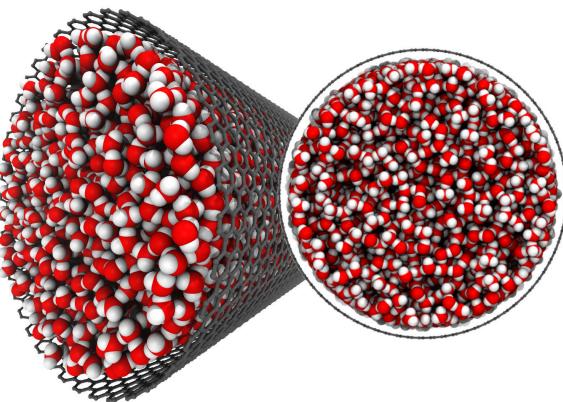
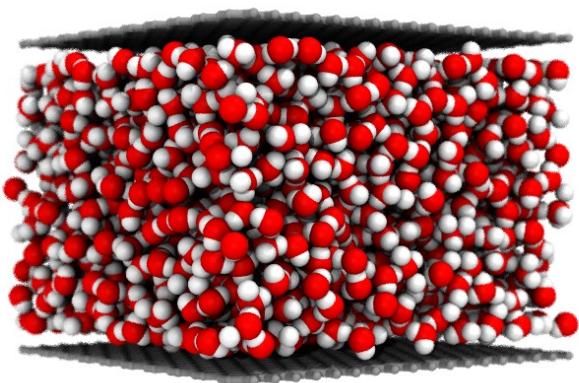


University of Stuttgart
Cluster of Excellence in Simulation Technology



MAICoS



Group website



MAICoS Docs

MAICoS: A Toolkit for the Molecular Analysis of Interfacial and Confined Systems

MDAnalysis User Group Meeting
September, 28th 2023

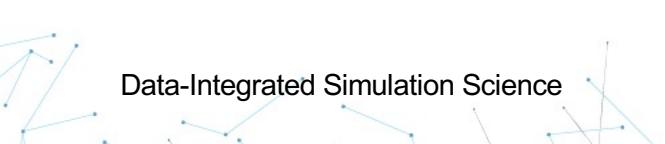
Henrik Jäger
Junior Research Group
for Multiscale Modelling
of Materials (M³)



SimTech

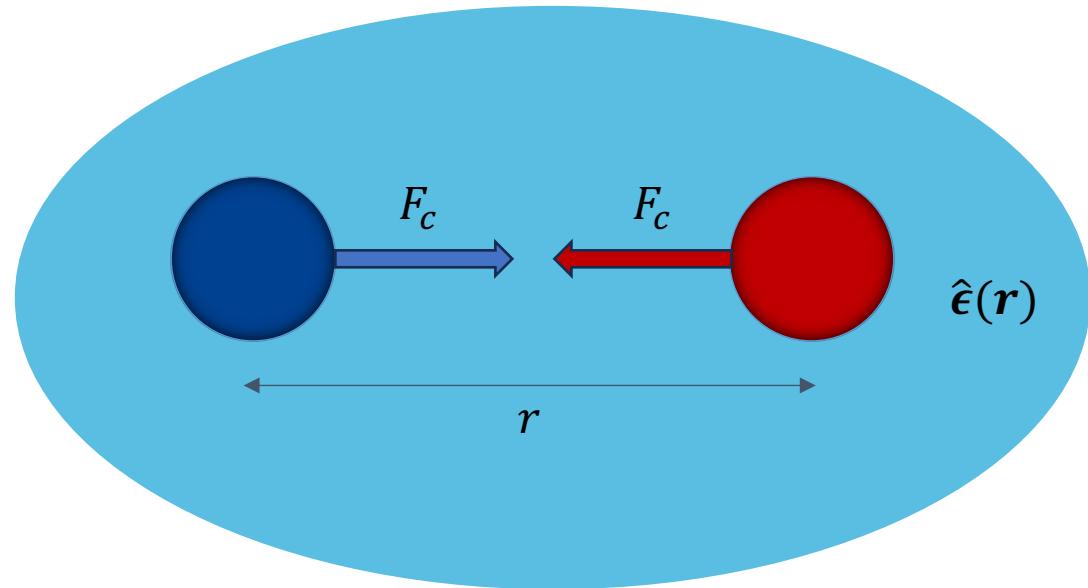
Overview

- A short history of MAICoS – Why we started it
- General design
- Applications



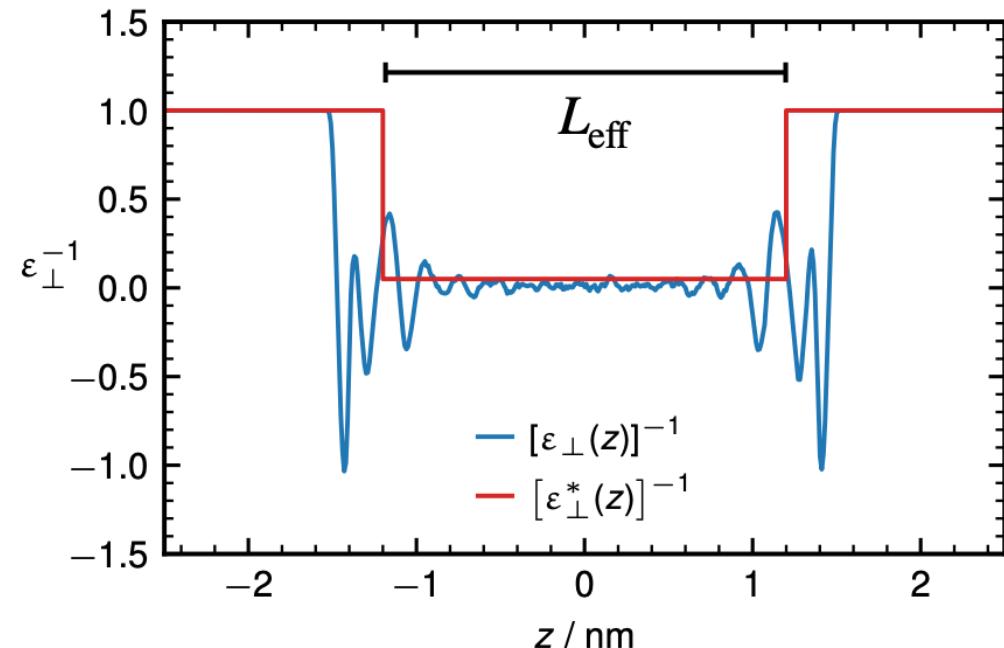
Dielectrics: A Motivating Example

Derivation, implementation and interpretation of spatially resolved dielectric analysis is not trivial



$$F_c = \frac{1}{4\pi\epsilon_0} \frac{|q||q|}{r^2}$$

Dielectric dividing surface



$$\frac{1}{\epsilon_{\perp}^{\text{eff}}} = 1 + \frac{\int_{-L/2}^{L/2} \epsilon_{\perp}^{-1}(z) dz - L}{L_{\perp}^{\text{eff}}}$$

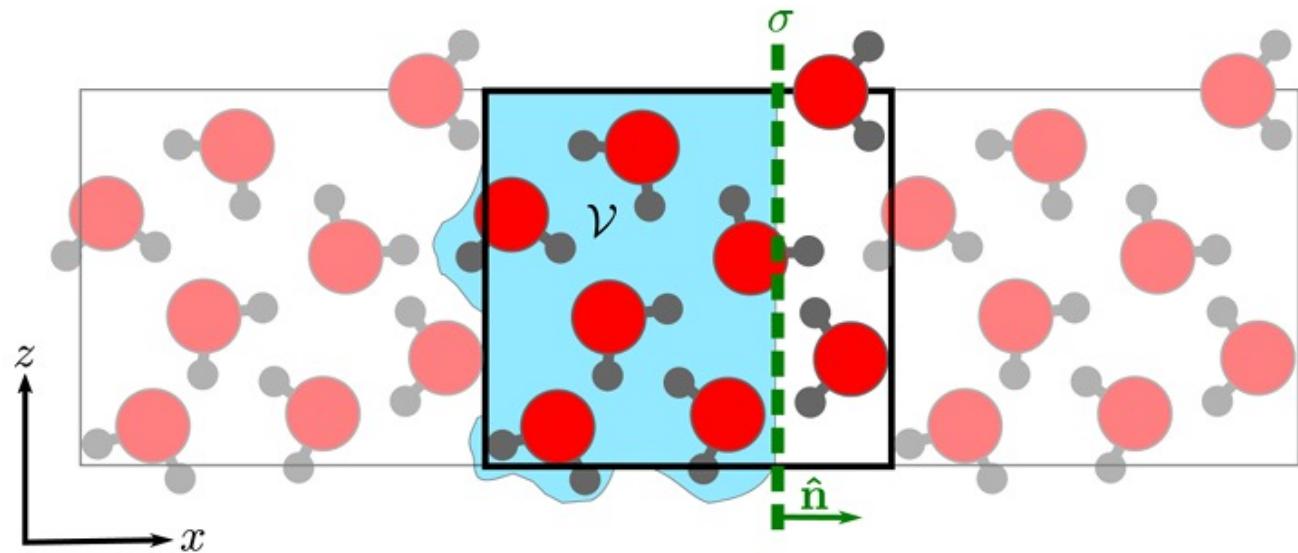
Dielectrics: A Motivating Example

Derivations for planar, cylindrical and spherical symmetries exist

$$\epsilon_{\perp}^{-1}(z) = 1 - \frac{c_{\perp}(z)}{\epsilon_0 k_B T + C_{\perp}}$$

$$\epsilon_{\parallel}(z) = 1 + \frac{c_{\parallel}(z)}{\epsilon_0 k_B T}$$

$$c_{\alpha}(z) = \langle m_{\alpha}(z) M_{\alpha} \rangle - \langle m_{\alpha}(z) \rangle \langle M_{\alpha} \rangle$$



Implementation caveats

- Box treatment
- Virtual site treatment
- Edge contributions (wrap/unwrap)

Physical caveats

- Electrostatic boundary conditions
- No free charges allowed

MAICoS – How it started



AS

Alexander Schlaich

Aw: static dielectric profile

An: Douwe Bonthuis

19. März 2014 um 18:04

Dear Douwe,

I think I managed through most of my problems and also your c-code is working now with the current gromacs-release.

However, I cannot obtain a bulk-like dielectric constant even for large slab separations.

Even with the c-code you sent me it seems more like $\text{eps} \sim 8$ in the center between two diamonds which are separated more than 3 nm.

What exactly did your system look like? Could you maybe send me some gro and corresponding mdp and itp files? Maybe you even have still have a trajectory I could use?

Thanks a lot,

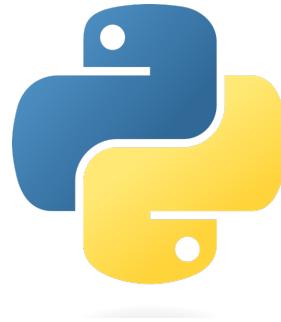
Best, Alex

MAICoS – How it started



mdtools

Project ID: 534



• 234 Commits ⚡ 5 Branches 🏷 0 Tags 📄 4.1 MB Files 🗑 4.1 MB Storage

A collection of scripts to analyse and build systems for molecular dynamics simulations.

27 Apr, 2017 2 commits



Move density.py from dielectric repo

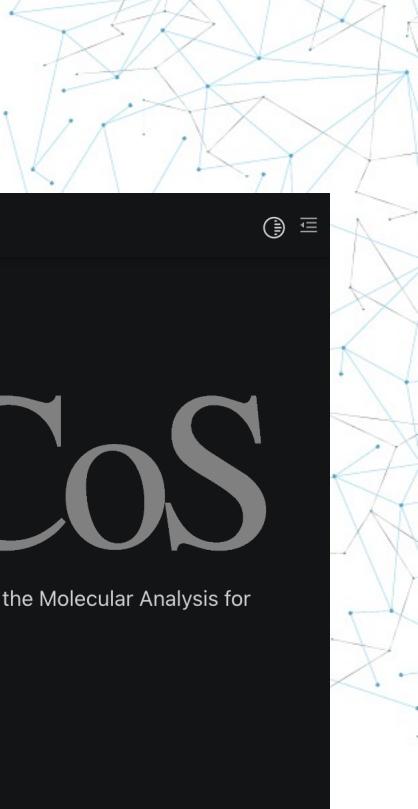
Schlaich, Alexander authored Apr 27, 2017



First version of README.md

Schlaich, Alexander authored Apr 27, 2017

Current state of MAICoS – Open Source and community driven



MAICoS > MAICoS

 MAICoS 
Project ID: 15092071 

  Unstar 15  Forks 10

981 Commits 13 Branches 12 Tags 4.2 GiB Project Storage 10 Releases

Topics: science Python molecular dy... + 3 more

Analyse molecular dynamics simulations of interfacial and confined systems.

[Read more](#)

powered by MDAnalysis pipeline passed docs development docs latest coverage 95.67%
pypi v0.7.2 Anaconda.org 0.7.2 discord 1 online Follow @maicos_analysis

lint docs build tests

lint	docs	build	tests
 lint 	 docs 	 build:linux  2	 tests:linux  2
		 build:macos  2	 tests:macos  2
		 build:windows  2	 tests:windows  2

Unit- and integration tests, physical validation with analytical solutions

MAICoS' Documentation



MAICoS

This documentation covers everything you need to know about MAICoS, the Molecular Analysis for Interfacial and Confined Systems toolkit. There are five sections:

- [Getting started](#)
- [How-to guides](#)
- [Reference guides](#)
- [Explanations](#)
- [Developer documentation](#)

If you are new to MAICoS, we recommend starting with the [Getting started](#) section. If you want to...

~15 Contributors



Current state of MAICoS - Design considerations



18 Analysis modules

DensityPlanar

DensityCylinder

DensitySphere

RDFPlanar

RDFCylinder

DielectricPlanar

DielectricCylinder

DielectricSphere

DielectricSpectrum

DipoleAngle

DiporderPlanar

DiporderCylinder

DiporderSphere

TemperaturePlanar

VelocityPlanar

VelocityCylinder

KineticEnergy

Saxs

Generalize analysis tasks

- Observables: Weights and normalization
- Geometry: Binning and symmetry

Ensure quality of research

- FAIR Workflow with full record of analysis
- Correlation and error analysis

Provide convenience functions

- Preliminary output for long trajectories
- Analyse multiple groups at once

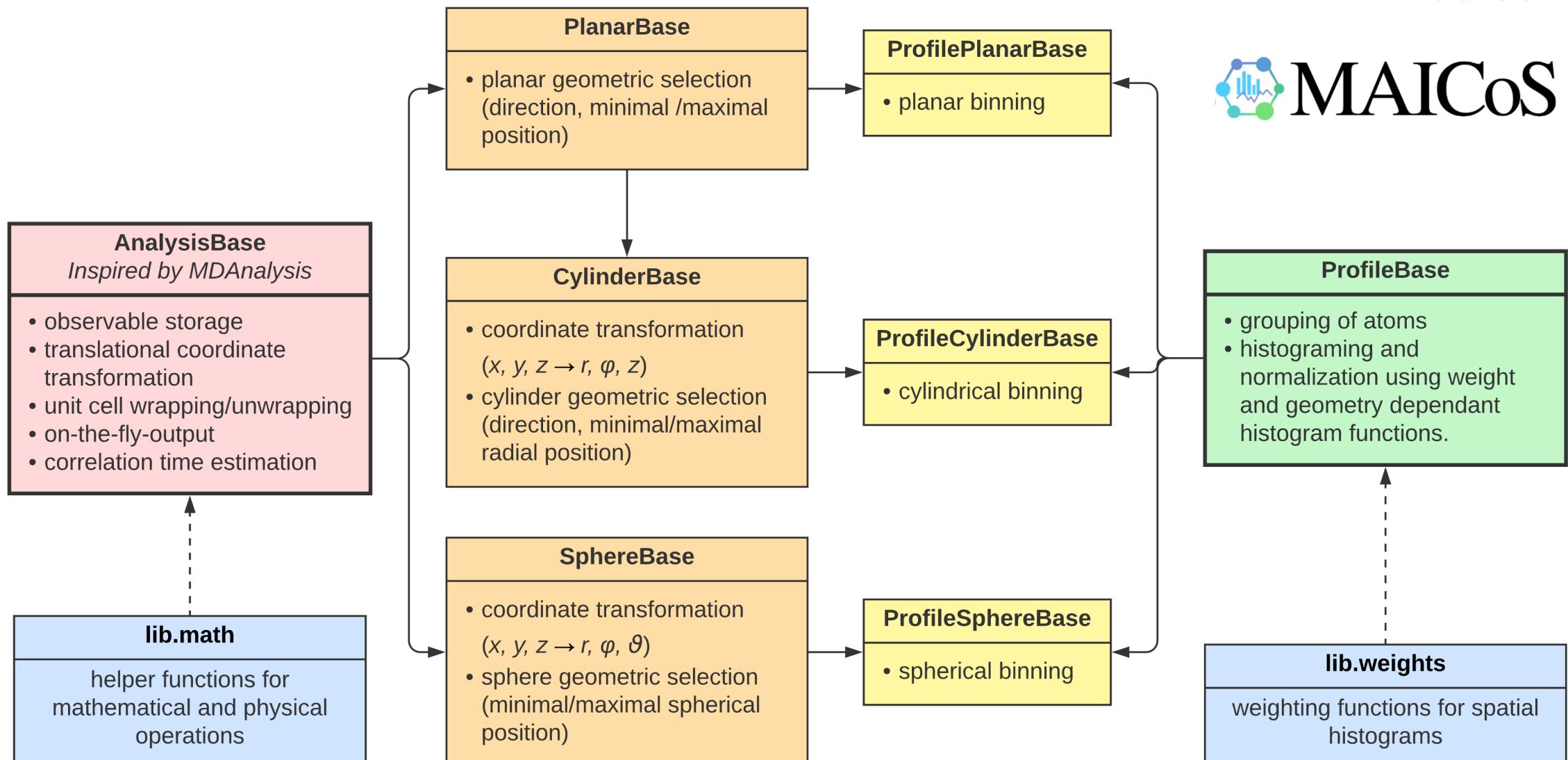
Prevent common mistakes

- Check for wrong physics
- Do preprocessing steps with sensible defaults



General design

Overview

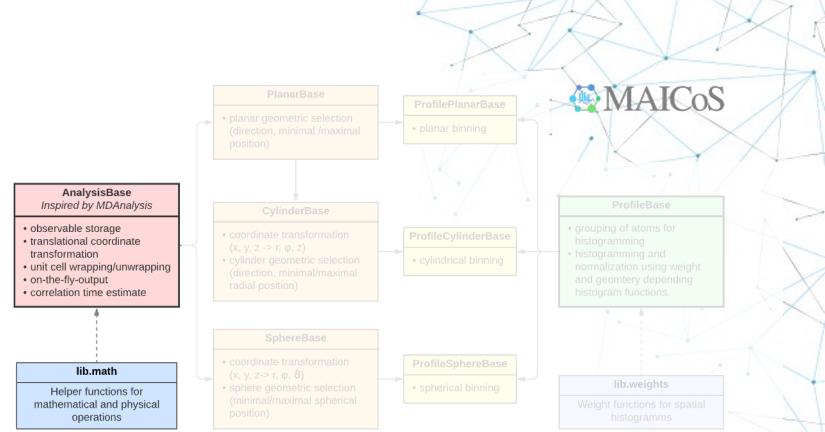


 **MAICoS**

AnalysisBase

Modified version of mda.AnalysisBase

Implements „generic“ analysis features



- **Observable management**
 - Saves observables from `_single_frame` and provides means and standard errors
 - Analyses correlation time of data and warns the user if calculated errors are underestimated
- **System reference**
 - Moves reference group to the box center
 - Manages wrap/unwrap on a case basis
- **FAIR Workflow**
 - Writes out full record of the analysis, including time, module input and software version
 - Prints relevant publications
- **Comfort functions**
 - Manages calls to `_conclude` to print out preliminary results

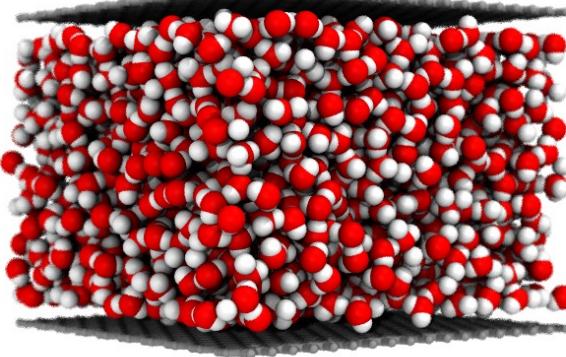
Geometric abstraction

For spatially dependent analysis, most systems can be split into three basic geometries.

Consistent definition of bin-width, -position, -edge, and –volume

Correct coordinate transformations

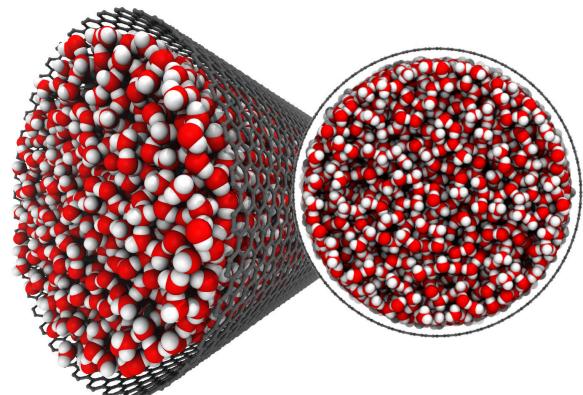
Planar



Slit pores
Lipid bilayers

...

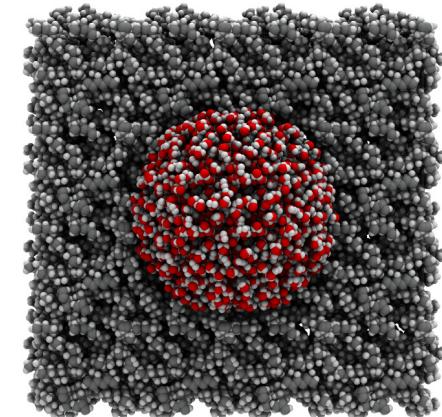
Cylindrical



Carbon Nanotubes
Cylindrical pores

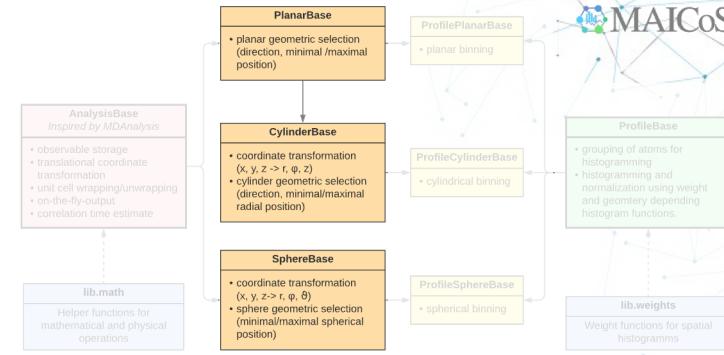
...

Spherical



Lipid micelles
Proteins

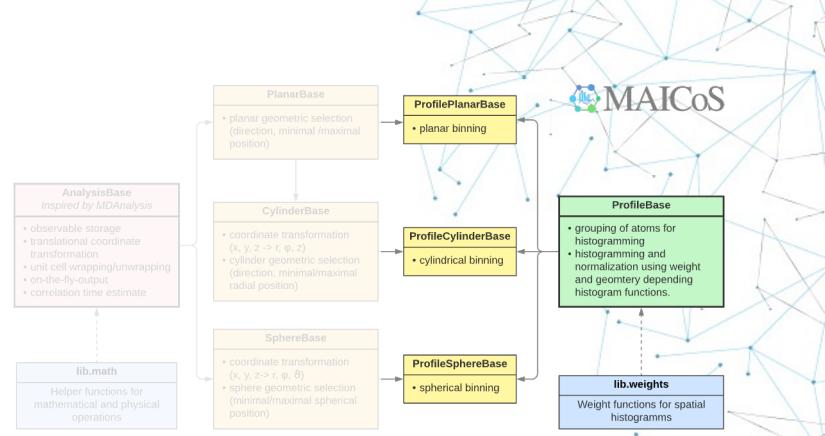
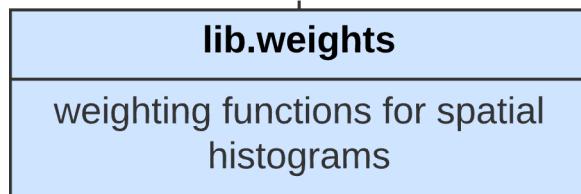
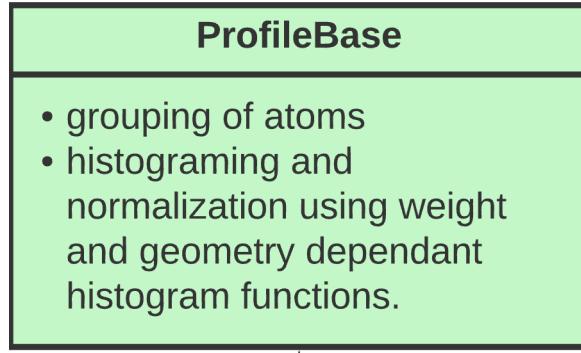
...



Observable abstraction

Most analysis is about counting observables:

- Densities (mass, charge)
- Means (Dipole orientation, velocity)



User defines weighting function.

ProfileBase manages grouping and histogramming.

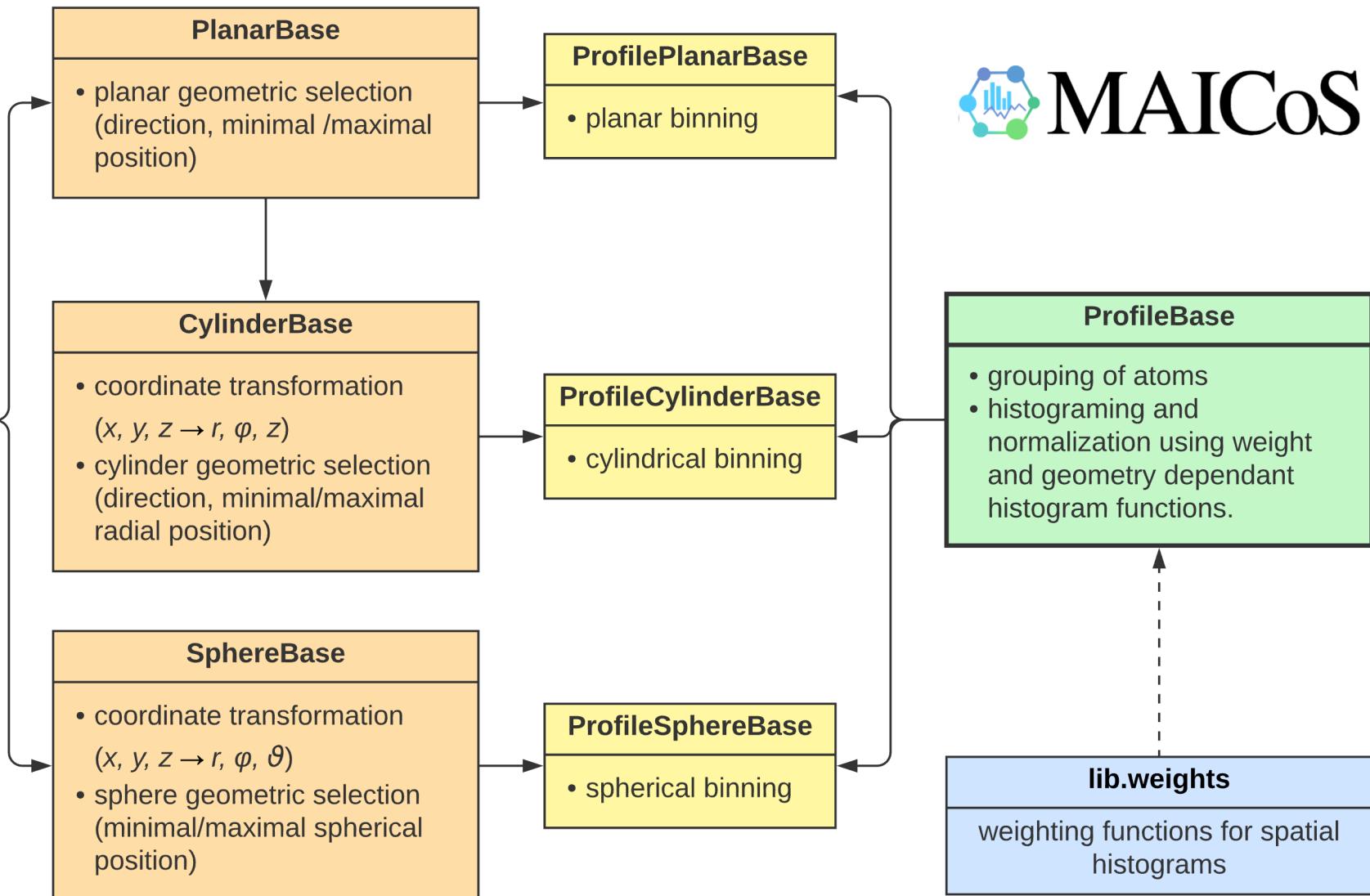
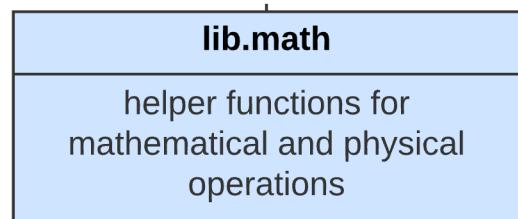
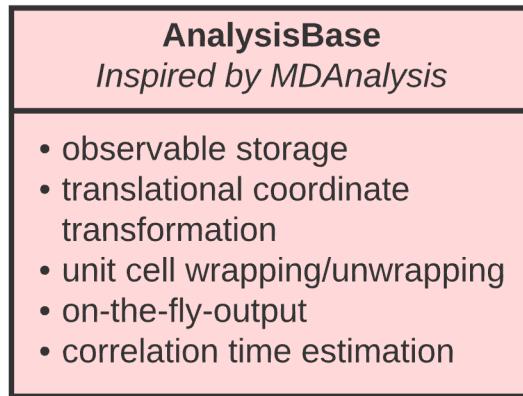
Implemented weights are independently tested.

Easy to implement new weights (numpy arrays)

Do you see your analysis here?



MAICoS



Application

Example 1: Shear in lipid bilayer

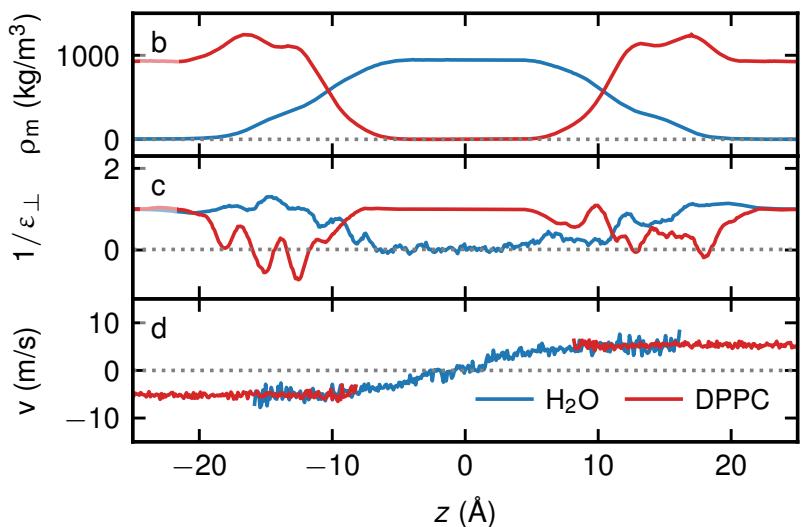
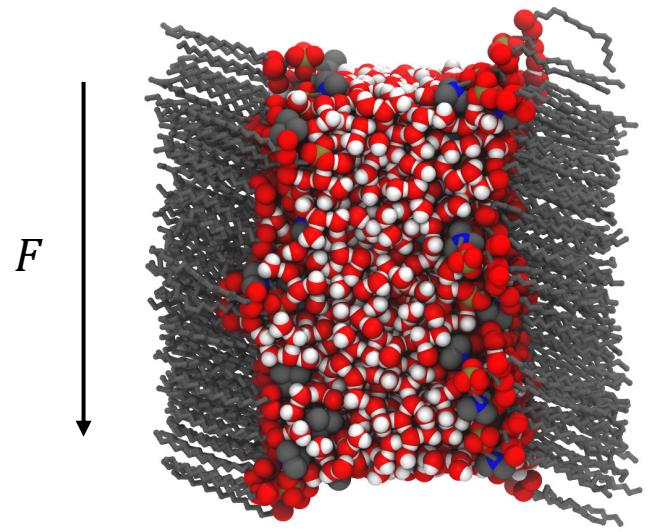
From the command line:

```
maicos VelocityPlanar \
-s run.tpr \
-f run.trr \
-atomgroups 'resname SOL' 'resname DPPC' \
-no-unwrap \
-grouping 'residues' \
-vdim 0 \
-bin_width 0.1 \
-v
```

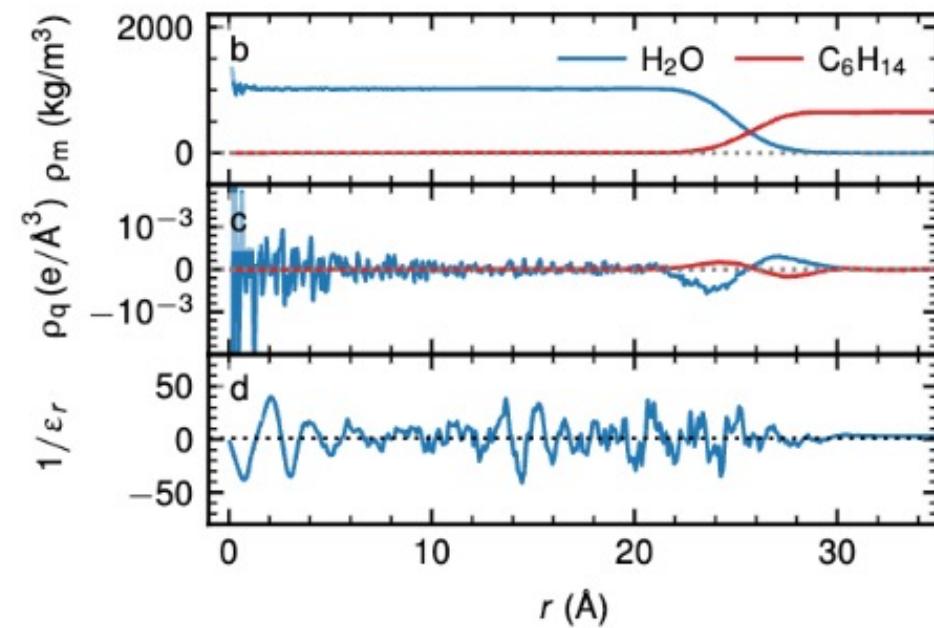
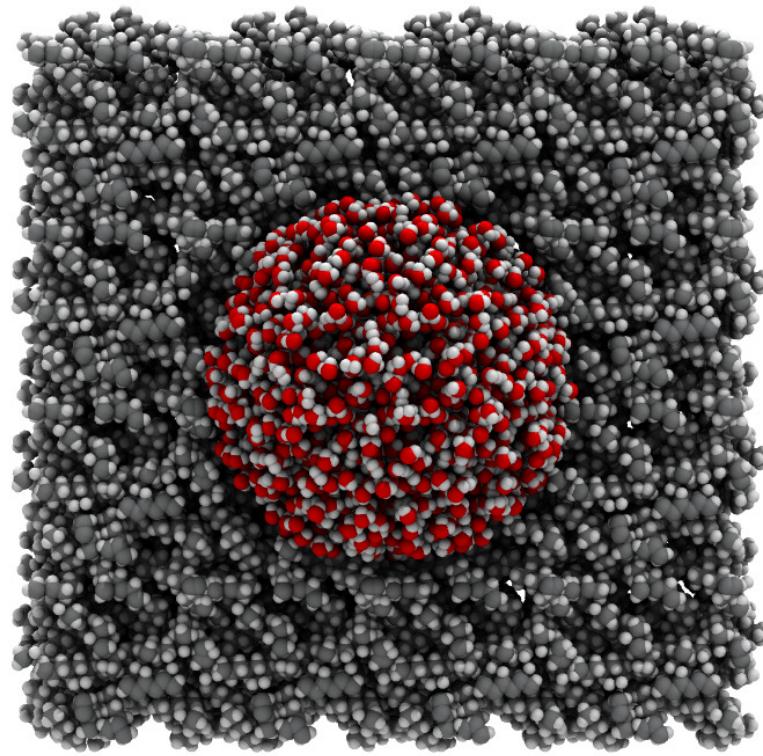


From the python interface:

```
vplan = VelocityPlanar(
    atomgroups=[group_H2O_NEMD, group_DPPC_NEMD],
    bin_width=bin_width_NEMD,
    vdim=0,
    grouping="residues")
vplan.run()
vplan.save()
```



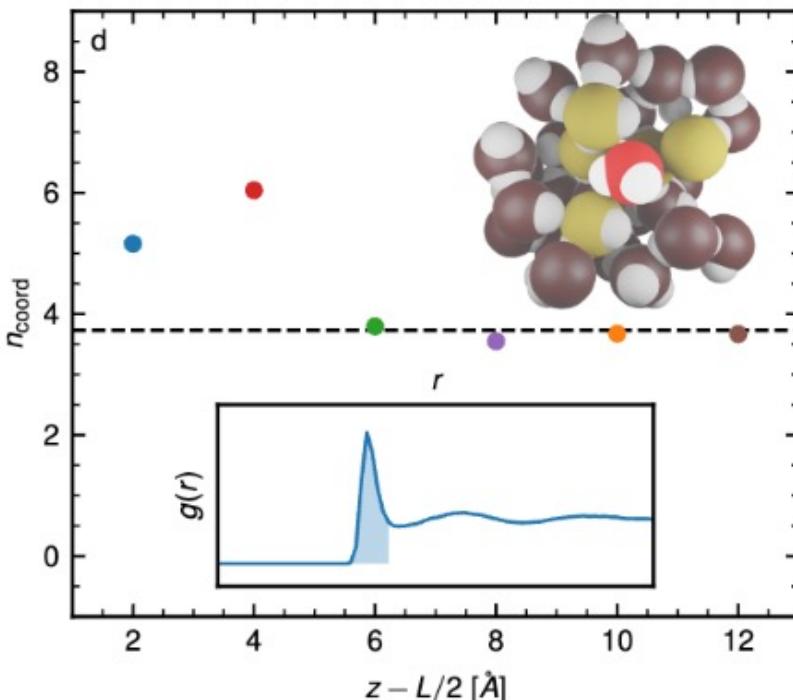
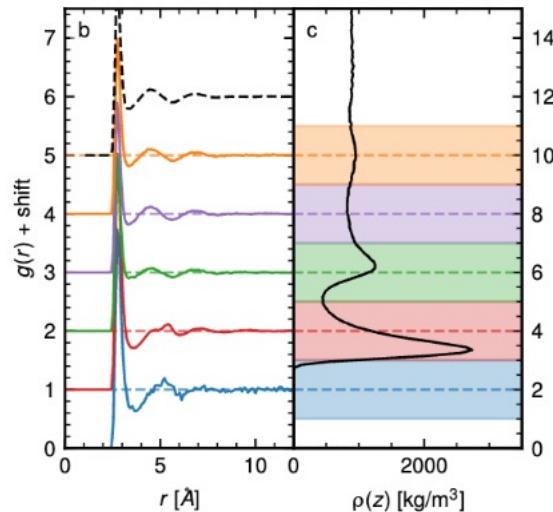
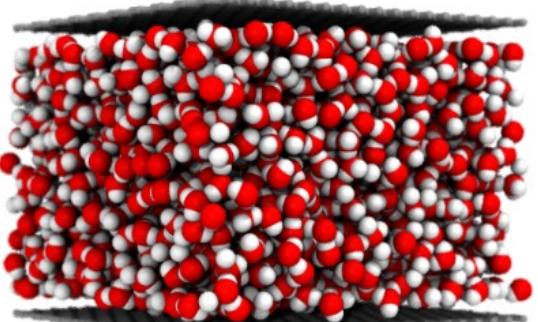
Example 2: Spherical analysis of a water droplet in oil



Example 3: RDF in planar confinement

```
# This file was generated by RDFPlanar on Sat, Sep 09 2023 at 04:35:28
#
# RDFPlanar is part of MAICoS v0.7.2
#
# Command line:
# Module input: RDFPlanar(g1, g2=None, rdf_bin_width=0.3, dzheight=0.1,
range=(0.0, None), bin_method='com', output='rdf.dat', refgroup=None,
unwrap=False, concfreq=0, dim=2, zmin=None, zmax=None,
bin_width=1).run((start=None, stop=None, step=None, verbose=None))
#
# Statistics over 20001 frames
#
# Considered atomgroups:
# (1) OW 1910
#
# First column represents the bin positions for the RDFs. The spatial bin
positions are reported in the header
#
# r [Å] | rdf at -15.00 Å [Å^-3] | rdf at -13.00 Å [Å^-3] | rdf at -11.00 Å [Å^-3]
| rdf at -9.00 Å [Å^-3] | rdf at -7.00 Å [Å^-3] | rdf at -5.00 Å [Å^-3] | rdf
at -3.00 Å [Å^-3] | rdf at -1.00 Å [Å^-3] 4.977616639894860001e-02
0.000000000000000e+00 0.000000000000000e+00
0.000000000000000e+00 0.000000000000000e+00
0.000000000000000e+00 0.000000000000000e+00
0.000000000000000e+00 0.000000000000000e+00
```

18



Conclusion

- MAICoS implements FAIR analysis modules for interfacial and confined systems
- Easily extendable by new analysis modules
- Robust codebase for a specialized application
- Features and generic design principles applicable to MDAnalysis



Outlook

- Growth of userbase through MDAKit integration
- More interesting Science!
- Preprint out very soon™



Acknowledgements

Maintainers



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Active developers



Adyant
Agrawal



Philipp
Stärk



Kira
Fischer



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Gravelle

And all the contributors

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Marc Sauter

Julian Kappler

Shane Carlson

Laura Scalfi

Dominik Wille

Julius Schulz



Gefördert durch



Deutsche
Forschungsgemeinschaft

Questions?



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