

MDAnalysis UGM 24

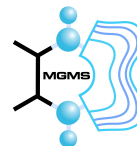
London, UK



Welcome

21 August 2024

Oliver Beckstein



NUMFOCUS
OPEN CODE = BETTER SCIENCE

**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. Poletto, 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/>

 @MDAnalysis



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Google Summer of Code

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Andrew Michael-Agrawal, Elizabeth Manning, **Oliver Beckstein**, Danny Parton, Philip Fowler, **Tyler Reddy**, Joseph Goose, **Jan Domanski**, Benjamin Hill, Paul Rigor, David Caplan, Christian Beck, **Stéphane Boutevin**, **Sébastien Buchoux**, Joshua L. Adelman, Lukas Gross, **Adam Komogiyi**, Lukas Stelzl, Jinju Lu, Joshua Xue, Xavier Deupi, **Manuel Nurnberg**, **David McGibbon**, **Richard J. Gowers**, Alejandro Berna, **Matthias van der Feltz**, Matthieu Chavenc, **Andriy Nesterenko**, Caio S. Souza, Sean **Dotson**, Carlos Yanez, **David Houston**, Isaac V. **Ke**, Gorman Stock, **Jonathan Baer**, **Prashant**, Balasubramanian, **Paola**, **Kenia**, Abhinav Gupta, **Eugen Hrusa**, **Chen**, **Fiona B. Naughton**, Robert **Boomsma**, **Matthias**, **Antanu Srivastava**, **Pe**, **Cortini**, Zhiyi **Shish Punjani**, Uth **Shobhit Ag**, **Rathore**, Akshay **Zamora**, Jon Kap **King**, Kathleen Clark, Dominik 'Rath **Nestor Wendt**, **Micaela**, **Jose Borre**, **Hen von Bülow**, Nabarun **Johannes Zeman**, Ayus **Shujie Fan**, Andrew R. McCluskey, Henry Mull, **Irfan Alibay**, **Philip Loc**, **W. Thom**, **Ehlen**, Daniele Padula, Ninad Bhat, Fer **Luís Pedro Borges**, Araújo, **A. Kognole**, **Rocco Meli**, **Lily Wang**, **Joao Miguel Correia Teixeira**, Charlie Cook, Yuanyu Cha **Ivan Hristov**, Michael Quev **Hugo MacDermott-Opeskin**, Anshul Angaria, Shubham Sharma, **Yuxuan Zhuang**, Cédric Bouysset, Abhish **Morgana L. Nance**, Faraz Shah **Toorn**, Siddha **Ameya Harmalkar**, Shakul Pathak, Andrea Rizzi, **Marcello Seg**, Edis Jakupovic, Nicholas Craven, Mieczyslaw Torch **rehuet**, Ha **Karthikeyan Singaravelan**, Ian Aditya Kama **neschi**, Henrik Jäger, Jan Stevens, Orion Cohen, Dimitrios Papageorg **Mannah Polla**, **to-Ojeda**, Paarth Thadani, Henry Kobin, Ko **Shah**, Alexander Yang, Filip T. Szczypiński, Marcelo C. R. Melo, Mark D. Driver, Kevin Boyd, **Yantong Cai**, Bjarne Feddersen, Pratik Gu **er**, Aya M. Alaa, Kazi Shudipto Amin, Alia Lescoulie, Manish Kumar, Aditi Tripathi, Sukeerti T, Kavya Bisht, Mark Ademtew, Uma D Kadam, Ta **Mingyi Xue**, Meghan Osato, Anirvinya G, R **Manish Kumar**, Aditi Tripathi, Sukeerti T, Kavya Bisht, Mark Verma, Marcelo D. Poletto, Ricky **R. Pappalardo**, Tengyu Xie, Raymond Zhao, H **Jennifer A Clark**, Jake Fennick, Utsav Khattu, 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. Swarouth Goddard**, Aditya Keshari, Philipp Stärk, Kai Niklas Spauszus, Sampurna Mukherjee, Leon Wehrhan, Valerij Talagayev, Kurt McKee, Fabian Zills, Laksh Krishna Sh

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

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



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Oliver Beckstein *Using MDAnalysis for Machine
Learning: Non-parametric
Bayesian Kinetic Clustering*

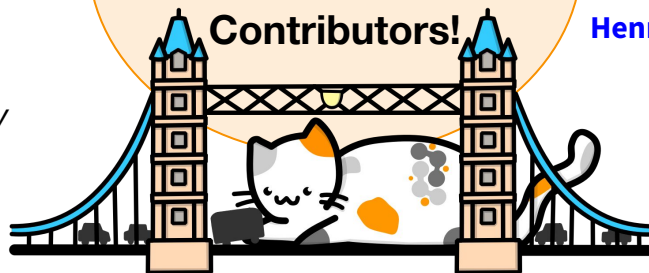
Hugo MacDermott-Opeskin *Building an Open
Source Antiviral Drug
Discovery Toolkit*

Hannah Pollak

*ClayCode: A Toolkit for Clay
Simulation Setup and
Analysis*

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

**UGM Talks and
Posters from
Code
Contributors!**



*Spatially Resolved
Impedance Spectra from
Molecular Dynamics
Simulations: A
Generalised Correlation
Analysis Approach*

Henrik Stooß

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

 @MDAnalysis

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

Code of Conduct



We are committed to providing a productive, harassment-free environment for everyone.
Everybody participating in the UGM agreed to abide by the CoC.

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



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

MDAnalysis Code of Conduct



Harassment or other CoC violations? Report!

Ombudspersons



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



Micaela Matta (at UGM)

- email: <micaela@mdanalysis.org>
- discord: @micamicamicaa



Richard Gowers (at UGM)

- email: <richard@mdanalysis.org>
- discord: @richard7377



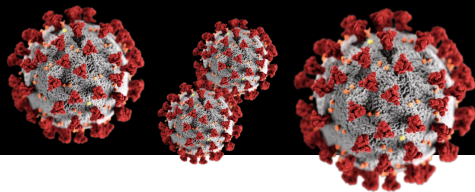
Jenna Swarthout Goddard (online)

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

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

MDAnalysis Code of Conduct





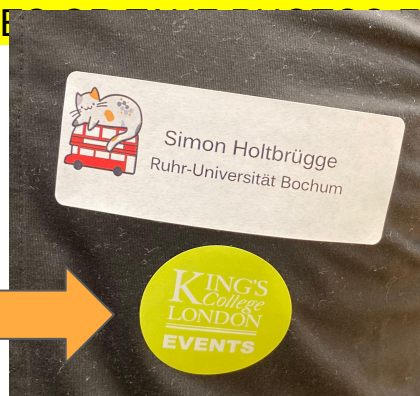
COVID19 – risk differs for everyone, so we want to make it possible for everyone to attend

- Please **do not attend if you are testing positive for SARS-Cov-2**
- Limited number of test kits at registration — ask if you need one.
- Testing positive during workshop?
 - Please do not attend.
 - Please notify the organizing committee ugm@mdanalysis.org (will handle information confidentially)
 - We will inform attendees about positive cases (*anonymously*)
- Masks are not required but welcome — we support your choice.
 - Masks available at registration
- Social distancing: your choice (not enforced)

Photography and recording policies & badges



- Use the #photos channel (and #mda-pets 🐱 🐶) on Discord generously, **BUT:**
 - Make sure you have permission from any people appearing in photos (if there's a **yellow dot** on their name tag, **please ask first**)
 - Respect presenters wishes: if you see **DO NOT RECORD NOTE** OR **THIS SESSION** then:
 - don't take pictures
 - don't take public notes
- Wear badges
- Have "Kings College Events" sticker always



"Please do NOT include me in pictures."

Locations



Talks

- King's College London (KCL) Bush House **Auditorium** (Ground Floor)
300 Strand, London, WC2B 4BG, United Kingdom

Coffee Breaks/Lunches

- KCL Bush House **Arcade** (Ground Floor)

Poster Reception (Wednesday only)

- KCL Bush House **Eighth Floor South** (8th Floor)

(6) Meeting Rooms (which will also be used for Hackathon breakouts)

- KCL Bush House **2.01-2.06** (2nd Floor)

Restrooms

Pub Night (Thursday only; pre-registered attendees)

- Bermondsey Bierkeller, 2-4 Tooley St., London, SE1 2SY, United Kingdom

Communications



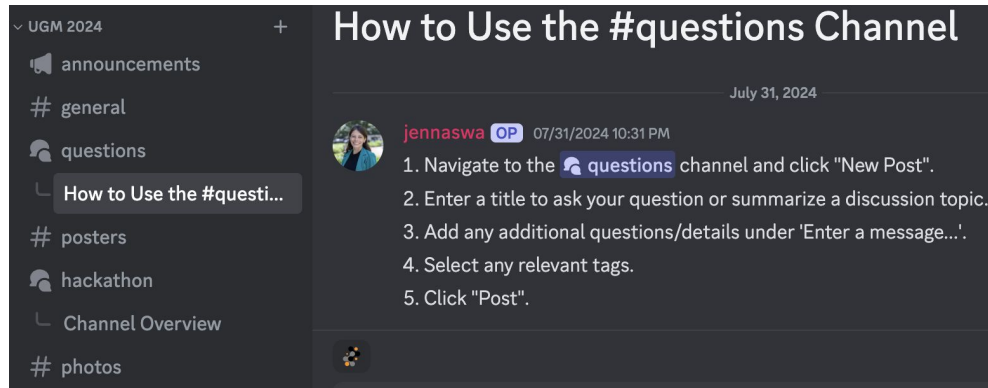
Discord



join our Discord

<https://discord.com/invite/kGaDXy7egd>

- UGM 2024 section



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.

GitHub Repository

<https://github.com/MDAnalysis/UGM2024>

- Presenters *encouraged*, but not required, to make materials available
- Includes specific details related to the **hackathon**



And now...



**...on to the MDAnalysis
State of the Union!**