Abstract

KERN is a bi-annually released set of radio astronomical software packages. It should contain most of the standard tools that a radio astronomer needs to work with radio telescope data. The goal of KERN is to save time and prevent frustration in setting up of scientific pipelines, and to assist in achieving scientific reproducibility.

Keywords: software, packaging, radio astronomy, reproducible science, containerisation

1. Introduction

The installation of scientific software for use in astronomy can be notoriously challenging. The radio astronomy community has a limited number of dedicated software engineers and often lacks the human resources to dedicate to industrial-quality software development and maintenance. It is not uncommon that poorly written and badly maintained software packages of high complexity are used by scientists around the world, as these provide some set of algorithmic features not available elsewhere.

KERN has been created to facilitate scientists and system administrators. KERN is the name of the project to structure and automate the packaging of scientific software. The main deliverable is the KERN suite, a bi-annually released set of 3rd party open source scientific software packages.

The primary goals of KERN are: to make it easier to install the scientific software, to supply a consistent working environment to a scientist and to improve interoperability and interchangeability.

Due to human resource limitations, we target KERN to one operating system and distribution. This is unfortunate, but recent development and adaptation of containerisation technology make it easier to deploy packaged software on most platforms. Limiting us to only one platform enables us to focus on performing the packaging only once, and to do this well. The choice of this one platform is then based on install base (desktop, server) and ease of use for user and developer (package creator).

The intended audience of this paper is threefold:

• the user, who is interested in using the software bundled with KERN,
• the developer, who wants his radio astronomy software available to a wider range of users and
• the system administrator who is setting up systems intended to be used for radio astronomical data reduction.

The name KERN means ‘core’ in Dutch and Afrikaans.

2. The target platform

A quick look around various astronomy institutes and universities shows that GNU/Linux and OS X are the most used personal computing platforms. On the server side it is without question GNU/Linux. Compared to OS X, GNU/Linux is an open source and a freely available platform, which is also a clear advantage. These facts combined result in the choice for Linux as the KERN platform.

However, further consideration was required before selection of the most suitable platform. There are various flavours of GNU/Linux, with different design philosophies and varying packaging formats. The most popular distributions can be split into two groups, RPM (Red Hat Package Manager) package and Debian package based distributions. There is no major advantage or disadvantage to either package format. Although there are diverse local trends, it is our experience that in the South African radio astronomy community, the majority of frequently utilised platforms are Debian based, specifically Ubuntu LTS. This distribution also appears to have popularity worldwide. Therefore, it was the most logical choice as KERNs target platform.

3. Other packaging methods

In this section we discuss other packaging systems available to us, and motivate our choice not to use these.

3.1. Anaconda

A packaging effort named Anaconda is currently gaining popularity. Anaconda is a cross platform set of scientific software, with a focus on Python. It supports GNU/Linux,
Windows and OS X. OS X is also often used as a desktop environment in radio astronomy. Supporting OS X would be advantageous for many end users.

We have performed experiments with packaging packages for Anaconda. Users have reported that Anaconda is easy to operate; however, at the time of writing, the packaging procedure is cumbersome for the developer. In effect, developers cannot generate the same high quality, seamlessly installable packages, as is achievable with native Linux packaging methods. Additionally, Anaconda lacks an equivalent to Debian’s Lintian, a packaging tool that dissects a Debian package and tries to find bugs and violations of the Debian policies.

Various software packages in KERN are not created with OS X support in mind thus requiring various modifications to the source code. Also, compilation procedures can vary greatly across platforms, doubling the packaging and maintenance effort if we would support OS X as a platform.

In addition, Linux distributions come with a large set of prepackaged software, which eliminates the need to package many dependencies. Using Anaconda would necessitate packaging up many dependencies ourselves.

The limitations of Anaconda led to the preference of Debian over Anaconda packages.

3.2. Python and pip

The Python programming language has become the most widely used language in astronomy. Python comes with a package manager called pip. Pip assists in downloading and installing Python packages from the Python package index (PyPi). Another useful tool for setting up Python environments is called virtualenv. Virtualenv enables a user to set up one or more isolated Python environments without system administrator rights. The combination of these two tools enables the end user to set up various custom environments with specific versions of dependencies. For pure Python projects, pip and virtualenv are cross platform and independent of the host operating system package manager. However, pip is less suited for impure Python projects. Some Python libraries depend on non-Python run time libraries and/or non-Python development headers compile time, making them “impure”. A recent improvement to the Python Packaging system is the introduction of wheels. Wheels are pre-compiled binary Python packages. These do not require compilation and will work if the packaged library does not have unusual requirements. An example of a independent binary wheel is Numpy. Numpy only depends on Python and a small set of system libraries. The Application Binary Interface (ABI) differs across host platforms and python versions, requiring a wheel for every platform and python combination. These are supplied on PyPi and the correct version is automatically selected by pip on installation.

Problems arise for example, with the python-casacore package, which has more unusual dependencies. Python-casacore depends on the casacore package and both packages need to have a matching ABI. If the version of casacore differs between compile time and run time, the library does not work. Pip does not have any control over reinforcing the shared library version. This would imply that we need to create, upload and maintain wheels for every casacore released. Moreover, with every casacore release we would also need to create a wheel for every OS and supported profile. The exponential growth of this cartesian product quickly becomes cumbersome for the package maintainers.

These limitations combined with pip’s inability to handle non-Python libraries, make pip an ill suited candidate for our packaging effort. Nevertheless, this does not mean pip and KERN cannot be combined.

The approach we adopt is that we prepackage impure python libraries and bundle them with KERN. These Python packages are then precompiled against a set of specific library versions. This guarantees the ABIs always match up. Users can then augment the system python installation, or a Python virtual environment, with packages from the packaging index using pip.

Although KERN supports both Python 2 and Python 3, most Python packages in KERN only support Python version 2. For now, the only package that supports Python 3 is python-casacore. The KERN Python 3 package for casacore is named python3-casacore.

3.3. Collaboration with Debian

Ubuntu is directly based on Debian and thus is similar to Debian. Nonetheless, due to version differences in the bundled libraries in each distribution, KERN packages are unlikely to run on Debian. Fortunately the packaging procedure is identical for Debian and Ubuntu, which makes creating true Debian packages a matter of a recompilation of the source package.

In contrast, the build system, dependency management and library management for RPM is completely different. Porting our packages to RPM is non-trivial, and maintaining support for RPM based distributions would imply doubling the required effort.

We have established a collaboration with Debian developers, and some packages from KERN (e.g. casacore and aoflagger) have been incorporated into Debian directly. These packages have been uploaded to the Debian archive, and changes are synchronised between KERN and the Debian archive.

Not all KERN packages are suitable for uploading to Debian. Packages with a small user base or packages that are fragile and receive continuous fixes (as opposed to formal release) are not well suited to this distribution model, since it can take some time before a package ends up in a Debian release. For the more stable packages in KERN, we expect a continuation of this effort, with more packages ending up in Debian in the future.
4. Usage

To use the packages of KERN, one needs to add the KERN remote repository to the system. It is recommended to use the latest released version, which is KERN-2 at time of writing. KERN-2 is packaged for Ubuntu 16.04: using the packages on a different distribution or version will most likely fail. If running Ubuntu 16.04 is not an option on a particular system, we recommend using Docker, Singularity (see below) or a virtual machine.

The add-apt-repository command should be used to add the KERN repository to a system. Some packages in KERN depend on Ubuntu packages in the multiverse and restricted repositories (CUDA is an example of such a dependency). Once the local cache is updated using apt-get update the package cache can be searched using apt-cache search PACKAGE and packages can be installed using the apt-get install PACKAGE command.

In case of an unexpected fault, it is important to ensure that the latest versions of all packages are being used (by running apt update and apt upgrade), before reporting new issues.

Missing packages can be nominated for inclusion in KERN by requesting the packaging on the issue tracker.

For further instruction on how to install and use KERN packages, we refer to the KERN suite documentation.

5. Notable packages

Here we discuss the important or non-trivial packages part of KERN. Note that this is not the full list of packages. The full list of packages contained in KERN-2 is provided in Table A.1.

5.1. casacore

Most of the packages in KERN depend on casacore. Casacore is a suite of C++ libraries for radio astronomy data processing. The most important library is the table system for working with Measurement Set, which is currently the most used data storage format in radio astronomy. Since it is such an important package, additional effort has been put in making this package quality high, and it should be seen as an example and reference for all other packages. The package has also been accepted in the main Debian repository and updates are synchronised between Debian and KERN.

5.2. casacore data

Casacore has a “soft” dependency on the “casacore data” package. The latter contains ephemerides, geometric data and other tables required for performing calculations such as coordinate conversions. Strictly speaking, the casacore data package is not required if one is not calculating e.g. coordinate conversions, but in practice many components of casacore will fail or give warnings if the data package is missing. The casacore data package is updated on a regular basis using a cron job. Updated content typically consists of accurate GPS movements of the tectonic plates, new or updated radio telescope positions, leap seconds, etc. There is no central authority controlling the content of the casacore data package, and various institutes around the world create their own versions. We base the KERN package on the data supplied and updated weekly by the Netherlands Institute for Radio Astronomy (ASTRON), which is published on its public FTP server.

5.3. MeqTrees

MeqTrees is a software suite developed at ASTRON and subsequently Rhodes and SKA SA. MeqTrees is aimed at implementing various versions of the Radio Interferometry Measurement Equation (RIME), which is used for simulation and calibration of radio interferometric data. MeqTrees consists of two core packages: Timba (the C++-based computational implementation) and Cattery (a set of Python frameworks providing end-user tools). Other packages in the suite include Tigger (a sky model and FITS image viewer), Owlcat (a set of Measurement Set manipulation utilities) and Pyxis (a scripting/pipelining framework).

5.4. CASA

CASA, Common Astronomy Software Applications, is a popular system for reduction of radio astronomy data. CASA is maintained by the National Radio Astronomy Observatory. It has proven to be one of the most challenging pieces of software to package up. CASA is delivered as one monolithic self-contained tarball, which bundles a complete set of dependencies, including its own python interpreter and IPython interface. This scheme has the advantage that it runs on most systems without modification or additional library requirements. However, the tarball is sizable (over 1Gb at time of writing). In addition, various dependencies bundled with CASA are dated (for example, the bundled IPython package is version 0.10, dating from 2010). This makes it hard to install updated packages into the CASA bundled Python, since CASA itself may break if packages are updated. Since CASA depends on so many old libraries, it is close to impossible to install it as an overlay on the default Debian filesystem and make use of the system Python interpreter and libraries. Some effort has been made towards unbundling an earlier version of CASA (4.3) into individual packages, but the CASA team was unable to dedicate resources to this effort in further releases. We have therefore adopted the single large package option as the only practical possibility for now. Other

https://github.com/kernsuite/packaging/issues
http://kernsuite.info/
https://packages.qa.debian.org/c/casacore.html

4https://github.com/casacore/casacore-data-update
5ftp://ftp.astron.nl/outgoing/Measures/
6http://casa.nrao.edu/
attempts have been made to bridge the gap between the system and CASA Python interpreter, but the result is still far from ideal.

We have decided to take a pragmatic approach and package a subset of CASA and instead of installing it as an overlay on the system, choosing to do so in a separate directory. Having a package simplifies the installation and helps us to manage dependencies, since there are packages that depend on CASA. We reduced the install size by unbundling the experimental Carta viewer, which reduced the final install footprint by about 1Gb. In case of CASA 4.7.1 the tarball is reduced by 60% to about 400MB. The software is installed in /opt/casa and a symlink to the casa binary is created under /usr/bin. The package works exactly like the naive CASA installation (apart from the omitted Carta), but unfortunately still cannot interoper-ate with the Debian system Python installation. Since the package is a modified version of the original release, we decided to rename the package to casalite.

5.5. AIPS

NRAO’s venerable Astronomical Image Processing System (AIPS) is the predecessor of CASA and, despite its age, maintains a wide and enthusiastic user base. AIPS has some of the oldest code of all the packages in KERN and depends on various (nowadays rather arcane and arcahiec) system configuration modifications. We bundle AIPS with a minimal configuration that assumes a single system (localhost) setup. All software is installed under /opt/aips, similar to CASA. The software requires a writable data folder in order to operate, thus when the package is installed, an aips group is created if it does not exist. Users who want to use AIPS need to be added to this group. Due to the complexity of AIPS compilation, the KERN packages are not compiled from source, but are rather based on the binary tarball distribution.

5.6. LOFAR

Another notable package is the lofar package. This package contains all the code bundled in the LOFAR imaging pipeline. Most of it is used by astronomers working with data from the LOFAR radio telescope, however, it has a number of general-interest components, such as the PyBDSM / PyBDSF source finder and the makems Measurement Set creation tool. For the reader familiar with building and using the LOFAR pipeline, it is relevant to know that the full “Offline” bundle is contained in the KERN package.

5.7. Pulsar software

KERN contains a number of software packages from the pulsar community such as tempo, presto and psrchive. These tools were particularly difficult to create packages from, since most of them do not perform normal release management and tend to have broken build scripts. For packages without version numbers, we introduce our own date-based versioning scheme and the packages are updated on request.

6. Containerisation

6.1. Docker

Docker is a mature and popular concept for distributing software and managing processes. Although it is easy to create a docker container from a piece of software, it is no replacement for proper software packaging. We think that proper packaging and containerisation go hand in hand: Debian packages provide robustness and dependency management while containerisation provides portability and distributability.

We have prepared an easy to use base docker image which can be used to create custom docker images containing all the KERN packages combined with end-user scripts. The Dockerfile below is all that is needed to set up a Docker container for any given package in KERN.

The example below is for aoflagger:

```bash
FROM kernsuite/base:2
RUN docker-apt-install aoflagger
```

The kernsuite Docker image is a clean Ubuntu system with the KERN suite repository enabled. It also contains an up-to-date pip so that one can directly install Python libraries. The `docker-apt-install` command is just a wrapper script that updates the apt cache before installing the package, then removes the cache. The latter is done to prevent cluttering of the Docker image, which could otherwise lead to exploding image sizes.

6.2. Singularity

A number of assumptions made by Docker creators have created security concerns and have made Docker a poor fit to the typical HPC environment. This has motivated the development of an alternative containerisation technology called Singularity. While this is presently less popular, Singularity is more suited for deploying software in a multi-tenant cluster environment, which is the most common environment in science. We have created scripts to easily set up Singularity images containing all KERN software; these can be used to deploy all of KERN on any cluster supporting Singularity.8

7. Project structure

All the packaging effort of KERN is strictly open source and open development. All source code is publicly available on Github. We use the Github bug tracker to interact with users. Users can report problems, ask questions

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1. https://github.com/kernsuite/singularity
2. http://github.com
and request new features via the bug tracker. Participation is encouraged by the means of pull requests. We have a central entry point website which contains a list of common questions and links to all related services and pages.

7.1. The release cycle

We anticipate a KERN release recycle of approximately six months. At the time of writing, the latest release is KERN-2, released on 13 March 2017. Every KERN release is “fixed”, in the sense that we do not plan any package updates post-release, unless some critical issues need to be addressed. In between KERN releases, development activity proceeds on an active development branch called KERN-dev. This repository will be constantly updated with new packages, but this should only be used for testing and experiments rather than for production science.

7.2. Technical structure

Our packaging procedure makes extensive use of git. Every release of every package added to KERN is mirrored on our packaging Github repository. Every new release is a new commit to the git repository. These commits are then augmented with Debian metadata files. The metadata files contain a description, build and runtime dependencies as well as a robust script to build, install and clean the package. These metadata files can be very minimal if properly written build scripts are provided by the original software authors, but can be more complex in the absence of these.

New packages are published to Launchpad which is a free to use service maintained by Canonical, the company responsible for the Ubuntu distribution. Packages are built on the Launchpad build farm and we simply upload the base source image. This is an extra quality check, since the build farm makes sure that the package compiles correctly and that all the dependencies are correctly defined.

If the original source is provided with (unit)tests, as is the case for casacore, we run these tests during the creation of the package. Unfortunately, most software packages in KERN do not have a test suite provided by the developers.

All scripts and packaging files are released under the conditions of the MIT License. The MIT license is a simple and permissive license, it only requires preservation of copyright and license notices. Licensed works, modifications and larger works may be distributed under different terms and without source code. Note that this only applies to the KERN files and not to the software contained by the KERN packages. The licenses of these packages is respected and is bundled with every package.

8. Recommended usage

KERN is freely available and maintained as a service to the community. If you use KERN in a published work, please state which version of KERN was used and include it as a citation and/or an acknowledgment.

9. Conclusions

Although the KERN project does not introduce any novel algorithmic techniques as such, we are of the opinion that it is a foundational block for a robust radio astronomy software environment. Radio astronomy software has historically been difficult to build and install for the end user. Radio astronomers world wide now use the packages distributed via KERN.

Based on a subjective observation of users within our team at SKA South Africa, ease of software installation was vastly improved after KERN became available. Subsequently, the KERN ready-to-install packages resulted in a noticeable reduction in time and effort required to achieve successful software installation. While we believe this experience will not be unique to SKA SA, a further quantitative survey of the global community could not be carried out.

We believe that these packages, as well as the regular release cycle, are a great improvement for reproducible science, problem isolation and discoverability of tools. KERN is not only of benefit to astronomers, but also to system administrators, who now have to spend less time installing software and tracking updates and changes.

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10. References

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http://kernsuite.info/
https://github.com/kernsuite-debian
## Appendix A. List of packages in KERN

| Package name     | Description and website                                                                 | Version in KERN-2 |
|------------------|----------------------------------------------------------------------------------------|-------------------|
| casacore-data    | Casacore data files http://casacore.github.io/casacore                                  | 20171002          |
| casacore         | Suite of c++ libraries for radio astronomy data processing http://casacore.github.io/casacore | 2.3.0             |
| 21cmfast         | A seminumeric modelling tool to efficiently simulate the cosmological 21-cm signal https://github.com/andreimesinger/21cmFAST | 1.2               |
| aips             | Calibration, data analysis, image display, plotting, and a variety of ancillary tasks on Astronomical Data http://www.aips.nrao.edu/ | 31dec16           |
| aoflagger        | Find RFI in radio astronomical observations http://sourceforge.net/projects/aoflagger/ | 2.9.0             |
| attrdict         | A dictionary that allows attribute-style access https://github.com/bcj/AttrDict          | 2.0.0             |
| casalite         | Stripped down version of NRAO’s CASA https://casa.nrao.edu/                              | 4.7.1             |
| casarest         | Standalone radio interferometric imager derived from CASA https://github.com/casacore/casarest/ | 1.4.1             |
| casasynthesis    | The synthesis CASA 4.4 submodule as a standalone project https://github.com/radio-astro/casasynthesis | 0.1               |
| cassbeam         | Cassegrain antenna modelling https://github.com/ratt-ru/cassbeam                        | 1.1               |
| chgcentre        | Change the phase centre of a measurement set https://sourceforge.net/p/wsclean/wiki/chgcentre/ | 1.5               |
| drive-casa       | A Python package for scripting the NRAO CASA pipeline routines https://github.com/timstaley/drive-casa | 0.7.4             |
| dspsr            | Library for digital signal processing of pulsar astronomical timeseries http://dspsr.sourceforge.net/ | 0+git20170125      |
| dysco            | A compressing storage manager for Casacore measurement sets https://github.com/aroffringa/dysco | 1.0               |
| galsim           | Simulating images of astronomical objects (stars, galaxies) in a variety of ways https://github.com/GalSim-developers/GalSim | 1.4.3             |
| karma            | Toolkit for interprocess communications, authentication, encryption, graphics display, user interface and manipulating the Karma network data structure http://www.atnf.csiro.au/computing/software/karma/ | 1.7.25            |
| katdal           | Data access library for the MeerKAT project https://github.com/ska-sa/katdal            | 0.7.1             |
| katpoint         | Karoo Array Telescope pointing coordinate library https://github.com/ska-sa/katpoint | 0.6               |
| katversion       | Provides proper versioning for Python packages https://github.com/ska-sa/katversion     | 0.7               |
| kittens          | Collection of Python utility functions for purr, tigger, meqtrees and others https://github.com/ska-sa/kittens | 1.3.3             |
| lofar            | LOFAR telescope user software http://www.lofar.org                                      | 2.20.2            |
| makems           | Tool to create empty Measurement Sets https://github.com/ska-sa/makems                  | 1.3.0             |
| meqtrees-cattery | MeqTrees-based frameworks for simulation and calibration of radio interferometers https://github.com/ska-sa/meqtrees-cattery | 1.5.1             |

Continued on next page
| Package name         | Description and website                                                                 | Version in KERN-2 |
|---------------------|------------------------------------------------------------------------------------------|-------------------|
| meqtrees-timba      | Implementing and solving arbitrary Measurement Equations                                 | 1.5.0             |
| montblanc           | A PyCUDA implementation of the RIME                                                       | 0.4.0             |
| msutils             | A set of CASA Measurement Set manipulation tools                                          | 0.2.2             |
| mt-imager           | High performance image synthesiser for radio interferometry                              | 1.0               |
| multinest           | A Bayesian inference tool                                                                  | 2.14+git20150803 |
| obit                | Obit for ParselTongue                                                                     | 22JUN10k          |
| oskar               | Simulator for the Open Square Kilometre Array Radio Telescope                            | 2.6.1             |
| owlcot              | Miscellaneous utility scripts for manipulating radio interferometry data                 | 1.4.2             |
| parsetongue         | Python scripting interface for classic AIPS                                               | 2.3               |
| presto              | A large suite of pulsar search and analysis software                                       | 2+git20160004     |
| psrcat              | The ATNF Pulsar Catalogue                                                                  | 1.55              |
| psrchive            | C++ development library for the analysis of pulsar astronomical data                     | 2012.12+20170131  |
| purify              | Collection of routines for radio interferometric imaging                                  | 2.0.0             |
| purr                | Data reduction logging tool, Useful for remembering reductions                            | 1.3.1             |
| pymoresane          | Python version of the MORESANE deconvolution algorithm                                    | 0.3.6             |
| python-casacore     | Python 2 bindings to the casacore library                                                 | 2.1.2             |
| pyxis               | Python Extensions for Interferometry Scripting                                            | 1.5.1             |
| rfimasker           | Tool to apply RFI masks                                                                   | 0.1               |
| rpfits              | Data-recording format                                                                     | 2.24              |
| sagecal             | Very fast, memory efficient and GPU accelerated radio interferometric calibration program | 0.2+20170130      |
| scatterbrane        | Adding realistic scattering to astronomical images                                        | 0.0+git20160122   |
| sigproc             | Pulsar search and analysis software                                                       | 0.0+git20161025   |
| sigpyproc           | Python-based pulsar search data manipulation package                                       | 0.0+git20160115   |
| simfast21           | Generates a simulation of the cosmological 21cm signal                                    | 2.0 beta          |
| simms               | Creates empty measurement sets using the the CASA simulate tool                           | 0.9.1             |
| sopt                | Sparse OPTimisation shared library                                                       | 2.0.0             |

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| Package name | Description and website | Version in KERN-2 |
|--------------|-------------------------|-------------------|
| sourcery     | Tools for creating high fidelity source catalogues from radio interferometric datasets | [https://github.com/radio-astro/sourcery](https://github.com/radio-astro/sourcery) | 1.2.6 |
| spdlog       | Very fast, header only, C++ logging library | [https://github.com/gabime/spdlog](https://github.com/gabime/spdlog) | 1.0.11.0 |
| stimela      | Dockerized Radio Interferometry Scripting Framework | [https://github.com/SpheMakh/Stimela](https://github.com/SpheMakh/Stimela) | 0.2.7 |
| tempo        | Pulsar timing data analysis package | [https://sourceforge.net/projects/tempo/](https://sourceforge.net/projects/tempo/) | 0+git20160709 |
| tempo2       | Pulsar timing package | [https://bitbucket.org/psrsoft/tempo2/](https://bitbucket.org/psrsoft/tempo2/) | 2017.2.1 |
| tigger       | FITS and MeqTrees LSM viewer | [https://github.com/ska-sa/tigger](https://github.com/ska-sa/tigger) | 1.3.7 |
| tirific      | Simulate kinematical and morphological models | [http://gigjozsa.github.io/tirific/](http://gigjozsa.github.io/tirific/) | 2.3.7 |
| tkp          | A transients-discovery pipeline for astronomical image-based surveys | [https://github.com/transientskp/tkp](https://github.com/transientskp/tkp) | 4.0 |
| tmv          | A fast, intuitive linear algebra library for C++ | [https://github.com/rmjarvis/tmv](https://github.com/rmjarvis/tmv) | 0.74 |
| transitions  | Lightweight, object-oriented finite state machine implementation | [https://github.com/tyarkoni/transitions](https://github.com/tyarkoni/transitions) | 0.4.3 |
| wsclean      | Fast generic widefield interferometric imager | [http://sourceforge.net/projects/wsclean/](http://sourceforge.net/projects/wsclean/) | 2.3 |