Introducing Maneage: Customizable framework for managing data lineage

[RDA Europe Adoption grant recipient. Submitted to IEEE CiSE (arXiv:2006.03018), Comments welcome]

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RDA Spain webinar July 9th, 2020

Most recent slides available in link below (this PDF is built from Git commit a678365): https://maneage.org/pdf/slides-intro-short.pdf























Challenges of the RDA-WDS Publishing Data Workflows WG (DOI:10.1007/s00799-016-0178-2)

Challenges (also relevant to researchers, not just repositories)

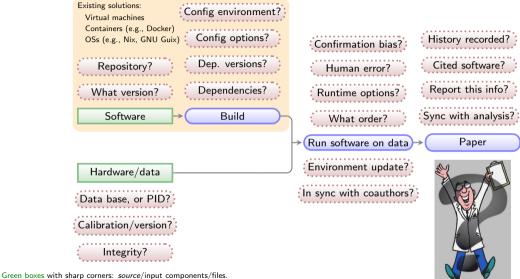
- ▶ Bi-directional linking: how to link data and publications.
- ▶ Software management: how to manage, preserve, publish and cite software?
- ► Metrics: how often are data used.
- ▶ Incentives to researchers: how to communicate benefits of following good practices to researchers.





"We would like to see a workflow that results in all scholarly objects being connected, linked, citable, and persistent to allow researchers to navigate smoothly and to enable reproducible research. This includes linkages between documentation, code, data, and journal articles in an integrated environment. Furthermore, in the ideal workflow, all of these objects need to be well documented to enable other researchers (or citizen scientists etc) to reuse the data for new discoveries."

General outline of a project (after data collection)



Blue boxes with rounded corners: built components. Red boxes with dashed borders: questions that must be clarified for each phase.

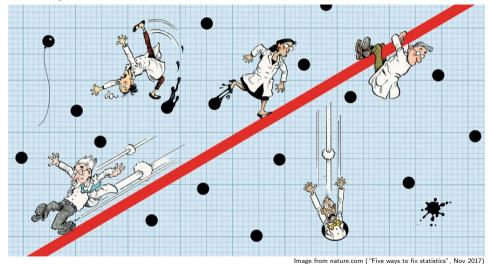








Science is a tricky business



Data analysis [...] is a human behavior. Researchers who hunt hard enough will turn up a result that fits statistical criteria, but their discovery will probably be a false positive.

Five ways to fix statistics, Nature, 551, Nov 2017.

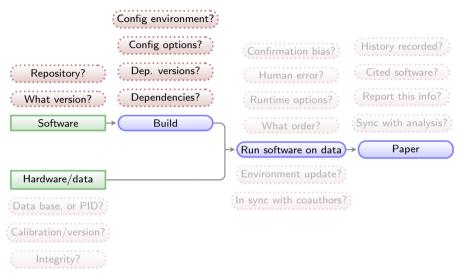
Founding criteria

Basic/simple principle:

Science is defined by its METHOD, not its result.

- Complete/self-contained:
 - ▶ Only dependency should be POSIX tools (discards Conda or Jupyter which need Python).
 - ▶ Must not require root permissions (discards tools like Docker or Nix/Guix).
 - ▶ Should be non-interactive or runnable in batch (user interaction is an incompleteness).
 - Should be usable without internet connection.
- ▶ **Modularity**: Parts of the project should be re-usable in other projects.
- Plain text: Project's source should be in plain-text (binary formats need special software)
 - This includes high-level analysis.
 - ▶ It is easily publishable (very low volume of ×100KB), archivable, and parse-able.
 - ▶ Version control (e.g., with Git) can track project's history.
- ▶ Minimal complexity: Occum's rasor: "Never posit pluralities without necessity".
 - Avoiding the fashionable tool of the day: tomorrow another tool will take its place!
 - Easier learning curve, also doesn't create a generational gap.
 - Is compatible and extensible.
- ▶ Verifable inputs and outputs: Inputs and Outputs must be automatically verified.
- ► Free and open source software: Free software is essential: non-free software is not configurable, not distributable, and dependent on non-free provider (which may discontinue it in N years).

General outline of a project (after data collection)



Green boxes with sharp corners: *source*/input components/files.

Blue boxes with rounded corners: *built* components.



Example: Matplotlib (a Python visualization library) build dependencies

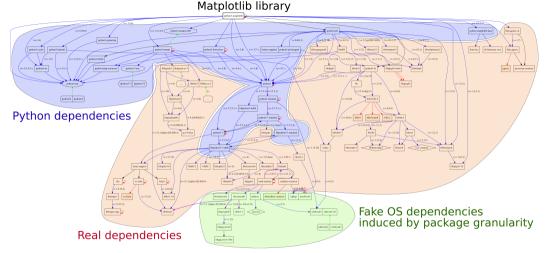


Fig. 1. Transitive dependencies of the software environment required by a simple "import matplotlib" command in the Python 3 interpreter.

Advantages of this build system

- ▶ Project runs in fixed/controlled environment: custom build of Bash, Make, GNU Coreutils (1s, cp, mkdir and etc), AWK, or SED, LATEX, etc.
- ▶ No need for root/administrator permissions (on servers or super computers).
- ► Whole system is built automatically on any Unix-like operating system (less 2 hours).
- Dependencies of different projects will not conflict.
- ► Everything in plain text (human & computer readable/archivable).



https://natemowry2.wordpress.com

Software citation automatically generated in paper (including Astropy)

Dayer every popul (ne). Your Month day



Figure 2: (a) An example image of the Wide-Field Planetury Comera 2 on housel the Hubble Server Education (1997 to 2009). This is one of the samele images from the FITS standard webpage, kept as examples for this file format, this Historyam of nixel volues in (a)

removes the necessity to add further dependencies (to create the plots) to your project. There are high-level language libraries like Matelatlib which also generate plats. However, the problem is that they require many dependencies (Python, Numpy and etc.). Installing these dependencies from source, is not easy and will harm the reproducibility of your paper. Note that after several years, the binary files of those biob-level libraries, that you easily install today, will no longer be available in common repositories. Therefore building the libraries from source is the only ontion to remendance your regards:

Furthermore, since PGFPlots is built by MBX it respects all the properties of your text (for example line width and fosts and etc). Therefore the final plot blends in your paper much more picals. It also has a mondarful manual!

This template also defines two ISTeX macros that allow you to mark text within your document as new and noter. For example, this test has been marked as new. If you comment the line (by adding a '5' at the start of the line or simply deleting the line) that defines by object to be some of them the one that was morked now will become black (totally blend in with the rest of the text) and the one marked topote will not be in the final PDE. You can thus use blight light changes to easily make conies of your research for existing counthors (who are just interested in the new parts or notes) and new co-authors (who don't want to be distracted by these issues in their first time reading).

2. NOTICE AND CITATIONS

To encourage other scientists to publish similarly reproducible papers, please add a notice close to the start of your paper or in the end of the abstract clearly mentioning that your work is fully

For the time being, we haven't written a specific paper only for this template. Until then, we would be grateful if you could cite the first paper that used the early versions of this template: Akhlashi and Ichikawa (2015).

After publication, don't forget to unload all the measurary data. software source code and the project's source to a long-lasting host like Zenodo (https://zenodo.org).

* http://mirrors.com.org/graphics/pgf/contrib/pgfplots/doc/pgfplots.pdf

YOUR NAME OF AL-

3. ACKNOWLEDGEMENTS

Please include the following two paragraphs in the Acknowledgement section of your narier. This reproducible narier termplate was developed in parallel with Grusstra, so it benefited from the some grants. If you don't use Consults in your final/outomized project, please remove it from the paragraph below, only mentioning the reproducible paper template.

This research was partly done using GNU Astronomy Utilities (Grasstro, ascl.net/1801.009), and the reproducible paper template v0-364-g268dfc0-dirty. Work on Graustro and the reproducible paper template has been funded by the Japanese Ministry of Education, Culture, Sports, Science, and Technolnew (MEXT) scholumbin and its Grant, in Aid for Scientific Research (21244012, 24253003), the European Research Council (ERC) advanced grant 339659-MUSICOS, European Union's Horizon 2020 research and innovation programme under Marie Sklodowska-Curie grant agreement No 721463 to the SUNDIAL. ITN: and from the Spanish Ministry of Economy and Competitisoners (MINECO) under grant number AVA2016-26219-P

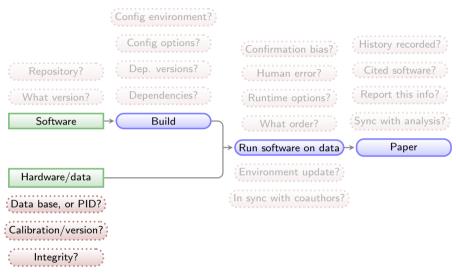
This research was done with the following free software progrows and libraries: Bain? 1.0.6. CETTSIO 3.45. CMake 3.14.2. cURL 7.63.0, Discoteg flock 0.2.3, File 5.36, FreeTyne 2.9. Gir 2015), GNU AWK 5.0.0, GNU Bash 5.0.7, GNU Birotils 2.32. GNU Compiler Collection (GCC) 9.1.0. GNU Coroutils 8.31. GNU Diffusils 3.7. GNU Finducils 4.6.0 199-e36: GNU Green 13. GNU Grin 1.10. GNU Integer Set Library 0.18. GNU Librard 2-4.6, GNU M4 L4-18, GNU Make 4-2-90, GNU Multiple Percision Arithmetic Library 6.1.2. GNU Multiple Precision. hibby 4.0.2. GNU NCURSES 6.1. GNU Rendline 8.0. GNU 120.3 GNU Which 2.31 GRI Ghostopies 9.26 UDES Shore: ince v9b. Library 1.6.37. Library 4.0.10. Lzin 1.20. Metastore (forked) 1.1.2.23-fa9170b. OnenBLAS 0.3.5. Onen MPI 4.0.1. OrenSSL LLLa PatchELF 0.9, rke-confir 0.29.2, Pethon 3.7.3. 2013). Cycler 0.10.0. Cython 0.29.6 (Rehnel et al. 2011). h5ny 2.9.0. Kiwisolver 1.0.1, Matplotlib 3.0.2 (Hamer 2007), Numery 1.16.2 (see der Welt et al. 2011), ekseyndig 1.5.1. Perkening 2.3. L python-dateutil 2.8.0. Sciev 1.2.1 (Oliphant 2007; Millman the PDF using the following nuckages: hiter 2.12, hiter 2.12. NNotes 3.12 NNotes 3.12 caption 2018-10-05 caption 2018datetime 2.60, datetime 2.60, ec 1.0, ec 1.0, etoolbox 2.5f, etool-3.05 fontones 1.0d. fontages 1.0d. footmise 5.5h. footmise 5.5h. fn 2 Ld fn 2 Ld Journa J.O. Journa J.O. navets J. 554, navets J. 554. pef 3.1.2, pef 3.1.2, pefplots 1.16, pefplots 1.16, preprint 2011, 3.14159265, texevre 2.501, texevre 2.501, times 2016-06-24. times 2016-06-24, titlesec 2.10.2, titlesec 2.10.2, tyfouts 2016-

06-24 referre 2016-06-24 olem 2016-06-24 olem 2016-06-24 scolor 2.12, scolor 2.12, skewad 2.7a and skewad 2.7a. We are very grateful to all their creators for freely providing this necessary infrastructure. This research (and many others) would not he nossible without them.

References Alabaria M. and T. Bridones (Sept. 2015). Audi., 220. 1.

Astropy Collaboration et al. (Oct. 2013). A&A, 558, A33. Astrony Collaboration et al. (Sept. 2018). AJ. 156, 123. Hauser, J. D. (2001). COSE, 9, 90. Millman, K. J. and M. Airazis (Mar. 2011). COSE, 13, 9. YOUR NAME OF AL-

General outline of a project (after data collection)



Green boxes with sharp corners: *source*/input components/files. Blue boxes with rounded corners: *built* components.



Input data source and integrity is documented and checked

Stored information about each input file:

- PID (where available).
- Download URL.
- MD5-sum to check integrity.

All inputs are $\frac{\text{downloaded}}{\text{during the analysis}}$.

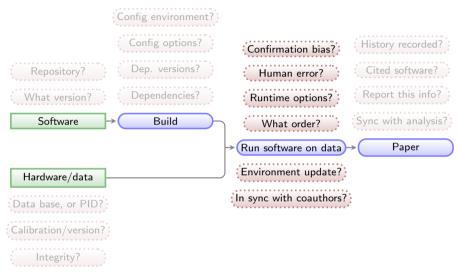
MD5-sums are checked to make sure the download was done properly or the file is the same (hasn't changed on the server/source).

Example from the reproducible paper arXiv:1909.11230. This paper needs three input files (two images, one catalog).





General outline of a project (after data collection)



Green boxes with sharp corners: *source*/input components/files.



Reproducible science: Maneage is managed through a Makefile

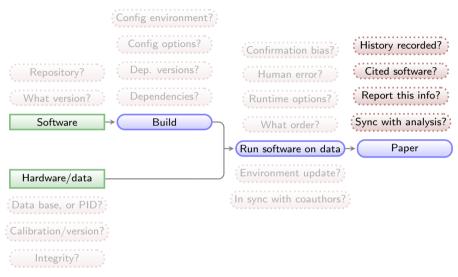
All steps (downloading and analysis) are managed by Makefiles (example from zenodo.1164774):

- Unlike a script which always starts from the top, a Makefile starts from the end and steps that don't change will be left untouched (not remade).
- A single rule can manage any number of files.
- Make can identify independent steps internally and do them in parallel.
- Make was designed for complex projects with thousands of files (all major Unix-like components), so it is highly evolved and efficient.
- ► Make is a very simple and small language, thus easy to learn with great and free documentation (for example GNU Make's manual).





General outline of a project (after data collection)



Green boxes with sharp corners: *source*/input components/files.

Blue boxes with rounded corners: *built* components.



Values in final report/paper

All analysis results (numbers, plots, tables) written in paper's PDF as LATEX macros. They are thus updated automatically on any change.

Shown here is a portion of the NoiseChisel paper and its LATEX source (arXiv:1505.01664).

```
\label{tsNeq1} $$ \left( S_n \right) = \left( S_n \right)^2 + \left( S_n \right)^2
```

\noindent

See Section \ref{SNeqmodif} for the modifications required when the input image is not in units of counts or has already been Sky subtracted. The distribution of {\scale \cong \cong\cong \cong \cong \cong \cong \cong \cong \cong \cong \cong \cong

smaller than —detenminarea are removed from the analysis in both R_s and R_d . In the examples in this section, it is set to 15. Note that since a threshold approximately equal to the Sky value is used, this is a very weak constraint. For each pseudo-detection, SNry can be written as.

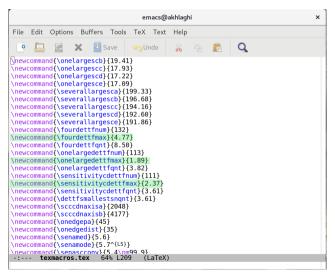
$$S/N_T = \frac{NF - NS_a}{\sqrt{NF + N\sigma_S^2}} = \frac{\sqrt{N}(F - S_a)}{\sqrt{F + \sigma_S^2}}.$$
 (3)

See Section 3.3 for the modifications required when the input image is not in units of counts or has already been Sky subtracted. The distribution of SN_T from the objects in R_s for the three examples in Figure 7 can be seen in column 5 (top) of that figure. Image processing effects, mainly due to shifting, rotating, and re-sampling the images for co-adding, on the real data further increase the size and count, and hence, the SN of false detections in real, reduced/co-added images. A comparison of scales on the SN histograms between the mock $\{(a.5.1)$ and $\{b.5.1\}$) and real $\{c.5.1\}$ examples in Figure 7 shows the effect quantitatively. In the histograms of Figure 7, the bin with the largest number of false pseudo-detections respectively has an SN of $\{1.89, 2.37, and 4.77\}$

The S/N_T distribution of detections in R_s provides a very ro-

Analysis step results/values concatenated into a single file.

All LATEX macros come from a single file.



Analysis results stored as LATEX macros

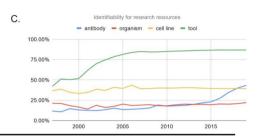
The analysis scripts write/update the LaTEX macro values automatically.

```
# Numbers for dettf.tex:
sant=9999999
function dettfhist
   # Set the file name.
   if [ \$2 == 4 \ 1 : then
                        obase=four:
   else
                                      obase=$2;
   fi
   if [ $2 == onelarge ]: then ind=" 7": else ind=" 12": fi
   name=$1$2$ind" detsn"$txt
   dettfnum=$(awk '/points binned in/{print $4; exit(0)}' $name)
   dettfgnt=$(awk '/quantile has a value of/{
                    printf("%.2f", $9); exit(0);}' $name)
   dettfmax=$(awk 'BEGIN { max=-999999 }
                  !/^{\#}/ \{ if(\$2>max)\{max=\$2: mv=\$1\} \}
                  END { printf("%,2f", mv) }' $name)
   addtexmacro $obase"dettfnum" $dettfnum
   addtexmacro $obase"dettfmax" $dettfmax
   addtexmacro $obase"dettfont" $dettfont
   # Find the smallest S/N quantile:
   sgnt=$(echo " " | awk '{if('$dettfant'<'$sgnt') print '$dettfant'}')</pre>
for base in 4 onelarge sensitivity3
do dettfhist $texdir/dettf/ $base: done
addtexmacro dettfsmallestsnant $sant
```

Let's look at the data lineage to replicate Figure 1C (green/tool) of Menke+2020 (DOI:10.1101/2020.01.15.908111), as done in arXiv:2006.03018 for a demo.

ORIGINAL PLOT

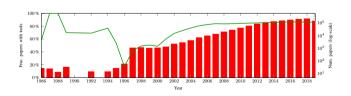
The Green plot shows the fraction of papers mentioning software tools from 1997 to 2019.



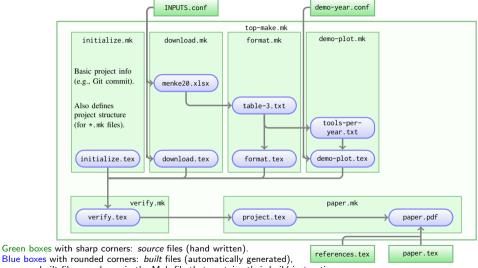
OUR enhanced REPLICATION

The green line is same as above but over their full historical range.

Red histogram is the number of papers studied in each year

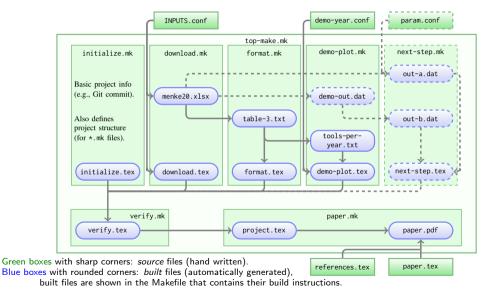


All analysis steps cascade down to paper.pdf (URL and checksum of input in INPUTS.conf).

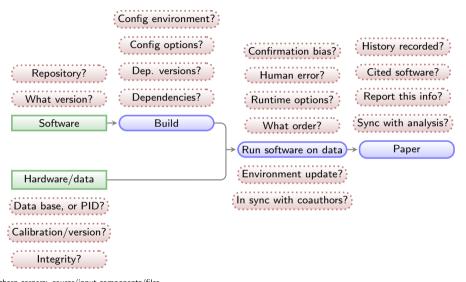


built files are shown in the Makefile that contains their build instructions.

It is very easy to expand the project and add new analysis steps (this solution is scalable)



All questions have an answer now (in plain text: human & computer readable/archivable).



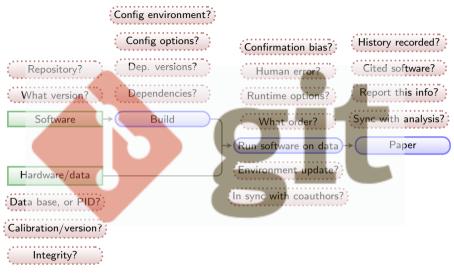
Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

Red boxes with dashed borders: questions that must be clarified for each phase.



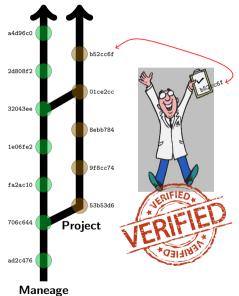
All questions have an answer now (in plain text: so we can use Git to keep its history).



Green boxes with sharp corners: *source*/input components/files.



New projects branch from Maneage



- Each point of project's history is recorded with Git.
- New project: a branch from the template.
 Recall that every commit contains the following:
 - Instructions to download, verify and build software.
 - Instructions to download and verify input data.
 - Instructions to run software on data (do the analysis).
 - ► Narrative description of project's purpose/context.
- Research progresses in the project branch.
- Template will evolve (improved infrastructure).
- Template can be imported/merged back into project.
- ► The template and project will evolve.
- During research this encourages creative tests (previous research states can easily be retrieved).
- Coauthors can work on same project in parallel (separate project branches).
- Upon publication, the Git checksum is enough to verify the integrity of the result.
 "Verified" image from vectorstock com

The Reales of the Low-Surface Brightness Universe Proceedings IAU Symposium No. 355, 2019 D. Valls-Galand, I. Travillo & S. Okamoto, eds.

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Carving out the low surface brightness universe with NoiseChisel

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Abstract. NoiseChisel is a program to detect very low signal-to-noise ratio (S/N) features with minimal assumptions on their morphology. It was introduced in 2015 and released within a collection of data analysis programs and libraries known as GNU Astronomy Utilities (Gnuastro). Over the last ten stable releases of Gaussiro. NoiseChisel has significantly improved detecting even fainter signal, enabling better user control over its inner workings, and many bug fives The most important change may be that NoiseChisel's segmentation features have been moved into a new program called Segment. Another major change is the final growth strategy of its true detections, for example NoiseChisel is able to eleter the outer wines of M51 down to S/N of 0.25, or 28.27 mag/arcsec2 on a single-exposure 8D6S smage (r-band). Segment is also able of 0.2.5, or 28.27 mag/arcsec⁻ on a single-expo of a plane (q-tonol), segment is also note to detect the localized HII regions as "clumps," he have five sensity. Finally, to orchestrate a controlled analysis, the concept of a "reproduct beautiful the used; this paper itself is exactly reproducible canaphoty sid-page-8505660.

Keywords, galaxies: halos, galaxies: photegraphy calaxies; structure, methods: data analysis, methods; reproducible, techniques; image processing techniques; photometric

1. Introduction

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Signal from the low surface brightness universe is buried does in the datasets noise and thus requires accurate detection methods. In Alchlaghi and Ichikawa (2015) (honosforth A115) a new method was introduced to detect such wars low signal to noise ratio (S.(N) signal from the images in a non-parametric manner. It allows accurate detection of the diffuse outer features of galaxies (that often have a different morphology from the centers). The software implementation of this method (NoiseChisel) is released as part of a larger collection of data analysis software known as GNU Astronomy Utilities! (Gnusstro). It was the first professional astronomical software to be independently referred by an independent panel (GNU Evaluation committee) and fully conforms with the GNU Coding Standardst

Since its release. NoiseChisel has been used in many studies. For example Baron et al. (2017) used it to identify objects that were missed by Rafelski et al. (2015) (henceforth R15) who used a combination of six SExtractor (Bertin and Arnouts 1996) runs with different configurations to avoid deblending problems, but still missed many sources with significant signal, see Figure 1. Borlaff et al. (2019). Miler et al. (2019), and Truillo et al. (2019) used it for accurate flat field and Sky subtraction to create deeper co-added images in galaxy fields for optimal detection of the low surface brightness features. Calvi et al. (2019) used it to find Lyman-\(\alpha\) emitters in spectra. For future studies, Laine et al.

1 https://www.gnu.org/prep/standards



The Sloan Digital Sky Survey extended point spread functions

Raúl Infante-Sainz 0,12* Ignacio Trujillo 01,2 and Javier Román 01,2,3

A robust and extended characterization of the point spread function (PSF) is crucial to extract the photometric information produced by deep imaging surveys. Here, we present the extended PSFs of the Sloan Digital Sky Survey (SDSS), one of the most productive astronomical surveys of all time. By stacking ~1000 images of individual stars with different brightness, we obtain the bidimensional SDSS PSFs extending over 8 arcmin in radius for all the SDSS filters (x, x, r. (-2). This new characterization of the SDSS PSEs is near a factor of 10 larger in extension. than previous PSFs characterizations of the same survey. We found asymmetries in the shape of the PSFs caused by the drift scanning observing mode. The flux of the PSFs is larger along the drift scanning direction. Finally, we illustrate with an example how the PSE models conbe used to remove the scattered light field produced by the brightest stars in the central region of the Come cluster field. This particular example shows the base importance of PSEs in the study of the low-surface brightness Universe, especially with the spectring of ultradeep surveys, such as the Large Synoptic Survey Telescope (LSST). Following a preeoducible science philosophy, we make all the PSE models and the scripts used to do the analysis of this paper publicly available (snapshot v0.4-0-pd966ad0).

Key words: instrumentation: detectors - methods: one trialway examples: image processing-techniques: photometric - galaxies: haloes ... IERIFIE

1 INTRODUCTION

The point second function (BSE) describes the resource of an imaging system to the light produced by a point source. Real PSFs have complex structures as their shapes depend on the optical note that light takes as it travels through the atmosphere and multiple period elements, mirrors, lenses, detectors, etc. For the vast majority of astronomical works, only a tirry nortion of the PSF (i.e. normally a few inner accreconds; see e.g. Traille et al. 2001a. b) is characterized. In practice, however, the light of both point and estanded courses are served ever the entire detector due to the offect of the PSF at large radii. Therefore, it is necessary to have a good understanding of its structure along the entire detector (typically entending over preminates or many)

Extended PSFs have become a vital tool to obtain reveise instance, Slater, Harding & Miles (2009) modelled the extended Schmidt telescope and showed that virtually all the pixels of the irease are deminated by the neutronal light by both stary and mlasin at 29.5 mag arrang 2 (V-hand). Truillo & Eliri (2016).

of the Strine \$2 survey and mad them to madel and correct the acottered light field resolved by stars to study the certical respective of the Galactic cirri. All the above works have shown that buring properties of astronomical objects at low-surface brightness levels One of the most commonly used surveys for measuring photo-

also characterized and used the extended PSF of the 10.4 m Gran

Telescopio Canarios (GTC) telescope to model and sorrove the

Even more troublesome for low-surface brightness studies is the

Spring (see a.g. Traille & Bolov 2011; Sanda 2014; 2015) that

the outer review of astronomical objects are accordy affected by

their own scattered light medical by the convolution with the PSE

In order to correct this effect. Karabal et al. (2017) reperated the PSF

and models of the internal reflections from images of the Canada-

France-Howaii Telescope (CFHT) to de-convolve a sample of three

Survey (SDSS: York et al. 2000) covering 14 555 deet on the sky Gust over 35 per cent of the full sky) in five photometric bunds (u. v. r, i, and z). Although SDSS is a relatively shallow survey compared

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E 2019 The Authoriti Published by Oxford University Press on behalf of the Reval Astronomical Society

Publication of the project

A reproducible project using Maneage will have the following (plain text) components:

- Makefiles.
- ► L^AT_EX source files.
- Configuration files for software used in analysis.
- Scripts/programming files (e.g., Python, Shell, AWK, C).

The volume of the project's source will thus be negligible compared to a single figure in a paper (usually ~ 100 kilo-bytes).

The project's pipeline (customized Maneage) can be published in

- ► arXiv: uploaded with the LATEX source to always stay with the paper (for example arXiv:1505.01664 or arXiv:2006.03018).
- Zenodo: Along with all the input datasets (many Gigabytes) and software (for example zenodo.3872248) and given a unique DOI.

Executing a Maneaged project (for example arXiv:2006.03018)

```
$ git clone https://gitlab.com/makhlaghi/maneage-paper
                                                         # Import the project.
$ ./project configure
                             # You will specify the build directory on your system,
                             # and it will build all software (about 1.5 hours).
$ ./project make
                             # Does all the analysis and makes final PDF.
```

Future prospects...

Adoption of reproducibility by many researchers will enable the following:

- ▶ A repository for education/training (PhD students, or researchers in other fields).
- ► Easy verification/understanding of other research projects (when necessary).
- ► Trivially test different steps of others' work (different configurations, software and etc).
- Science can progress incrementally (shorter papers actually building on each other!).
- Extract meta-data after the publication of a dataset (for future ontologies or vocabularies).
- ► Applying machine learning on reproducible research projects will allow us to solve some Big Data Challenges:
 - Extract the relevant parameters automatically.
 - Translate the science to enormous samples.
 - Believe the results when no one will have time to reproduce.
 - ► Have confidence in results derived using machine learning or AI.



Summary:

Maneage and its principles are described in arXiv:2006.03018. It is a customizable template that will do the following steps/instructions (all in simple plain text files).

- ► Automatically downloads the necessary *software* and *data*.
- Builds the software in a closed environment.
- ▶ Runs the software on data to generate the final research results.
- ▶ Modification of part of the analysis will only result in re-doing that part, not the whole project.
- Using LaTeX macros, paper's figures, tables and numbers will be Automatically updated after a change in analysis. Allowing the scientist to focus on the scientific interpretation.
- ► The whole project is under version control (Git) to allow easy reversion to a previous state. This encourages tests/experimentation in the analysis.
- ▶ The Git commit hash of the project source, is printed in the published paper and saved on output data products. Ensuring the integrity/reproducibility of the result.
- These slides are available at https://maneage.org/pdf/slides-intro-short.pdf.
- Longer slides are available at https://maneage.org/pdf/slides-intro.pdf.

For a technical description of Maneage's implementation, as well as a checklist to customize it, and tips on good practices, please see this page:

https://gitlab.com/maneage/project/-/blob/maneage/README-hacking.md