

# MDAnalysis SURF / PRACE workshop 2021: Closing remarks

# Special thanks

- SURF / PRACE
  - Carlos Teijeiro Barjas



# Special thanks

- MDAnalysis community & developers
  - 136 code authors inc. 15 core developers
- MDAnalysis course team:
  - Fiona, Lily, Oliver, Richard, Jonathan, Manuel, Micaela(, Irfan)
- You!

# End of course questionnaire

- SURF / PRACE questionnaire
  - Should have been sent to you yesterday
  - <https://events.prace-ri.eu/event/1201/>
- Any comments appreciated!
  - Help us improve materials & create future workshops

# Course certificates

- Available to everyone that participated in all days
- Must be requested from SURF / PRACE
  - [training-research@surf.nl](mailto:training-research@surf.nl)

# Installing MDAAnalysis

- Code available on github: <https://github.com/MDAnalysis/mdanalysis>
- Current workshop uses the 2.0.0-beta release
  - If you have any issues please do report!
  - ``pip install MDAnalysis==2.0.0b0 MDAnalysisTests==2.0.0b0``
  - Will release new version
- Usually, can install via both conda or pip
  - ``pip install MDAnalysis``
  - ``conda install MDAnalysis -c conda-forge``

# Workshop materials

- All workshop materials are available on github
  - <https://github.com/MDAnalysis/WorkshopPrace2021/>
  - Please report any issues/comments!
  - PRACE will hold a link to it
- Access to LISA (SURF jupyter hub) until the next of the next week
- Can also run locally or via Binder
- Happy to answer extra questions – discord/workshop-2021

# Getting in contact

- See: <https://www.mdanalysis.org/#participating>
- Github
  - “Code” issues / feature requests
- Mailing lists
  - Users
    - Code usage questions
  - Developers
    - Anything related to developing (using) MDAnalysis
- Discord



# Contributing to MDAnalysis

- Volunteer-led project, all contributions appreciated!
- How you can contribute:
  - Code [help wanted, new starter issues]
  - Answering mailing list questions
  - Raising issues
  - Blogs
  - Documentation
  - Generally being a member of the MDAnalysis community
  - etc...

# Google summer of code

- Hosted by Google
- Paid 10 weeks code development projects for students
  - Just needs to be (recently) registered at a learning institution
- MDAnalysis usually takes ~ 2 students (depends on capacity)

# Google summer of code

- Two projects this year
- Estefania Barreto-Ojeda
  - Curvature analysis of biological membranes
- Orion Cohen
  - Solvation module for MDAnalysis

# Google summer of code

- Process
  - Organization announcements ~ Early March
  - Student application period March -> April
    - 1 commit merged into MDAnalysis
    - Write a proposal
  - Projects announced ~ May
  - Coding period ~ June -> August

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# Future MDAnalysis events

- “Social hours”
  - Discord
  - Games, etc...
  - Next: Saturday 29<sup>th</sup> May (see #mda-social for poll)
- Future workshops? Future user/developer conference?
  - Let us know what you’d like to see!
  - Any help is appreciated 😊

Thanks for attending!