

Packaging considerations with **MDAnalysis** toolkits



Dependencies



- MDAKits *must* have MDAnalysis as a dependency
- This means that you will also inherit the following:
 - NumPy
 - SciPy
 - GridDataFormats
 - tqdm
 - threadpoolctl
 - packaging
 - fasteners
 - mda-xdrlib
 - cython
 - mmtf-python
 - joblib
 - matplotlib
 - waterdynamics
 - pathsimanalysis
 - mdahole2

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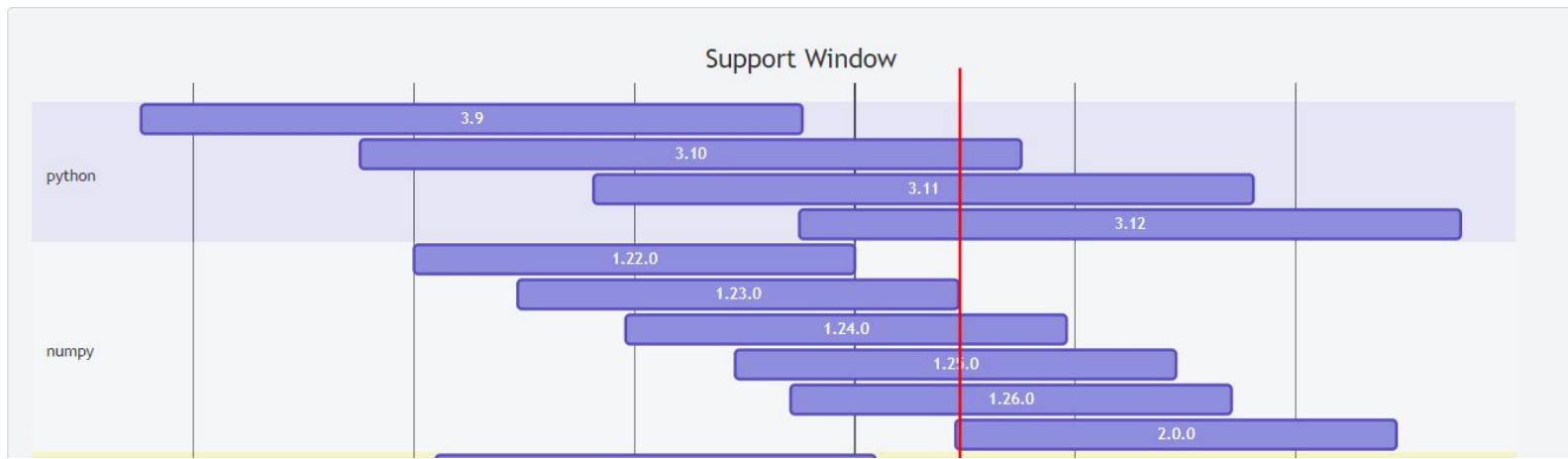
Will be removed in v3.0

- mmtf-python
- joblib
- matplotlib
- waterdynamics
- pathsimanalysis
- mdahole2

Dependencies: SPEC0



- MDAAnalysis minimally supports dependencies following SPEC0
 - <https://scientific-python.org/specs/spec-0000/>
- Minimum of **3 years** of Python version support
- Minimum of **2 years** of core package version support



Dependencies: MDAnalysis



- MDAnalysis does not currently have a set release schedule
 - Aim for quarterly, closer to twice yearly
- MDAnalysis follows semver
 - Major API breaks only done in major versions (i.e. v3.0)
 - API changes will follow a deprecation -> removal cycle
 - DeprecationWarning for at least one release before a change
 - Major version changes are generally > yearly (~3 years since the last one)
 - Bug fix releases are only made for the latest version release and only when absolutely necessary



- We recommend **pytest** as your testing framework
 - It is what we use within the core library
 - It is what we support the most within the mdakits registry
- MDAnalysisTests.datafiles has a useful repository of small input files for tests
 - Exists to test the MDAnalysis library
 - Limited scope for adding new files
- MDAnalysisData stores larger files
 - Encouraged to add new files

Packaging: management & repositories



- MDAAnalysis primarily supports **pypi** and **conda-forge**
 - Alternate dependency management tooling (e.g. Poetry is officially unsupported)
 - MDAKits are encouraged to be deployed to either, or both, of these
- The MDAKit registry currently only supports installs through the following:
 - Git
 - PyPi
 - conda



- MDAAnalysis is currently released as a GPLv3+ package
- This means that, by our interpretation, all downstream packages must fall under the terms of its license
 - I.e. all mdakits may have their own license but are packaged under GPLv3+
- We are currently in the process of relicensing to LGPLv2.1+ removing this limitation