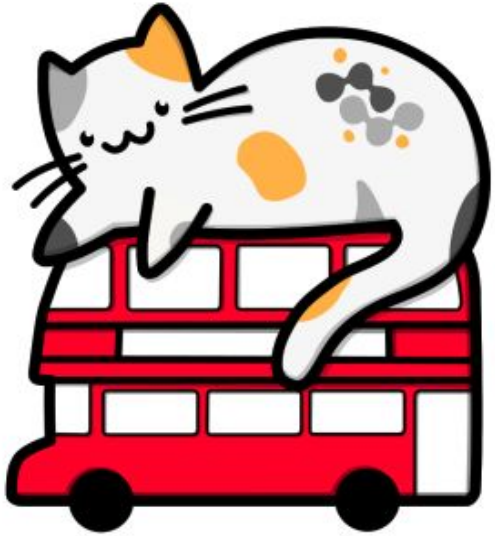
MDAnalysis

UGM 24

London, UK



Closing Remarks

22 August 2024

Oliver Beckstein

THE THOMAS YOUNG CENTRE TyC

MGMS

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Best Talk Voting

Scan this QR code to vote for your top ONE talk!

NOTE: If you are a presenter, please do not vote for your own talk 😸

Applications in Materials Science and Soft Matter *(Chair: Micaela Matta)*
Josh Dunn - Kinisi: Bayesian Analysis of Mass Transport from Molecular Dynamics Simulations
Shivani Grover - Choline Based Plastic Crystals as Barocaloric Materials: Insights from Ab Initio Molecular Dynamics

Toolkit Showcase *(Chair: Fiona Naughton)*
Sarah Fegan - CodeEntropy Software Development
Raquel López-Ríos de Castro - PySoftK 2.0: Tool for the Analysis of Interfaces, Interactions and Self-Assembly in Soft Matter Simulations
Hannah Pollak - ClayCode: A Toolkit for Clay Simulation Setup and Analysis

Toolkit Showcase *(Chair: Hugo MacDermott-Opeskin)*
Ferdoos Hossein Nezhad - MDGraphEmb: A Toolkit for the Encoding of Molecular Dynamics Data Using Graph Embedding
Namir Oues - MDAutoMut: A Toolkit for the Automated Evaluation of the Impact of Mutations on Protein Dynamics
Lexin Chen - Molecular Dynamics Analysis with N-ary Clustering Ensembles (MDANCE), A Novel Clustering Package Based on N-ary Similarity

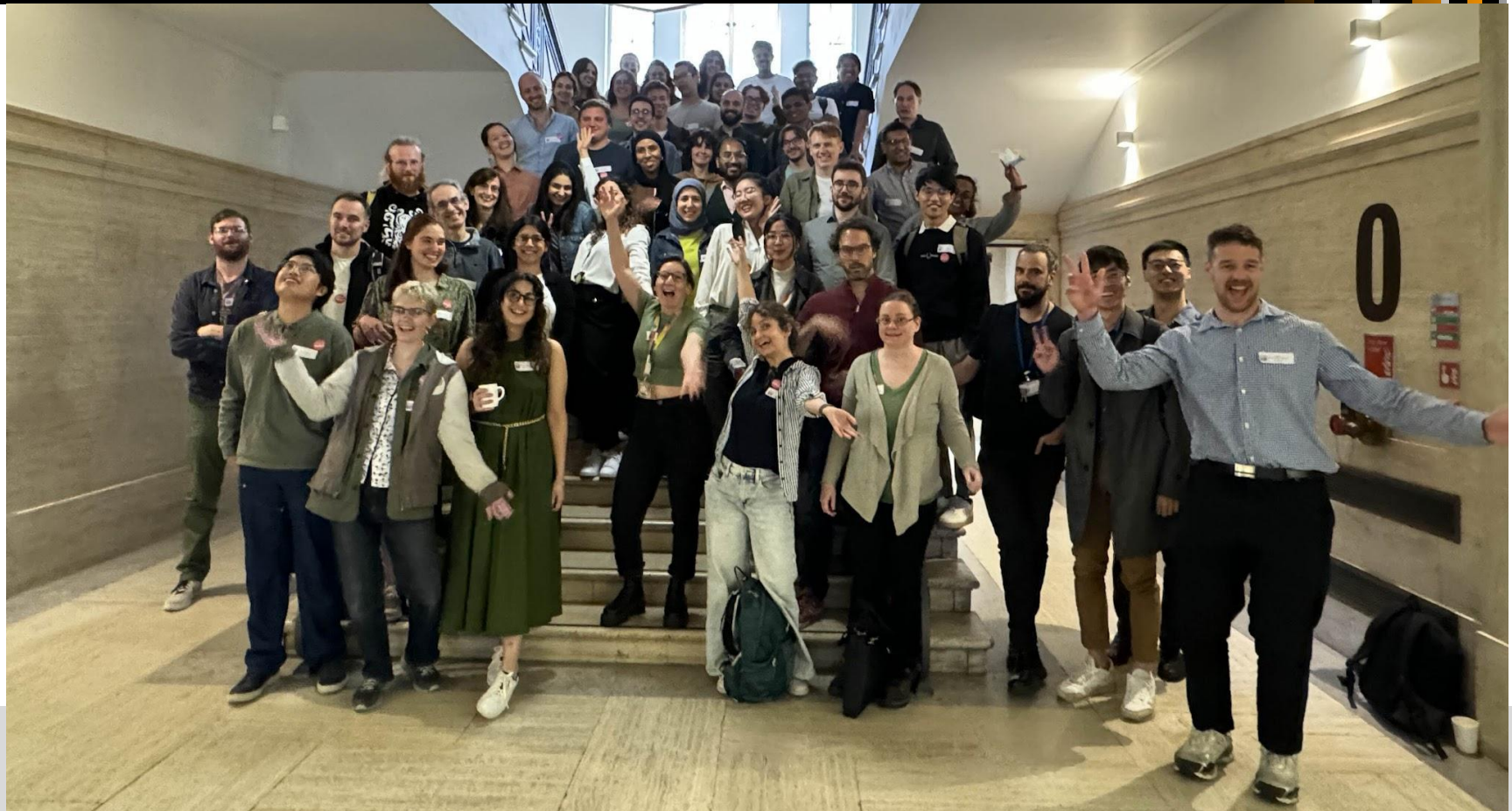
Applications in Drug Discovery and Therapeutics *(Chair: Richard Gowers)*
Özge Özkılınç - Exploring Lipase Biocatalysis in Sugar-Based Natural Deep Eutectic Solvents for Production of Novel Polymeric Compounds
Hugo MacDermott-Opeskin - Building an Open Source Antiviral Drug Discovery Toolkit
Evelyn Qiu - Investigating Allosteric Inhibitory Mechanisms of the Soluble Epoxide Hydrolase
Ivan Man - The Effect of Missense Mutations on the Binding Pocket Dynamics of Skeletal Mysoin
Sana Akhter - Mechanism of Ligand Binding to Target RNA Aptamer

Machine Learning and Multiscale Modeling with MD *(Chair: Yuxuan Zhuang)*
Henrik Stooß - Spatially Resolved Impedance Spectra from Molecular Dynamics Simulations: A Generalised Correlation Analysis Approach
Michal H. Kolar - Computer Simulations of the Ribosome
Matteo Degiacomi - Molearn: Streamlining the Design of Generative Models of Biomolecular Dynamics
Oliver Beckstein - Using MDAnalysis for Machine Learning: Non-parametric Bayesian Kinetic Clustering

https://forms.gle/ksePi73FuZE6dxew6

*This is also your last chance to vote by emoji reaction for **ALL STAR PETS** in the #mda-pets Discord channel!*

Closing Summary



Hackathon

Friday, 23 August

King's College London, Bush House, Auditorium

Time (BST)	
09:00 - 09:30	Check-In/Registration
09:30 - 10:15	A Bird's Eye View of Contributing to and Maintaining Open Source Software *(Oliver Beckstein; Fiona Naughton)*
10:15 - 10:30	Hackathon Introduction & Project Setup *(Yuxuan Zhaung, Hugo MacDermott-Opeskin)*
10:30 - 12:30	Work on Hackathon Projects
12:30 - 14:00	Lunch (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
14:00 - 16:00	Work on Hackathon Projects
16:00 - 17:00	Project Showcase (*Chair: Yuxuan Zhuang, Hugo MacDemott-Opeskin)*

Join the UGM **#hackathon** channel on Discord!

More details and proposed projects on GitHub:

How does it work?

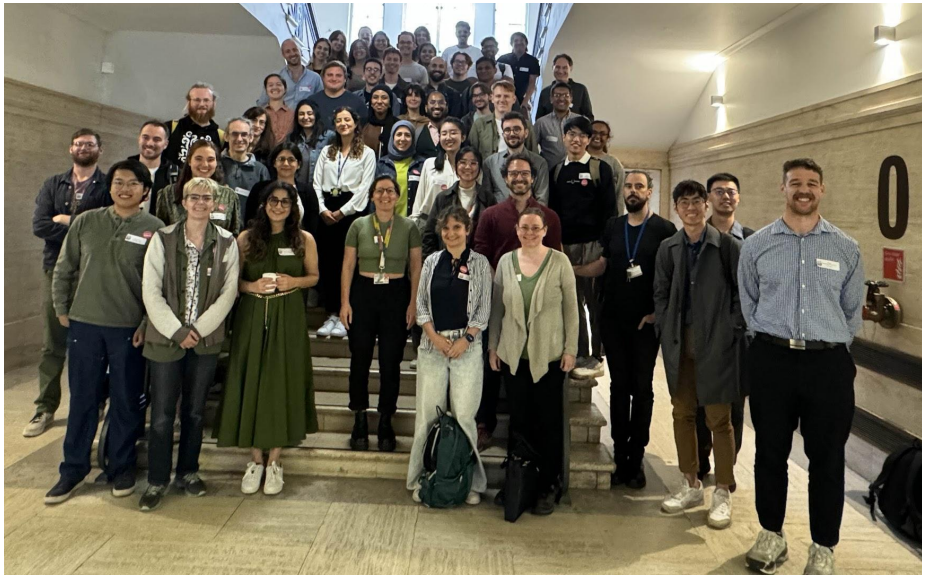
1. Find something you'd like to contribute to MDAnalysis!
2. Propose the idea to the discord UGM 2024 **#hackathon** channel.
3. Gather a team of like-minded attendees!
   Teams aren't required, but are strongly encouraged

https://github.com/MDAnalysis/UGM2024/tree/main/hackathon

Acknowledgements

THANK YOU! 🙏 to:

- All of our speakers and attendees
  - **Keynotes:** Antonia Mey, Francesca Stanzione
  - **Panelists:** Sarah Fegan, Shozeb Haider, Edina Rosta, Michelle Sahai
- UGM Organising Committee
- Partners and sponsors



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MDAnalysis
UGM 24
London, UK

11 core developers | **>208 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 B. 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 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, Sumit Gupta, Heet Vekariya, Lawson Woods, Johannes Stöckelmaier, **Jenna M. Swarthout Goddard**, Aditya Keshari, Philipp Stärk, Kai Niklas Spauszus, Sampurna Mukherjee, Leon Wehrhan, Valerij Talagayev, Kurt McKee, Fabian Zills, Laksh Krishna Sharma

https://www.mdanalysis.org/

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MD ANALYSIS

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OUTREACHY

Google Summer of Code

NSF

We'd love to hear your feedback!

MDAnalysis Community Survey

OUTREACHY

Adetutu Oluwasanmi

Develop a Communications Strategy for a Growing MDAnalysis User and Contributor Base

https://www.mdanalysis.org/2024/07/31/survey-announcement/

UGM Feedback Survey

NOTE: Please complete tomorrow if you plan to attend the hackathon

https://forms.gle/N9vBLCTaBypteEFU8

Want to contribute to MDAnalysis?

Participating

Ask **questions** on the GitHub Discussions forum and **be part of the conversation**. You can also join the MDAnalysis Discord Server to talk with other users and developers. (In order to join our Discord server, use the invitation link https://discord.gg/fXTSfDJyxE.)

Please report **bugs** or **enhancement requests** through the Issue Tracker.

MDAnalysis is **open source** and welcomes *your* contributions. Fork the repository on GitHub and submit a pull request. Participate on the GitHub Discussions (Development) forum.

MDAnalysis regularly takes part in various **mentoring and outreach programs**, such as Google Summer of Code, Google Season of Docs, Outreachy, the Station1 Frontiers Fellowship, and the CompChemURG mentorship schemes. Many of the current core developers joined the project through these mentoring schemes. The project also frequently offers **teaching workshops**, both online and in-person; recordings are often made available on the MDAnalysis YouTube channel. Follow our blog, LinkedIn, Twitter, and Bluesky pages for updates on how to participate.

https://www.mdanalysis.org/

MDAnalysis is looking to hire a contract-based **Technical Writer** (fully remote, full- or part-time for 200 hours) to help reorganise/consolidate the MDAnalysis website and learning resources.

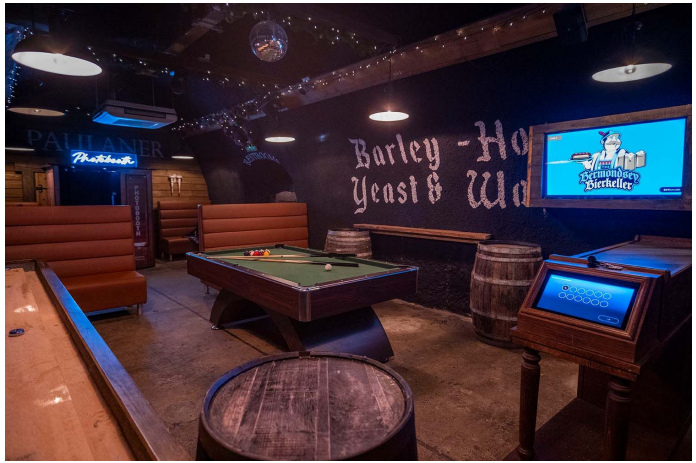
For more information, please talk to one of the core devs!

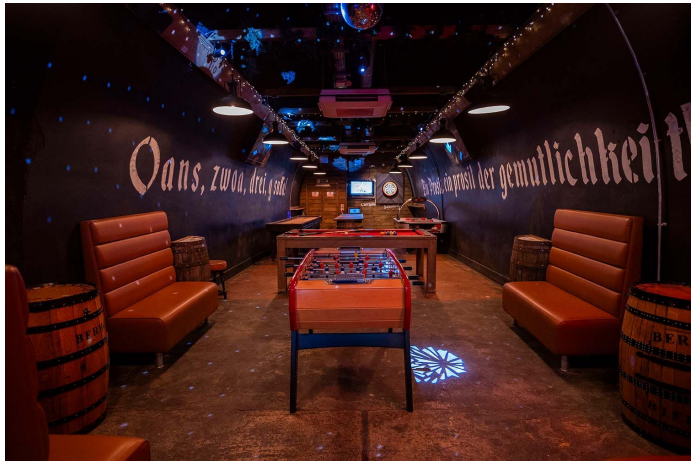
Social at Bermondsey Bierkeller tonight

Join us in the games room (Cellar Arch) from 7pm!

2-4 Tooley Street, London, SE1 2SY
Nearest Tube: London Bridge
https://www.bermondseybierkeller.co.uk/

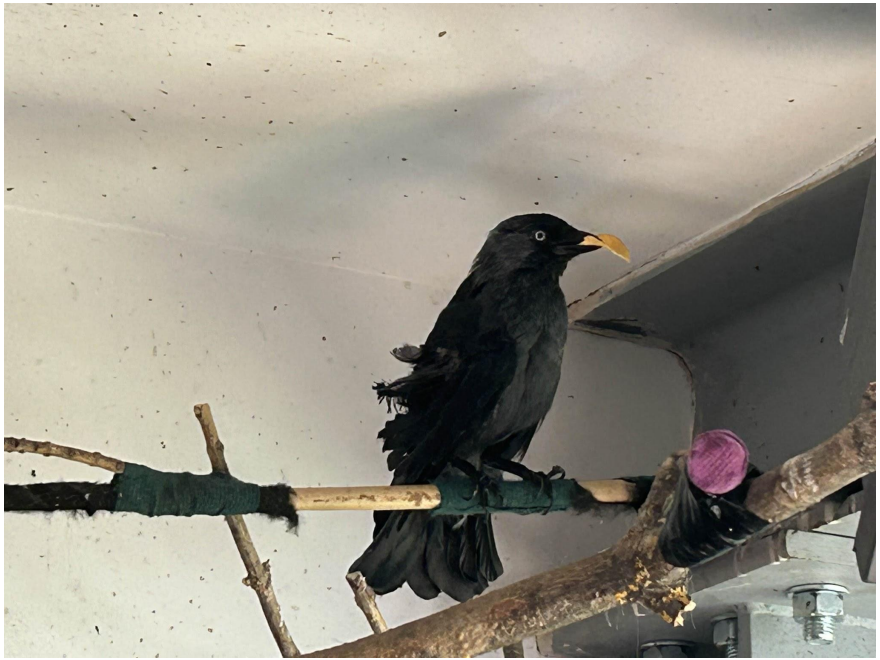
Food & drink tokens included if you RSVP'd,
Otherwise just pay directly at the venue!





Awards: All Star Pet

Pom



Awards: Best Poster

1. **Asal Azar** - Structural Dynamics of a Metalloprotease Enzyme: Insights from Molecular Dynamics Simulations

2. **Simon Holtbrügge** - Isotropic, Semi-isotropic, and Anisotropic Rotational Diffusion from Molecular Dynamics Trajectories

2. **Valerij Talagayev** - OpenMMDL: A Workflow for Molecular Dynamics Simulations of Protein-Ligand Complexes Setup, Simulation and Analysis

Awards: Best Talk

1. **Raquel López-Ríos de Castro**

PySoftK 2.0: Tool for the Analysis of Interfaces, Interactions and Self-Assembly in Soft Matter Simulations

2. **Lexin Chen**

Molecular Dynamics Analysis with N-ary Clustering Ensembles (MDANCE), A Novel Clustering Package Based on N-ary Similarity

3. **Namir Oues**

MDAutoMut: A Toolkit for the Automated Evaluation of the Impact of Mutations on Protein Dynamics

Honorable mentions

Michal H. Kolar - Computer Simulations of the Ribosome

Matteo Degiacomi - Molearn: Streamlining the Design of Generative Models of Biomolecular Dynamics

Thank you!

MDAnalysis UGM 24 London, UK

See you tomorrow at the Hackathon!

or

Safe travels!