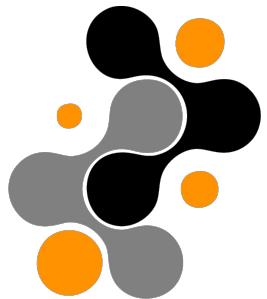


What's new and coming soon?

MDAnalysis
UGM 24
London, UK



Outreach



Teaching Workshops



This year we have delivered teaching workshops:

Various online workshops, with recordings available on Youtube (search mdanalysis).

10th May: CCPBioSim MDAnalysis workshop @ TYC London

24-25th June: MDAnalysis/MolSSI Workshop @ ASU AZ

& Upcoming:

5th September: CCPBioSim Training Week at Sheffield University

YouTube mdaanalysis

In [9]:

```
1 ow = peg_u.select_atoms('type Ow') # water oxygens
2 op = peg_u.select_atoms(['resname UNL and element O']) # PEG oxygens
```

We use the `rdf.InterRDF` function to calculate the radial distribution function:

In [10]:

```
1 00_rdf = rdf.InterRDF(ow, # O water
                      op, # O PEG
                      rrange=(0,10))
```

We need to `.run()` the radial distribution function, and optionally select an interval of frames:

In [11]:

```
1 RDF = 00_rdf.run(start=0, stop=90)
```

This returns a `results` dictionary reporting the bins and rdf values:

In [12]:

```
1 RDF.results['bins']
```

Out[12]:

```
array([0.06666667, 0.13333333, 0.2, 0.26666667, 0.33333333, 0.4, 0.46666667, 0.5, 0.56666667, 0.6, 0.66666667, 0.7, 0.76666667, 0.8, 0.86666667, 0.9, 0.96666667, 1.0, 1.06666667, 1.1, 1.16666667, 1.2, 1.26666667, 1.3, 1.36666667, 1.4, 1.46666667, 1.5, 1.56666667, 1.6, 1.66666667, 1.7, 1.76666667, 1.8, 1.86666667, 1.9, 1.96666667, 2.0, 2.06666667, 2.1, 2.16666667, 2.2, 2.26666667, 2.3, 2.36666667, 2.4, 2.46666667, 2.5, 2.56666667, 2.6, 2.66666667, 2.7, 2.76666667, 2.8, 2.86666667, 2.9, 2.96666667, 3.0, 3.06666667, 3.1, 3.16666667, 3.2, 3.26666667, 3.3, 3.36666667, 3.4, 3.46666667, 3.5, 3.56666667, 3.6, 3.66666667, 3.7, 3.76666667, 3.8, 3.86666667, 3.9, 3.96666667, 4.0, 4.06666667, 4.1, 4.16666667, 4.2, 4.26666667, 4.3, 4.36666667, 4.4, 4.46666667, 4.5, 4.56666667, 4.6, 4.66666667, 4.7, 4.76666667, 4.8, 4.86666667, 4.9, 4.96666667, 5.0, 5.06666667, 5.1, 5.16666667, 5.2, 5.26666667, 5.3, 5.36666667, 5.4, 5.46666667, 5.5, 5.56666667, 5.6, 5.66666667, 5.7, 5.76666667, 5.8, 5.86666667, 5.9, 5.96666667, 6.0, 6.06666667, 6.1, 6.16666667, 6.2, 6.26666667, 6.3, 6.36666667, 6.4, 6.46666667, 6.5, 6.56666667, 6.6, 6.66666667, 6.7, 6.76666667, 6.8, 6.86666667, 6.9, 6.96666667, 7.0, 7.06666667, 7.1, 7.16666667, 7.2, 7.26666667, 7.3, 7.36666667, 7.4, 7.46666667, 7.5, 7.56666667, 7.6, 7.66666667, 7.7, 7.76666667, 7.8, 7.86666667, 7.9, 7.96666667, 8.0, 8.06666667, 8.1, 8.16666667, 8.2, 8.26666667, 8.3, 8.36666667, 8.4, 8.46666667, 8.5, 8.56666667, 8.6, 8.66666667, 8.7, 8.76666667, 8.8, 8.86666667, 8.9, 8.96666667, 9.0, 9.06666667, 9.1, 9.16666667, 9.2, 9.26666667, 9.3, 9.36666667, 9.4, 9.46666667, 9.5, 9.56666667, 9.6, 9.66666667, 9.7, 9.76666667, 9.8, 9.86666667, 9.9, 9.96666667, 10.0, 10.06666667])
```

90 just to make sure I think we definitely have at least 90 frames sorry 98 98 okay and then we

Intro to Molecular Dynamics Trajectory Analysis using MDAnalysis



Mentoring



This year we have had 4 students come through mentoring programs

Via Google Summer of Code:



- Lawson Woods - Enhancing the Interoperability and Efficiency of the Zarr MDAKit
- Valerij Talageyev - 2D Visualization for Small Molecules
- Luna Morrow - Extend MDAnalysis Interoperability with OpenBabel

Via Outreachy:



- Adetutu Oluwasanmi - Develop a Communications Strategy for a Growing MDAnalysis User and Contributor Base



MDAnalysis Community Survey



This year we have had 4 students come through mentoring programs



- Dr. Morrow - Extend MD
<https://www.mdanalysis.org/2024/07/31/survey-announcement/>
Interoperability with OpenBabel

Via Outreachy:



- Adetutu Oluwasanmi - Develop a Communications Strategy for a Growing MDAnalysis User and Contributor Base



What's GSOC?



What is Google Summer of Code?

GSOC is a summer internship to work on open source software projects.

Google sponsors the scheme and students are paid over the summer.

Projects are usually to develop a new “feature” for MDAnalysis.

MDAnalysis has participated since 2016.

<https://summerofcode.withgoogle.com>



Google Summer of Code

What is Google Summer of Code?

Google Summer of Code is a global, online program focused on bringing new contributors into open source software development. GSoC Contributors work with an open source organization on a 12+ week programming project under the guidance of mentors.

How to get involved



How to participate/assist in these activities

We are always open to opportunities to hold teaching sessions etc.

Additionally materials are available on GitHub which are freely licensed for reuse.

For mentoring programs, project ideas (both to mentor and be mentored) are welcome, probably around February for GSOC 2025 deadline.

MDAnalysis / WorkshopMDMLEdinburgh2022

Code Issues 6 Pull requests 1 Discussions 1 Action

WorkshopMDMLEdinburgh2022 Public

Project 1: Bead and Ring Groups

It is common to want to consider a group of atoms as a single site/particle, for example defining the position of a water molecule (or a larger solvent) as its center of mass. It then follows that it is useful to consider many such groupings as an array of quasi-particles, leading to something like an `AtomGroup` -Group, e.g. a Group representing a solvent where each item in the Group is a single molecule. The goal of this project is to make two such groupings, `BeadGroup` and `RingGroup`:

- `BeadGroup` : groups of atoms that can be represented as a single site/particle. This could be used for analysis purposes, as well as to define coarse-grained beads.
- `RingGroup` : aromatic rings (eg benzene, nucleobases etc.) can be defined by their position (the geometric center of the ring) and their normal vector (the direction they are facing). This class would be implemented as a special case of `BeadGroup` which also defines a directionality.

Objectives

1. Design and implement a `BeadGroup` class to represent a container of many groupings of atoms
2. Generalise existing methods (e.g. `center_of_mass`) to `BeadGroup`
3. Implement `RingGroup` , as a special case of `BeadGroup`
4. Implement ring finding functions to quickly define these groups
5. Implement basic `RingGroup` analysis functions, eg angle between rings, π-stacking identification.

Relevant skills

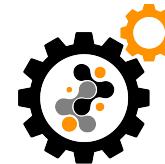
- Python
- Graph theory (eg the `NetworkX` package)

MDAKits





- Two major aims
 - Enabling reproducible MDAnalysis-using code development
 - Improving performance
- One way we are tackling reproducibility is by introducing the **MDAKITS** ecosystem



76 PROC. OF THE 22nd PYTHON IN SCIENCE CONF. (SCIPY 2023)

MDAKits: A Framework for FAIR-Compliant Molecular Simulation Analysis

Irfan Alibay^{‡†*}, Lily Wang^{‡†}, Fiona Naughton^{§†}, Ian Kenney^{¶†}, Jonathan Barnoud^{||}, Richard J Gowers[‡], Oliver Beckstein[¶]

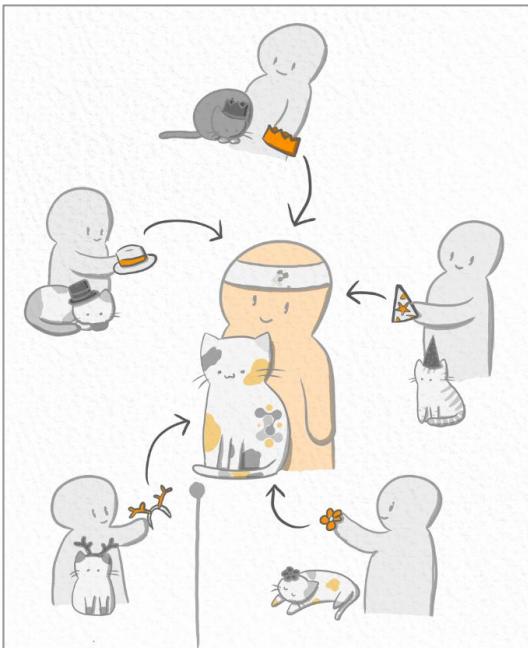


<https://mdakits.mdanalysis.org/>

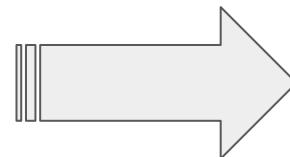
Growing Community & Code Base = Maintenance



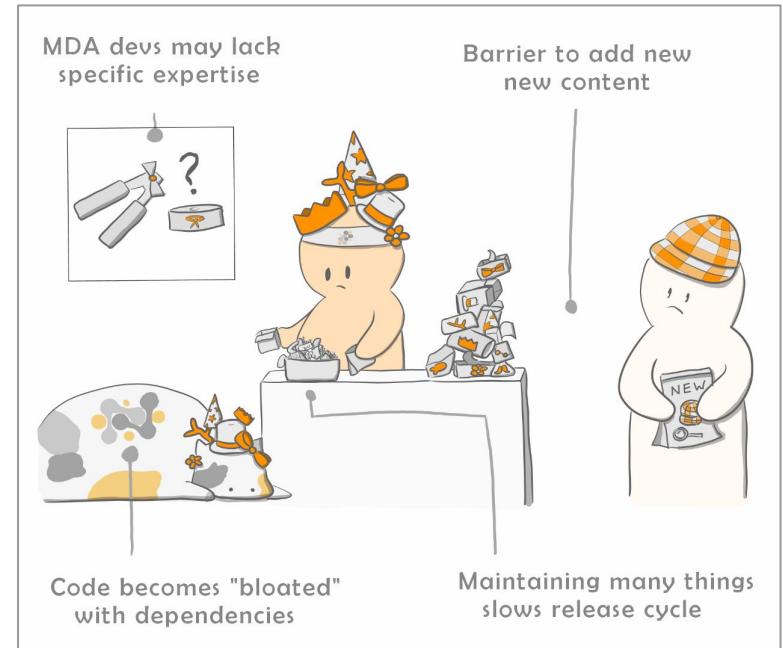
>200 code contributors and countless community members



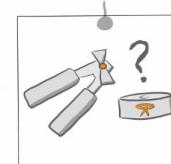
Asking for **MDAnalysis** contributions has many advantages...



...but a centralized solution is unsustainable for us



MDA devs may lack specific expertise



Barrier to add new new content



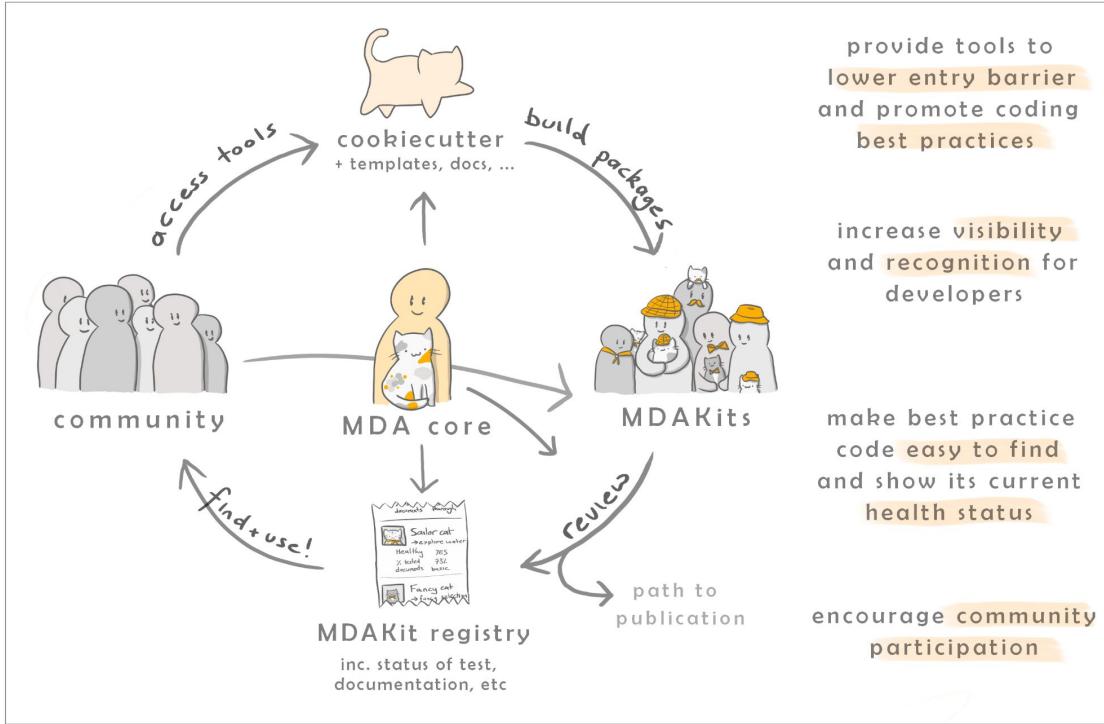
Code becomes "bloated" with dependencies

Maintaining many things slows release cycle



“MDAKits” can reduce barriers to participation

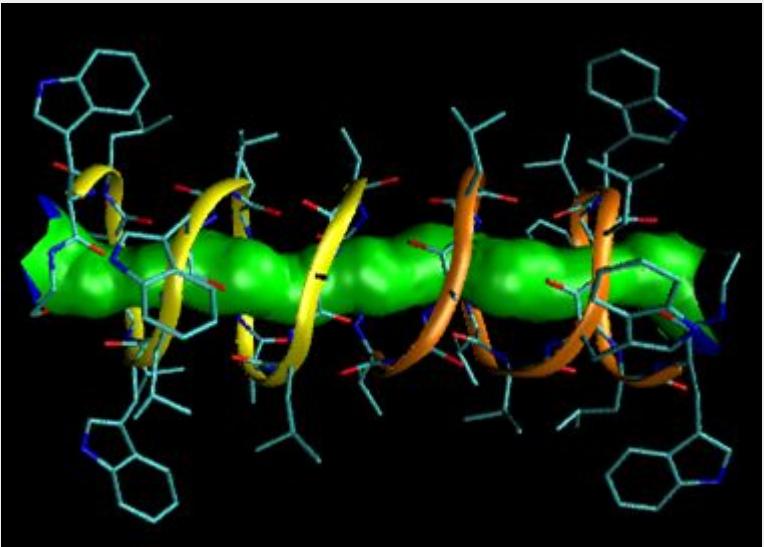
MDAKits, an ecosystem of downstream packages, may be more sustainable





MDAKit showcase: mdahole2

- Analysis of pathways through molecular channels
- Migrated core library specialized analysis
- Depends on external programs
 - Binaries made available on conda-forge



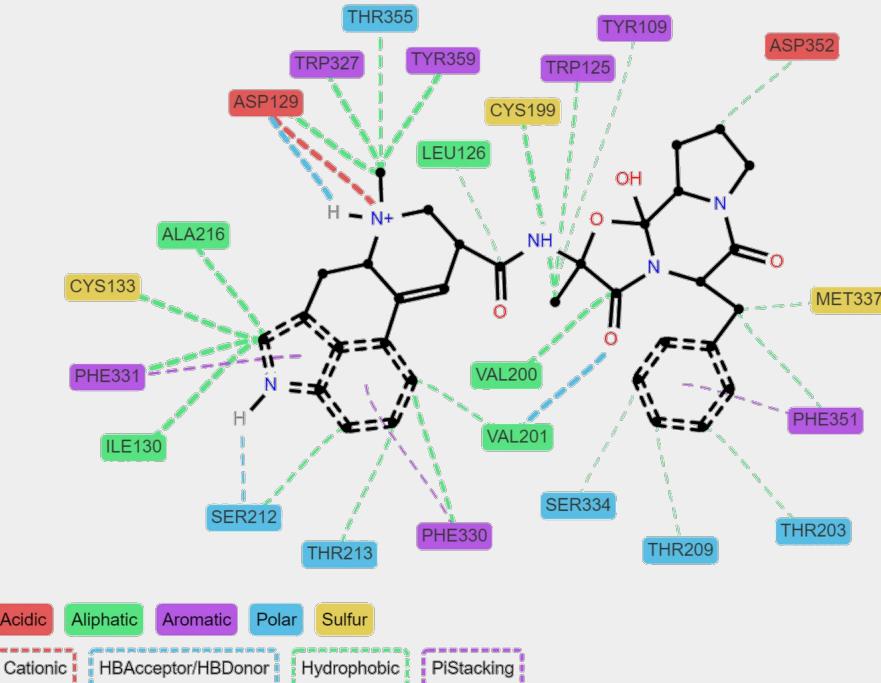
Smart, O. S., Goodfellow, J. M., & Wallace, B. A. (1993). The pore dimensions of gramicidin A. Biophysical Journal, 65(6), 2455–2460. [https://doi.org/10.1016/S0006-3495\(93\)81293-1](https://doi.org/10.1016/S0006-3495(93)81293-1)

Image from <https://holeprogram.com>



MDAKit showcase: ProLIF

- Generate interaction fingerprints for molecular complexes from simulation trajectories or experimental structures
- Package from Cédric Bouysset
- Code predating MDAKits



Acidic Aliphatic Aromatic Polar Sulfur
Cationic HBAcceptor/HBDonor Hydrophobic PiStacking

Bouysset, C., & Fiorucci, S. (2021). ProLIF: A library to encode molecular interactions as fingerprints. Journal of Cheminformatics, 13(1), 72. <https://doi.org/10.1186/s13321-021-00548-6>

Journal of
Cheminformatics



Modified image from publication.



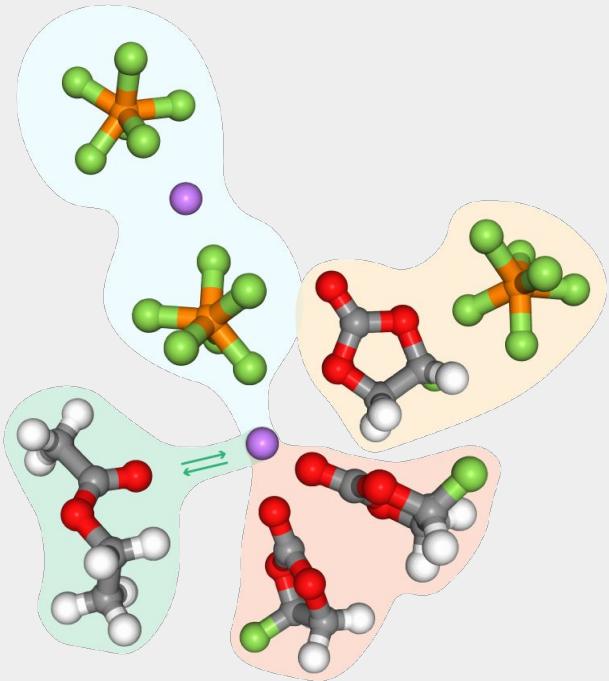
MDAKit showcase: SolvationAnalysis

- Implementation of routinely repeated analyses for solvated systems
- GSoC project from Orion Cohen
- JOSS publication

JOSS paper



Cohen, O. A., Macdermott-Opeskin, H., Lee, L., Hou, T., Fong, K. D., Kingsbury, R., Wang, J., & Persson, K. A. (2023). SolvationAnalysis: A Python toolkit for understanding liquid solvation structure in classical molecular dynamics simulations. *Journal of Open Source Software*, 8(84), 5183. <https://doi.org/10.21105/joss.05183>



Modified image from publication.

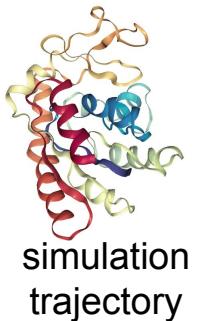
Performance





- Two major aims
 - Enabling reproducible MDAnalysis-using code development
 - Improving performance
- Performance improvements are arriving targeting both faster file reading and distance calculations

MDAnalysis library: heterogeneous data → uniform API



simulation
trajectory

dcd, xtc, trr,
ncdf, trj, pdb,
pqr, gro, crd,
dms, trz, mol2,
xyz, config,
history, gms, ...

psf, tpr,
prmtop, dms,
mol2, hoomd
xml, ...

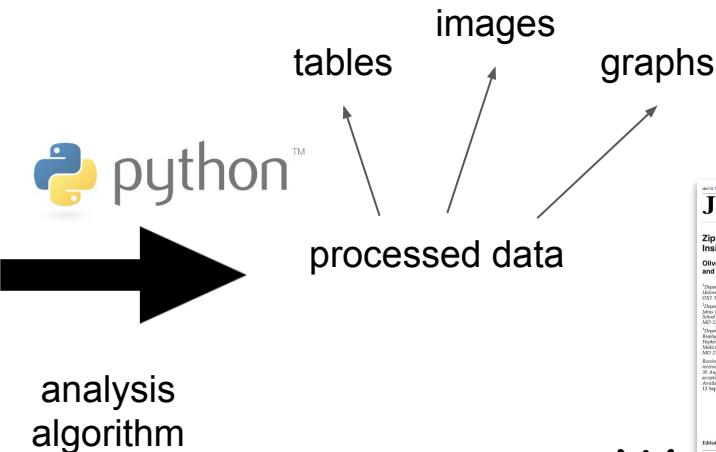
Oh nooooo!



“accessible”
structured data
`numpy.ndarray()`



> 40 file formats



1 analysis script



Insights &
publication!





Faster Reading - ASCII Files

While easy to read visually, ASCII files are a single stream of bytes with newline characters

To rewrite this in a compiled form (Cython) an interface for providing a seekable, line by line access to files was required.

First newlines characters in a block of read data must be identified, then pointers to these are served up sequentially.

Compressed files are the similar, but must be expanded out into an uncompressed form, then iterated

ATOM	1	N	PHE	A	1	-8.154	-0.523	-1.535	1.00	1.91	N
ATOM	2	CA	PHE	A	1	-8.345	0.512	-0.486	1.00	1.58	C
ATOM	3	C	PHE	A	1	-7.175	1.489	-0.464	1.00	1.22	C
ATOM	4	O	PHE	A	1	-6.056	1.146	-0.844	1.00	1.22	O
ATOM	5	CB	PHE	A	1	-8.499	-0.149	0.886	1.00	1.51	C
ATOM	6	CG	PHE	A	1	-7.392	-1.106	1.220	1.00	1.21	C
ATOM	7	CD1	PHE	A	1	-6.227	-0.654	1.818	1.00	1.63	C
ATOM	8	CD2	PHE	A	1	-7.517	-2.456	0.937	1.00	0.98	C
ATOM	9	CE1	PHE	A	1	-5.206	-1.533	2.128	1.00	1.89	C

ATOM	1	N	PHE	A	1	-8.154	-0.523	-1.535	1.00	1.91	N	ATOM		
2	CA	PHE	A	1	-8.345	0.512	-0.486	1.00	1.58	C	ATOM	3	C	
PHE	A	1	-7.175	1.489	-0.464	1.00	1.22	C	ATOM	4	O	PHE	A	1
-6.056	1.146	-0.844	1.00	1.22	O	ATOM	5	CB	PHE	A	1	-8.499		
-0.149	0.886	1.00	1.51	C	ATOM	6	CG	PHE	A	1	-7.392	-1.106		
1.220	1.00	1.21	C	ATOM	7	CD1	PHE	A	1	-6.227	-0.654	1.818		
1.00	1.63	C	ATOM	8	CD2	PHE	A	1	-7.517	-2.456	0.937	1.00		
0.98	C	ATOM	9	CE1	PHE	A	1	-5.206	-1.533	2.128	1.00	1.89		

```
^<8B>^H^H9<BD><C4>f^@^Cfoo.pdb^@u<D2>;<92><C3> ^L^F<E0>><A7><E0>^B<D1>
!<A5><C3>z<92>&q<8A><DC><FF>;<91><E4>d<CD><CE>^B<85>`^<C6><F8><E3>^W<F2><F2><DA><EE><CE>
^F:<F7><90><E9>y[ □ u<9C>`^K` d<99>=d
2#<C4>^P<E5>5x<AF><CF><FA><D9>g<E3>qZ~9r<AE>-#. <B0>|<EE><84>C2<96>K:<B8>X:<AE>u<9C>`^<DD>
^<E9>2 V^N<85><A9>;<97><F8><E0><88><90><EC><D9>^F`^B`_<93>q<C8> `&C2>3n<EB>8<89><D0>;<A3>
><B9><A:AB><U><FE>><T><DB><DF>><9E>N<F6><B4><EB><A8><D8>P<C9>Z<80>~O1<E4><BB>t3.<CB><F2><G>
^G<C5>^ReK<97><B4><C3>"`T,"`<97>U+0084>+<CA><D1>
]D<E5>^H<D8><EE><D0>C^M<F9><CB><C9><D6>Y<B9><98><B6><FE><FE>O^W<81><B4>H<FB><DF>4
^AR<97>N<BB><DD>qo<93>%<EC><C7>B^@^@
```

Faster Reading - TPR Files



The Gromacs TPR format is a binary format used to store the complete state of a simulation setup.

It is not *intended* to be read externally, however it is the best file format for working with Gromacs data.

This has also been rewritten from the ground up to fix performance issues. Additionally coordinates and velocities can now be read from these files.

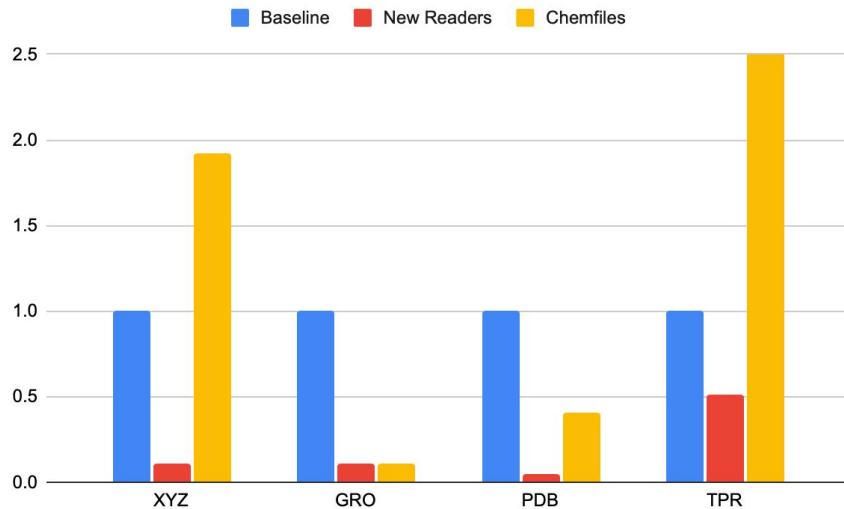
Faster Reading - ASCII



In total, rewriting into Cython has improved the speed of reading these files by orders of magnitude.

In comparison to ChemFiles (another compiled language solution) performance in best case seems competitive, indicating that the “true” best performance has been achieved.

These improvements are coming to MDAnalysis soon(™) and won’t require any changes to use.



Faster Reading - Conclusions



Generally these rules should be followed as much as possible:

- Don't allocate memory
- Don't copy data
- Don't interact with the OS

This is mostly driven by other work in the field, especially Lemire's work.

The screenshot shows a red-themed arXiv preprint page. At the top, it says "arXiv > cs > arXiv:1902.08318". Below that is the category "Computer Science > Databases". A timestamp indicates it was submitted on 22 Feb 2019 (v1) and last revised on 23 Jul 2024 (this version, v7). The title of the paper is "Parsing Gigabytes of JSON per Second". The authors listed are Geoff Langdale and Daniel Lemire.

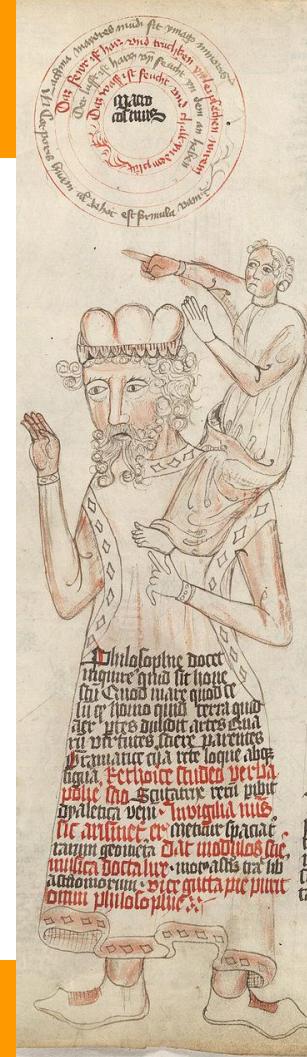
The screenshot shows a GitHub repository page for "fast_float" by "fast_float". The repository is public. The header includes links for Code, Issues (16), Pull requests (2), Actions, and Projects. The repository name "fast_float" is prominently displayed along with its status as "Public".

Community driven development

These contributions are the product of
community effort

Most Reader contributions come from outside
sources

TPR format has had 11 authors contributing to
it over 12 years



Acknowledgements



208+ code contributors and countless community members

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 Segà, 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 Kobiń, Kosuke Kudo, Sulay Shah, Alexander Yang, Filip T. Szczypinski, 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



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GSOC & Outreachy Mentors Team:

Hugo MacDermott-Opeskin, Cedric Bouysset, Yuxuan Zhuang, Richard, Jenna, Micaela, Xu Hong Chen

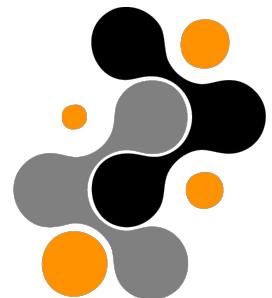
MDAKits Group:

Fiona Naughton, Ian Kenney, Irfan Alibay, Lily Wang and Oliver Beckstein

Performance Warriors:

Hugo & Richard

And now over to you...



Day 1



Wednesday, 21 August

King's College London, Bush House, Auditorium

Time (BST)	
09:00 - 09:30	Check-In/Registration
09:30 - 09:35	Welcome and Opening Remarks
09:35 - 10:15	MDAnalysis State of the Union
10:15 - 10:45	Coffee Break and Meet and Greet (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
10:45 - 11:45	Keynote Talk Antonia Mey - From a Molecular Movie of a Protein to Quantitative Data
11:45 - 12:45	Applications in Materials Science and Soft Matter Josh Dunn - Kinisi: Bayesian Analysis of Mass Transport from Molecular Dynamics Simulations Özge Özkilinç - Exploring Lipase Biocatalysis in Sugar-Based Natural Deep Eutectic Solvents for Production of Novel Polymeric Compounds Shivani Grover - Choline Based Plastic Crystals as Barocaloric Materials: Insights from Ab Initio Molecular Dynamics
12:45 - 14:15	Lunch (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
14:15 - 15:15	Toolkit Showcase 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
15:15 - 15:45	Coffee Break (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
15:45 - 16:45	Panel Discussion Communities and Resources for Computational Molecular Scientists Panelists: Sarah Fegan (CCPBioSim), Shozeb Haider (MGMS), Edina Rosta (TYC), Michelle Sahai (CompChemURG)
16:45 - 17:30	Lightning Talks Valerij Talagayev - OpenMMDL: A Workflow for Molecular Dynamics Simulations of Protein-Ligand Complexes Setup, Simulation and Analysis Simon Holtbruegge - Isotropic, Semi-isotropic, and Anisotropic Rotational Diffusion from Molecular Dynamics Trajectories Kira Fischer - Calculating Pair Distribution Functions in Anisotropic Geometries Asal Azar - Structural Dynamics of a Metalloprotease Enzyme: Insights from Molecular Dynamics Simulations Zhiwen Zhong - Unraveling the Molecular Dance: Insights into TREM2/DAP12 Complex Formation in Alzheimer's Disease through Molecular Dynamics Simulations Midhun Mohan Anila - Scrutinising the Conformational Ensemble of the Intrinsically Mixed-Folded Protein Galectin-3 Yu-Yuan (Stuart) Yang - Deep Learning for Binding Site Segmentation in Protein Ensembles
17:30 - 17:35	Day 1 Closing Remarks
17:35 - 21:00	Reception and Poster Session (Bush House, 8th Floor (South), https://www.kcl.ac.uk/kingsvenues/rooms/bh-8fs)

Try to meet ≥ 2 people you don't know!

Day 2



Thursday, 22 August

King's College London, Bush House, Auditorium

Time (BST)	
09:00 - 09:25	Check-In/Registration
09:25 - 09:30	Day 2 Opening Remarks
09:30 - 10:30	Keynote Talk Francesca Stanzione - Molecular Dynamics for Drug Discovery: Insights into Protein, Ligand, and Protein-Ligand Complexes
10:30 - 11:00	Coffee Break (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
11:00 - 12:00	Toolkit Showcase 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
12:00 - 12:45	Everything You Wanted to Know About MDAnalysis, But Didn't Dare Ask!
12:45 - 14:15	Lunch (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
14:15 - 15:30	Applications in Drug Discovery and Therapeutics 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 Myosin Sana Akhter - Mechanism of Ligand Binding to Target RNA Aptamer
15:30 - 16:00	Coffee Break (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
16:00 - 17:15	Machine Learning and Multiscale Modeling with MD 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
17:15 - 17:30	Presentation of Awards and Day 2 Closing Remarks
19:00 - 21:00	(Optional) Social Pub Night (Bermondsey Bierkeller, 2-4 Tooley Street, London, SE1 2SY, https://www.bermondseybierkeller.co.uk/) Pre-registered Attendees

Group photo time!

Keep talks/posters in mind so you can vote!

And post in #mda-pets



Day 3



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
10:15 - 10:30	Hackathon Introduction & Project Setup
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

Suggest
projects and
organise into
teams in
#hackathon!