# 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
  - https://events.prace-ri.eu/event/1201/

- Any comments appreciated!
  - Help us improve materials & create future workshops

# Installing MDAnalysis

- 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!

- 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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# Thanks for attending!