIENCE

Naveen Michaud-Agrawal, Elizabeth J. Denning, Oliver Beckstein

9 core developers 188 code contributors + hundreds of community members + thousands of users

Naveen Michaud-Agrawal, Elizabeth J. Denning, **Oliver Beckstein**, Danny Parton, Philip Fowler, **Tyler Reddy**, Joseph Goose, Jan Domanski, Benjamin Hall, Paul Rigor, David Caplan, Christian Beckstein (logo), *Sébastien Buchoux*, Joshua L. Adelman, Lukas Grossar, Andy Somogyi, Lukas Stelzl, Jinju Lu, Joshua L. Phillips, Zhuyi Xue, Xavier Deupi, *Manuel Nuno Melo*, Robert McGibbon, **Richard J. Gowers**, Alejandro Bernardin, Lennard van der Feltz, Matthieu Chavent, Joe Jordan, Alex Nesterenko, Caio S. Souza, Sean L. Seyler, *David L. Dotson*, Carlos Yanez S., Kyle J. Huston, Isaac Virshup, *Max Linke*, Gorman Stock, *Jonathan Barnoud*, Hai Nguyen, Balasubramanian, Mattia F. Palermo, Utkarsh Saxena, Abhinav Gupta, John Detlefs, Eugen Hruska, Bart Bruininks, **Fiona Naughton**, Robert Delgado, Wouter Boomsma, *Matteo Tiberti*, Tone Bengtsen, Shantanu Srivastava, Pedro Reis, Ruggero Cortini, Zhiyi Wu, Kashish Punjani, Utkarsh Bansal, Shobhit Agarwal, Vedant Rathore, Akshay Gupta, Juan Eiros Zamora, Jon Kapla, Sang Young Noh, Andrew William King, Kathleen Clark, Dominik 'Rathann' Mierzejewski, Nestor Wendt, **Micaela Matta**, Jose Borreguero, Sören von Bülow, Nabarun Pal, Mateusz Bieniek, Paul Smith, Navya Khare, *Johannes Zeman*, Ayush Suhane, Davide Cruz, Shujie Fan, Andrew R. McCluskey, Henry Mull, **Irfan Alibay**, *Philip Loche*, Matthew W. Thompson, Ali Ehlen, Daniele Padula, Ninad Bhat, Fenil Suchak, Yibo Zhang, Luís Pedro Borges Araújo, Abhishek A. Kognole, **Rocco Meli**, **Lily Wang**, Matthijs Tadema, Joao Miguel Correia Teixeira, Charlie Cook, Yuanyu Chang, Guillaume Fraux, Ivan Hristov, Michael Quevillon, Hao Tian, **Hugo MacDermott-Opeskin**, Anshul Angaria, Shubham Sharma, Yuxuan Zhuang, Cédric Bouysset, Abhishek Shandilya, Morgan L. Nance, Faraaz Shah, Wiep van der Toorn, Siddharth Jain, Ameya Harmalkar, Shakul Pathak, Andrea Rizzi, William Glass, Marcello Sega, Edis Jakupovic, Nicholas Craven, Mieczyslaw Torchala, Ramon Crehuet, Haochuan Chen, Karthikeyan Singaravelan, Ian Kenney, Aditya Kamath, Leonardo Barneschi, Henrik Jäger, Jan Stevens, Orion Cohen, Dimitrios Papageorgiou, Hannah Pollak, Estefania Barreto-Ojeda, Paarth Thadani, Henry Kobin, Kosuke Kudo, Sulay Shah, Alexander Yang, Filip T. Szczypiński, Marcelo C. R. Melo, Mark D. Driver, Kevin Boyd, Atharva Kulkarni, Yantong Cai, Bjarne Feddersen, Pratik Gupta, Alexander Gorfer, Aya M. Alaa, Kazi Shudipto Amin, Alia Lescoulie, Henok Ademtew, Uma D Kadam, Tamandeep Singh, Mingyi Xue, Meghan Osato, Anirvinya G, Rishabh Shukla , Manish Kumar, Aditi Tripathi, Sukeerti T, Kavya Bisht, Mark Verma, Marcelo D. Poleto, Ricky Sexton, Rafael R. Pappalardo, Tengyu Xie, Raymond Zhao, Haleema Khan, Jennifer A Clark, Jake Fennick, Utsav Khatu, Patricio Barletta, Mikhail Glagolev, Christian Pfaendner, Pratham Chauhan, Meet Brijwani, Vishal Parmar, Moritz Schaeffler, Xu Hong Chen, Domenico Marson, Ahmed Salah Ghoneim, Alexander Schlaich, Josh Vermaas, Xiaoxu Ruan, Egor Marin, Shaivi Malik, Daniel J. Evans, Mohit Kumar, Shubham Kumar, Zaheer Timol, Geongi Moon

https://www.mdanalysis.org/

@MDAnalysis

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Google Summer of Code

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Fiona Naughton

Micaela Matta

Irfan Alibay

Lily Wang

Yuxuan Zhuang

Ian Kenney

Jenna Swarthout-Goddard
(Community & Project Manager,
UGM Mastermind)

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ClayCode: A Tool for Automatingthe Setup of Atomistic Clay Models for Molecular Dynamics Simulations with GROMACS

Hannah Pollak

Keynote: *Encoding Interactions as Fingerprints in MD Simulations*

Cédric Bouysset

MAICoS: A Toolkit for the Molecular Analysis of Interfacial and Confined Systems

Henrik Jäger

Parallelization of MDAnalysis

Egor Marin

https://www.mdanalysis.org/

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Code of Conduct

We are committed to providing a productive, harassment-free environment for everyone.

- In short: Be respectful to each other. Think about your words and actions. Be mindful that we are from different backgrounds.
- https://www.mdanalysis.org/pages/conduct/
- **Everybody participating in the UGM agreed to abide by the CoC.**

Code of Conduct

If you feel or felt being made uncomfortable, unwelcome, threatened or endangered, please **contact**
- one of the CoC Committee members
- any of the other organizers

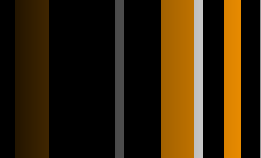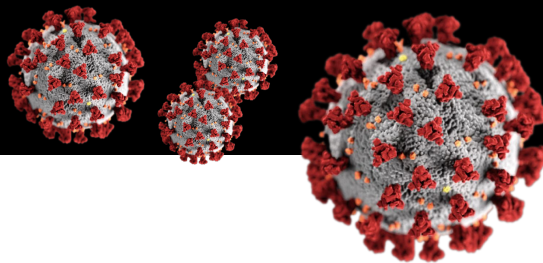or **submit a report to MDAnalysis** (can be anonymous) with links in https://www.mdanalysis.org/pages/conduct/

Jenna Swarthout-Goddard

Micaela Matta

Richard Gowers

COVID19 policies

- Recommended: vaccinated against COVID19 with up-to-date boosters
- Testing: not required BUT please test yourself if you were at risk of contracting COVID19 — limited number of self tests available at check-in
- Testing positive for SARS-CoV-2/COVID19:
    - Please do not attend.
    - Please notify the organizing committee ugm@mdanalysis.org (will handle information confidentially)
- Face coverings: not required but welcomed — we support your personal choice, whichever it is.
- Social distancing: your choice (not enforced); respect other's preferences (signaled with the "dot")

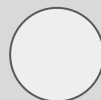"Please keep some distance."   "I am comfortable with handshakes."

Photography and recording policies

- Respect presenters wishes: if you see <mark>DO NOT RECORD NOTES OR TAKE PHOTOS FOR THIS SESSION</mark> then
    - don't take pictures
    - don't take public notes

"Please do not take photos of me."   "I am happy to appear in pictures."

Locations

Day 1 and 2 (talks)

- Faculty of Sciences of the University of Lisbon (ULisboa), Campo Grande, 1749-016 Lisbon
- Talks: Auditorium, **Building C1**
- Coffee break/lunch location: **Building C6**
- Restrooms

Day 3 (hackathon)

- SANA Metropolitan Hotel, Madrid Room
- R. Soeiro Pereira Gomes 2, 1600-198 Lisbon

MDAnalysis UGM 2023
Faculty of Sciences of the University of Lisbon
Campo Grande, 1749-016 Lisbon, Portugal

Source of Map: https://ciencias.ulisboa.pt/en/conferencia/ilter/meeting-place
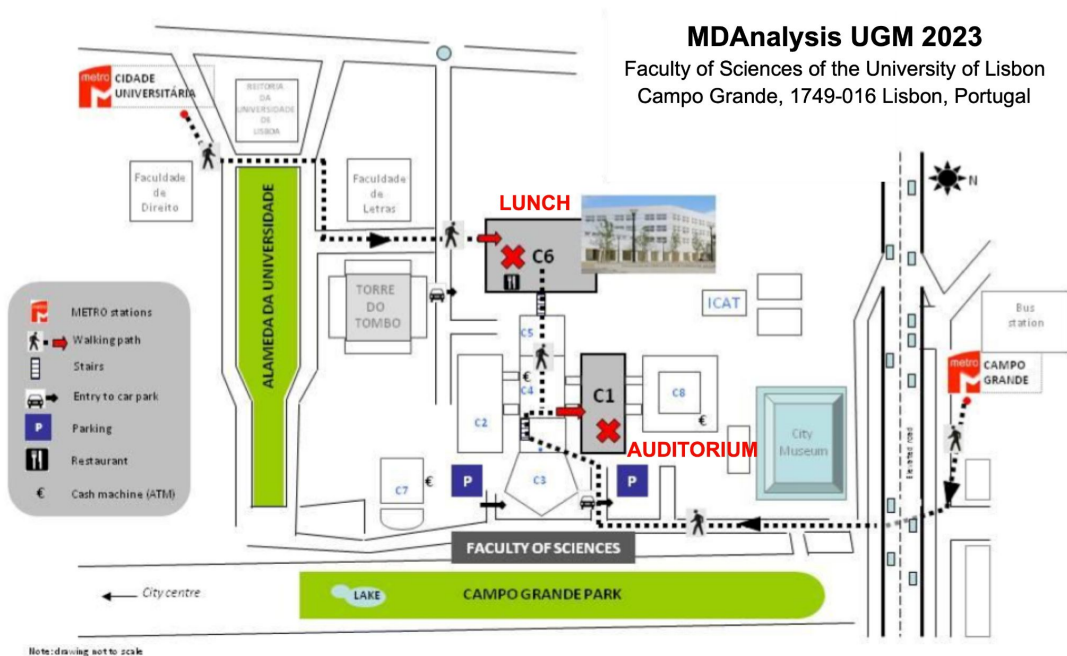
Communications

Discord

join our Discord

https://discord.gg/sAKgZZnPv4

- **UGM 2023** section
- e-posters in **#posters**
- discussions

Shared Google Doc

- You were registered with your email from conference sign up. Request access if necessary.

- All are invited to participate.
- Respect speakers notes to not record talk.

MDAnalysis and the Future: Defining the Path Forward Beyond 3.0

Panel   General

September 15, 2023   NEW

jennaswa [she/her] OP 09/15/2023 6:38 PM
Questions/comments for the speakers of the MDAnalysis and the Future: Defining the Path Forward Beyond 3.0 open discussion

React to Post   Follow

👋 Start the conversation!
Be the first to share what you think!

Program Overview

Day 1 (here)

12:00 – 12:30	Registration
12:30 – 12:45	Welcome
12:45 – 13:30	MDA State of the Union
13:30 – 16:30	Talks and Career Panel
16:45 – 17:45	Keynote: Giovanni Pavan
17:45 – 18:00	Closing remarks Day 1
19:30 – 21:00	Conference Dinner @ Rice ME

Day 2 (here)

9:00 – 9:30	Registration
9:30 – 13:00	Talks
13:00 – 14:00	Lunch
14:00 – 15:00	Keynote: Cédric Bouysset
15:00 – 15:30	Talks
16:00 – 17:00	Open Discussion: Future of MDAnalysis
17:00 – 17:30	Awards & Closing

Day 3 (SANA Metropolitan Hotel, Madrid Room)

10:00 – 15:00	Hackathon