# Maneage: a proof-of-concept for rigorous reproducible research paper criteria

(Akhlaghi+2021, CiSE 23, 82 DOI:10.1109/MCSE.2021.3072860, arXiv:2006.03018)

#### Boud Roukema

Institute of Astronomy, Nicolaus Copernicus University

Ten Years of Guix 16 September 2022 @Université de Sorbonne

Slides' main authors: Akhlaghi + Roukema; pdf built from git commit 348ad50; this pdf: https://cosmo.torun.pl/ $\sim$ boud/Roukema20220916TYG.pdf

# Reproducibility crisis in scientific research: astronomy

#### Snakes on a Spaceship – An Overview of Python in Heliophysics

"...inadequate analysis descriptions and loss of scientific data have made scientific studies difficult or impossible to replicate". From Burrell+2018, (arXiv:1901.00143).

#### Perspectives on Reproducibility and Sustainability of Open-Source Scientific Software

"It is our interest that NASA adopt an open-code policy because without it, reproducibility in computational science is needlessly hampered". From Oishi+2018, (arXiv:1801.08200).

#### Schrödinger's code: source code availability and link persistence in astrophysics

"We were unable to find source code online ... for 40.4% of the codes used in the research we looked at". From Allen+2018, (arXiv:1801.02094).

#### and in biology, other sciences, economics

#### Repeatability of published microarray gene expression analyses

loannidis $\pm 2009$  evaluated the replication of data analyses in 18 articles ... in Nature Genetics and reproduced only 2 in principle.". DOI:10.1038/ng.295.

#### Is Economics Research Replicable? 60 papers from Thirteen Journals Say "Usually Not"

Chang & Li (2015) were are able to replicate less than half of 67 papers in prestigiuos journals, with help from the authors. DOI:10.17016/FEDS.2015.083

#### An empirical analysis of journal policy effectiveness for computational reproducibility

Stodden+2018 studied a random sample of 204 scientific papers in *Science* and were able to obtain artifacts from 44% and reproduce the findings for 26%. DOI:10.1073/pnas.1708290115

#### "Reproducibility crisis" in the sciences?

Baker 2016, Nature 533, 452: 70% of researchers couldn't reproduce another scientist's results; half couldn't reproduce their own. nature.com/articles/533452a

# Replicability (hardware/statistical)

- Involves data collection.
- Inherently includes measurement errors (can never be exactly reproduced).
- Example: Raw telescope image/spectra.
- ► NOT DISCUSSED HERE.

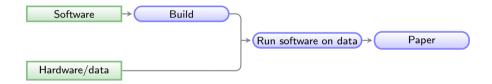


(C) CC BY-SA 2006, R. Feiler

#### Reproducibility (software/deterministic)

- Involves data analysis, or simulations.
- Starts after data is collected/digitised.
- Example: 2 + 2 = 4 (i.e., sum of datasets).
- **▶** DISCUSSED HERE.

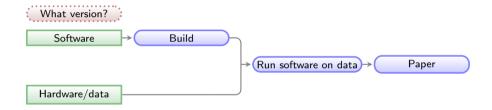




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.





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

Blue boxes with rounded corners: built components.



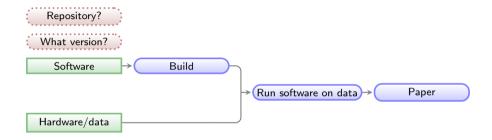
# Different package managers have different versions of software (repology.org, 2021/12/02)

# Astropy Packaging status Debian Experimental Rasphian Oldstable Raspbian Stable Raspbian Testing Ubuntu 20.04 Ubuntu 21.04

Ubuntu 22.04

#### GNU Astronomy Utilities (Gnuastro)

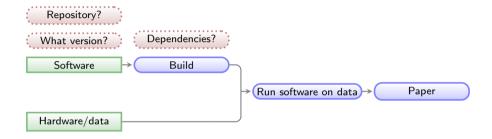




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

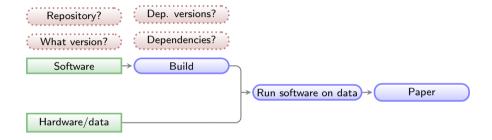




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.



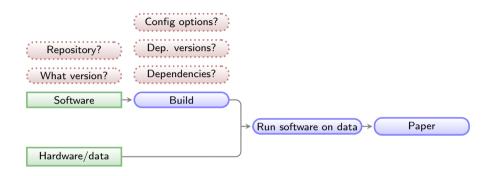


Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: *built* components.

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

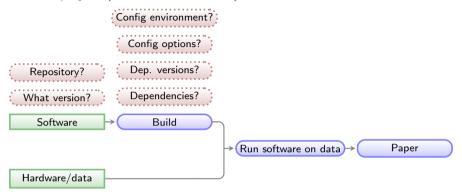




Green boxes with sharp corners: *source*/input components/files.

Blue boxes with rounded corners: *built* components.





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

Blue boxes with rounded corners: built components.



# Example: Matplotlib (a Python visualization library) build dependencies

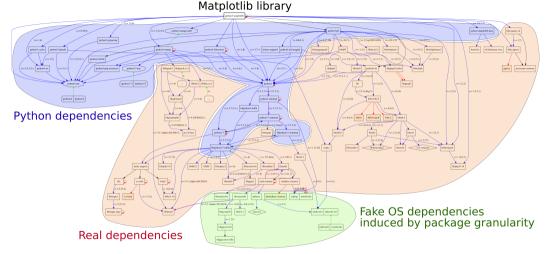
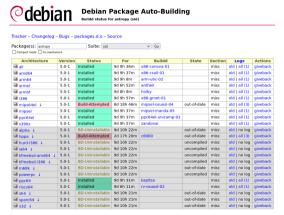
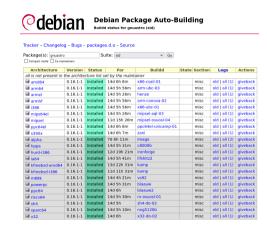


Fig. 1. Transitive dependencies of the software environment required by a simple "import matplotlib" command in the Python 3 interpreter.

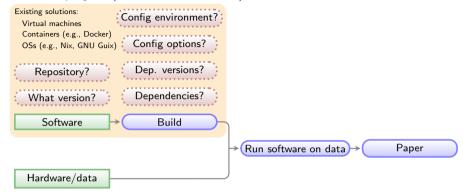
# Impact of "Dependency hell" on native building in various hardware (CPU architectures), retrieved from Debian on 2021/12/02



Astropy depends on Matplotlib



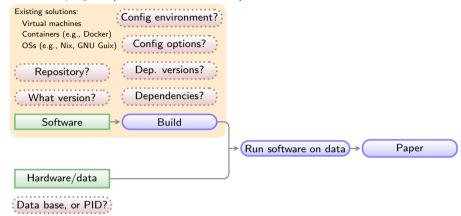
GNU Astronomy Utilities doesn't.



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

Blue boxes with rounded corners: built components.

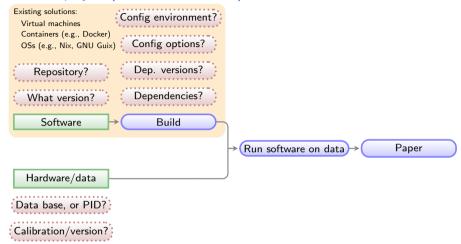




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

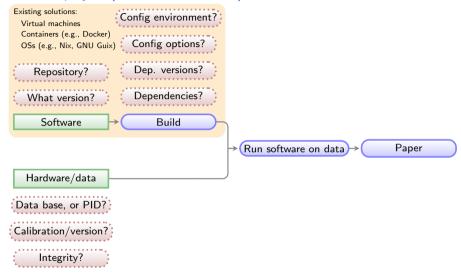




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

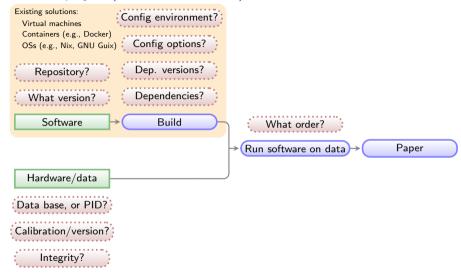




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

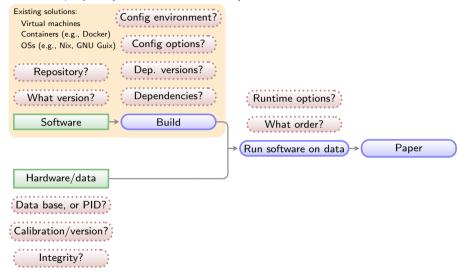




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

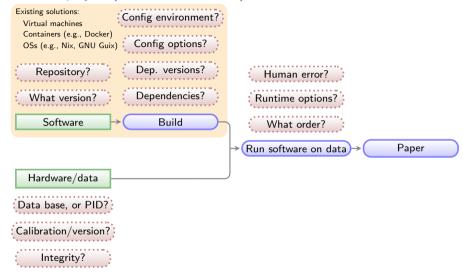




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

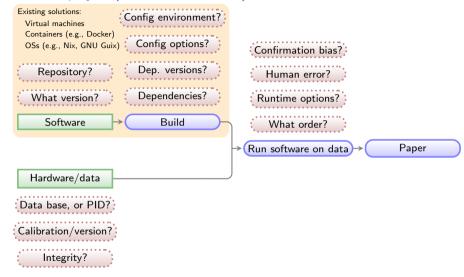




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

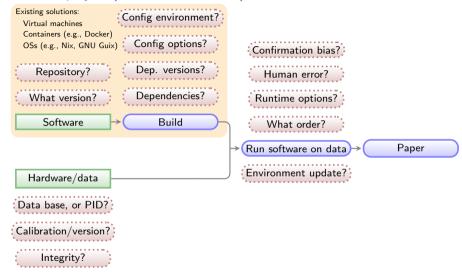




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

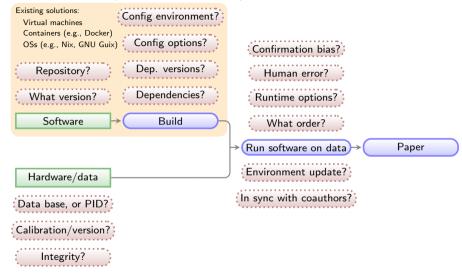




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

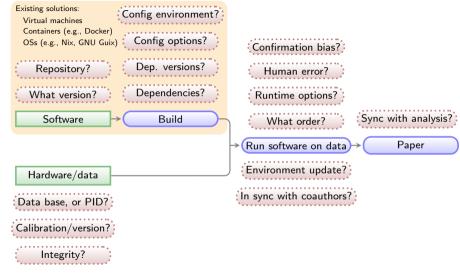




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

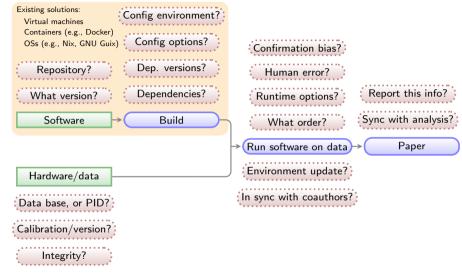




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

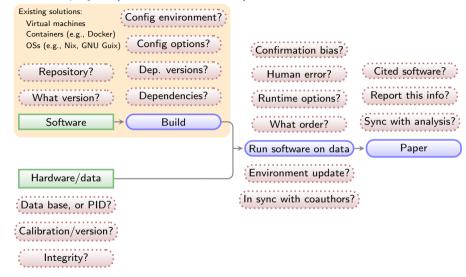




Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.





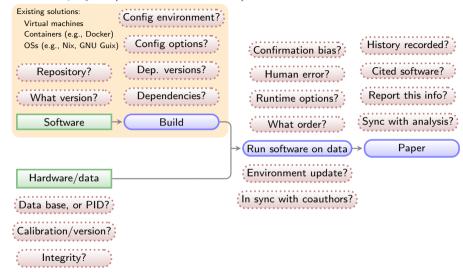
Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.



Di Cosmo & Pellegrini (2019) Encouraging a wider usage of software derived from research

"Software is a hybrid object in the world research as it is equally a driving force (as a tool), a result (as proof of the existence of a solution) and an object of study (as an artefact)".



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

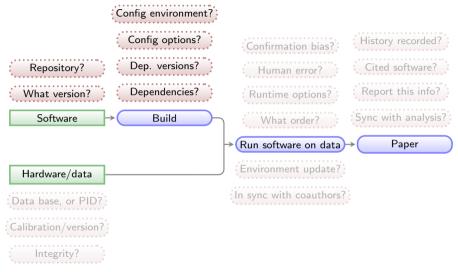
Blue boxes with rounded corners: built components.



#### Buckheit & Donoho (1996) Lecture Notes in Statistics (vol 103, DOI:10.1007/978-1-4612-2544-7\_5)

"An article about computational science [today: almost all sciences] ... is not the scholarship itself, it is merely ADVERTISING of the SCHOLARSHIP.

The ACTUAL SCHOLARSHIP is the complete software development environment and the complete set of instructions which generated the figures."



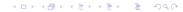
Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.



#### Criteria for a solution

- ▶ 1. Completeness (self-contained-ness):
  - ▶ (1) Only dependency should be POSIX tools (discards Conda or Jupyter which need Python).
  - (2) Plain text: Project's source should be in plain-text (binary formats need special software)
  - (3) No impact on host OS libraries, programs, env variables.
  - (4) Must not require root permissions (discards tools like Docker or Nix/Guix).
  - (5) Builds its own controlled software + env variables.
  - ▶ (6) Should be usable without an internet connection.
  - (7) Contains full instructions for inputs, software building, and outputs: analysis + narrative + graphical output (e.g. pdf or html)
  - (8) Should be non-interactive or runnable in batch (user interaction is an incompleteness).
- ➤ 2. Modularity: Parts of the project should be re-usable in other projects.
- ▶ 3. Minimal complexity: Occam's razor: "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.
- 4. Scalability: an implementation should easily scale to arbitrarily large, complex projects.



#### Criteria for a solution

- ▶ 5. Verifiable inputs and outputs: Inputs and Outputs must be automatically verified.
- ▶ 6. Recorded history: Exploratory research involves modifying methods, reducing over-ambitious goals, serendipity; hypothesis testing should have a fixed, predefined method did the authors modify the method? how? what? which? when?
- 7. Including the narrative that is associated with the analysis: a workflow alone lacks motivations, interpretations.
- ▶ 8. 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).

# Our solution: CiSE 23 (3), pp 82-91: DOI:10.1109/MCSE.2021.3072860, arXiv:2006.03018



"solutions") have been proposed, which mostly rely on the common technology of the day starting

Digital Object Identifier 10.1109/MCSE 2021.3072860

However, these technologies develop fast, e.g., code written in Python 2 (which is no longer officially maintained) often cannot run with Python 3. The cost of staying up to date within this rapidly evolving landscape is high, Scientific projects, in particular, suffer the most: Scientists have to focus on their own research domain, but to some degree, they need to understand the technotons of their tools because it determines their results



https://maneage.org

#### Predefined/exact software tools

#### Reproducibility & software

Reproducing the environment (specific software versions, build instructions and dependencies) is also critically important for reproducibility.

- Containers or Virtual Machines are a binary black box.
- Maneage installs fixed versions of all necessary research software and their dependencies.
- ► Installs similar environment on GNU/Linux, or macOS systems.
- Works very much like a package manager (e.g., apt or brew).





#### Controlled environment and build instructions



```
emacs@akhlaghi
File Edit Options Buffers Tools Makefile Help
                       Save ← Undo 
       # not 'LIBS'
       # On Mac systems, the build complains about 'clang' specific
       # features, so we can't use our own GCC build here.
       if [ x$(on mac os) = xves 1: then \
         export CC=clang: \
         export CXYsclang++: \
       41. 1
       cd $(ddir) \
       && rm -rf cmake-$(cmake-version) \
       && tar xf $< \
       && cd cmake-$(cmake-version) \
       && ./bootstrap --prefix=$(idir) --system-curl --system-zlib \
                      --system-bzip2 --system-liblzma --no-qt-gui \
       && make -1$(numthreads) LIBS="$$LIBS -1ssl -1crvpto -1z" VERBOSE=1 \
       && make install \
       && cd .. \
       && rm -rf cmake-$(cmake-version) \
       && echo "CMake S(cmake-version)" > 50
$(ibidir)/ghostscript: $(tdir)/ghostscript-$(chostscript-version).tar.gz
       $(call obuild, $<, ohostscript-$(ohostscript-version)) \
       && echo "GPL Ghostscript $(ghostscript-version)" > $0
B(ibidir)/gguastro: $(tdir)/gguastro-$(gguastro-version).tar.lz \
                   $(ibidir)/ghostscript \
                   $(ibidir)/libings \
                   $(ibidir)/libtiff >
                   $(ibidir)/libgit2 )
                   $(ibidir)/wcslib \
                   $(ibidir)/asl
ifen ($(static build) ves)
       staticonts="--enable-static=ves --enable-shared=no":
       $(call qbuild, $<, qnuastro-$(qnuastro-version), static, \
                      $$staticopts. -i$(numthreads). \
                      make check - i$(numthreads)) \
       && on $(dtexdir)/onwastro tex $(ictdir)/ \
       && echo "GNU Astronomy Utilities $(gnuastro-version) \citep(gnuastro)" > *
$(ibidir)/imagemagick: $(tdir)/imagemagick-$(imagemagick-version).tar.xz \
                      $(ibidir)/libipeg \
                      $(ibidir)/libtiff \
                      $(ibidir)/zlib
       $(call qbuild, $<, ImageMagick-$(imagemagick-version), static, \
                      --without-x --disable-openmo, V=1) \
       && echo "ImageMagick $(imagemagick-version)" > $0
Il'... high-level mk 67% 1584 Git master (Makefile)
```

#### Controlled environment and build instructions

```
emacs@akhlaghi
File Edit Options Buffers Tools Makefile Help
                      Save Save
include reproduce/software/config/installation/texlive.mk
include reproduce/software/config/installation/versions.mk
lockdir = $(BDIR)/locks
tdir = $(BDIR)/software/tarballs
ddir = $(BDIR)/software/build-tmp
idir = $(BDTR)/software/installed
ibdix = $/RDIR\/software/installed/bin
ildir = $(BDIR)/software/installed/lib
dtexdir = $(shell pwd)/reproduce/software/bibtex
itidir = $(BDIR)/software/installed/version-info/tex
ictdir = $(RDIR)/software/installed/version-info/cite
ipydir = $(BDIR)/software/installed/version-info/python
ibidir = $(BDIR)/software/installed/version-info/proglib
# Set the top-level software to build.
all: $(foreach p, $(top-level-programs), $(ibidir)/$(p)) \
     $(foreach n. $(top-level-python). $(invdir)/$(p)) \
     $(itidir)/texlive
# Other basic environment settings: We are only including the host
# operating system's PATH environment variable (after our own!) for the
# compiler and linker. For the library binaries and headers, we are only
# using our internally built libraries.
# To investigate:
    1) Set SHELL to '$(ibdir)/env - NAME=VALUE $(ibdir)/bash' and set all
       the parameters defined bellow as 'NAME-VALUE' statements before
       calling Bash. This will enable us to completely ignore the user's
       native environment
    2) Add '--noprofile --norc' to '.SHELLFLAGS' so doesn't load the
       uper's environment
ONE SHELL
CHELLELACE
                        := --noprofile --norc -ec
export CCACHE DISABLE := 1
export PATH
                       := $(ibdir)
export SHELL
                       := $(ibdir)/bash
export CRRELAGS
                       := -I$(idir)/include
export PKG CONFIG PATH := $(ildir)/pkgconfig
export PKG CONFIG LIBDIR := $(ildir)/pkgconfig
export LD RUN PATH := $(ildir):$(il64dir)
export ID LIBRARY PATH := $(ildir):$(il64dir)
export IDELAGS
                       := $(reath command) -1$(ildir)
# We want the download to happen on a single thread. So we need to define a
lock, and call a special script we have written for this job. These are
Ill... high-level mk 4% 181 Git-master (Makefile)
```

```
emacs@akhlaghi
File Edit Options Buffers Tools Makefile Help
                       Save ← Undo 
       # not 'LIBS'
       # On Mac systems, the build complains about 'clang' specific
       # features, so we can't use our own GCC build here.
       if [ x$(on mac os) = xves 1: then \
         export CC=clang: \
         export CXYsclang++: \
       41. 1
       cd $(ddir) \
       && rm -rf cmake-$(cmake-version) \
       && tar xf $< \
       && cd cmake-$(cmake-version) \
       && ./bootstrap --prefix=$(idir) --system-curl --system-zlib \
                      --system-bzip2 --system-liblzma --no-qt-gui \
       && make -1$(numthreads) LIBS="$$LIBS -1ssl -1crvpto -1z" VERBOSE=1 \
       && make install \
       && cd .. \
       && rm -rf cmake-$(cmake-version) \
       && echo "CMake S(cmake-version)" > 50
$(ibidir)/ghostscript: $(tdir)/ghostscript-$(chostscript-version).tar.gz
       $(call obuild, $<, ohostscript-$(ohostscript-version)) \
       && echo "GPL Ghostscript $(ghostscript-version)" > $0
(ibidir)/gnuastro: $(tdir)/gnuastro-$(gnuastro-version).tar.lz \
                   $(ibidir)/ghostscript \
                   $(ibidir)/libings \
                   $(ibidir)/libtiff >
                   $(ibidir)/libgit2 )
                   $(ibidir)/wcslib \
                   $(ibidir)/asl
ifen ($(static build) ves)
       staticonts="--enable-static=ves --enable-shared=no":
       $(call qbuild, $<, qnuastro-$(qnuastro-version), static, \
                      $$staticopts. -i$(numthreads). \
                      make check - i$(numthreads)) \
       && on $(dtexdir)/onwastro tex $(ictdir)/ \
       && echo "GNU Astronomy Utilities $(qnuastro-version) \citep(qnuastro)" > *
$(ibidir)/imagemagick: $(tdir)/imagemagick-$(imagemagick-version).tar.xz \
                      $(ibidir)/libipeg \
                      $(ibidir)/libtiff \
                      $(ibidir)/zlib
       $(call qbuild, $<, ImageMagick-$(imagemagick-version), static, \
                      --without-x --disable-openmo, V=1) \
       && echo "ImageMagick $(imagemagick-version)" > $0
Il'... high-level mk 67% 1584 Git master (Makefile)
```



## Example: Matplotlib (a Python visualization library) build dependencies

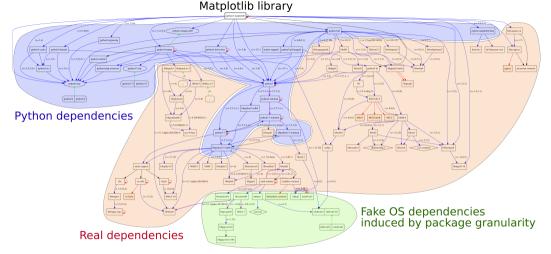


Fig. 1. Transitive dependencies of the software environment required by a simple "import matplotlib" command in the Python 3 interpreter.

#### All high-level dependencies are under control (e.g., NoiseChisel's dependencies)

#### **GNU/Linux distribution**

#### macOS

### \$ 1dd .local/bin/astnoisechisel

libgnuastro.so.7 => /PROJECT/libgnuastro.so.7 (0x00007f6745f39000) libgit2.so.26 => /PROJECT/libgit2.so.26 (0x00007f6745df1000)

libtiff.so.5 => /PROJECT/libtiff.so.5 (0x00007f6745d77000)
liblzma so 5 => /PROJECT/liblzma so 5 (0x00007f6745d4f000)

libipeg.so.9 => /PROJECT/libipeg.so.9 (0x0000716745d41000)

libucs.so.6 => /PROJECT/libucs.so.6 (0x00007f6745ba8000)

libcfitsio.so.8 => /PROJECT/libcfitsio.so.8 (0x000071674588b000)

libcurl.so.4 => /PROJECT/libcurl.so.4 (0x00007f6745811000)

libssl.so.1.1 => /PROJECT/libssl.so.1.1 (0x00007f6745777000)

libcrypto.so.1.1 => /PROJECT/libcrypto.so.1.1 (0x00007f6745491000)

libz.so.1 => /PROJECT/libz.so.1 (0x00007f6745474000)
libgsl.so.23 => /PROJECT/libgsl.so.23 (0x00007f67451e3000)

libgs1.so.23 => /PROJECT/libgs1.so.23 (0x00007f67451e3000)

libgslcblas.so.0 => /PROJECT/libgslcblas.so.0 (0x00007f67451a1000) linux-vdso.so.1 (0x00007fffdcbf7000)

libpthread.so.0 => /usr/lib/libpthread.so.0 (0x00007f6745006000) libm.so.6 => /usr/lib/libm.so.6 (0x00007f6745027000)

libc.so.6 => /usr/lib/libc.so.6 (0x00007f6744e43000)

libdl.so.2 => /usr/lib/libdl.so.2 (0x00007f6744e1e000)

/lib64/ld-linux-x86-64.so.2 => /usr/lib64/ld-linux-x86-64.so.2

#### \$ otool -L .local/bin/astnoisechisel

/PROJECT/libgnuastro.7.dylib (comp ver 8.0.0, cur ver 8.0.0)
/PROJECT/libgit2.26.dylib (comp ver 26.0.0, cur ver 0.26.0)
/PROJECT/libtiff.5.dylib (comp ver 10.0.0, cur ver 10.0.0)
/PROJECT/libtjma.5.dylib (comp ver 8.0.0, cur ver 8.4.0)
/PROJECT/libjeg.9.dylib (comp ver 8.0.0, cur ver 8.4.0)
/PROJECT/libwcs.6.2.dylib (comp ver 6.0.0, cur ver 6.2.0)
/PROJECT/libcifitsio.8.dylib (comp ver 8.0.0, cur ver 6.2.0)
/PROJECT/libcitl.4.dylib (comp ver 10.0.0, cur ver 10.0.0)
/PROJECT/libssl.1.1.dylib (comp ver 11.0, cur ver 11.0)
/PROJECT/libsrl.1.dylib (comp ver 1.1.0, cur ver 1.1.0)
/PROJECT/libg.1.dylib (comp ver 10.0.0, cur ver 1.2.11)
/PROJECT/libgsl.3.dylib (comp ver 25.0.0, cur ver 25.0.0)
/PROJECT/libgsl.3.dylib (comp ver 1.0.0, cur ver 1.0.0)
/Usr/lib/libSystem.B.dylib (comp ver 1.0.0, cur ver 1252.50.4)

Project libraries: High-level libraries built from source for each project (note the same version in both OSs). GNU C Library: Project specific build is in progress (http://savannah.nongnu.org/task/?15390). Closed operating system files: We have no control on low-level non-free operating systems components.

#### 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 ( $\sim$  2–3 hours; Sep 2022).
- Dependencies of different projects will not conflict.
- ► Everything in plain text (human & computer readable/archivable).

### 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, (b) Histogram 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 'h' 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 tonote will not be in the final PDF. You can thus use blight light changes to easily make conies of your research for cristing 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 narror. This reproducible narror template 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 2.21.0 (D.I.) Autonomy Dillities 0.9 (Alddachi and Edikson 2015), GNU AWK 5.0.0, GNU Bosh 5.0.7, GNU Birutils 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 3.3. GNU Gain 1.10. GNU Integer Set Library 0.18. GNU Librard 2.4.6 CINIU MA LA LE CINIU Maior 4.2.90 CINIU Malei. ple Precision Arithmetic Library 6.1.2. GNU Multiple Precision. Country library, GNU Multiple Precision Floating-Point Rehighly 4.0.2. GNU NCURSES 6.1. GNU Rendline 8.0. GNU Scientific Library 2.5, GNU Sed 4.7, GNU Ter 1.32, GNU Wort 120.3 GNU Which 2.21 GRI Ghostocriet 9.26 UDES Shores 1.10.5. ImageMarick 7.0.8-46. Libbot 0.9.1. Librar 2.0.26.0. Libince v9b. Library 1.6.37. Library 4.0.10. Lain 1.20. Metastore (forked) 1.1.2-23-fa9170b. OpenBLAS 0.3.5. Open MPI 4.0.1. OpenSSL L.I. La. PatchELF 0.9. plos confin 0.29.2. Pethon 3.7.3. Dizin 6.0. WCSLIB 6.2, XZ Utils 5.2.4, Zip 3.0 and Zlib 1.2.11. (Astrony Collaboration et al. 2013: Astrony Collaboration et al. 2018). Cyclor 0.10.0. Cython 0.29.6 (Rehnel et al. 2011). h5m: 2.9.0. Kiwisolver 1.0.1, Matphotlib 3.0.2 (Harner 2007), Numery 1.16.2 (see der Welt et al. 2011), eksesselle 1.5.1. Perkening 2.3.1, python-dateutil 2.8.0, Scipy 1.2.1 (Oliphant 2007; Millman and Alexais 2011). Saturations 40.9.0. Separated areas 3.3.0 and Six 1.12.0. The ISTeX source of the paper was compiled to make the PDF using the following nuckages: hither 2.12, hither 2.12. NNotes 3.12 NNotes 3.12 caption 2018-10-05 caption 2018-10.05 courier 2016.06.24 courier 2016.06.24 counter 5.24 datetime 2.60, datetime 2.60, ec 1.0, ec 1.0, etoolbox 2.5f, etool-3.05 funtaces 1.0d. fentages 1.0d. footmise 5.5h. footmise 5.5h. fn 2 Ld fn 2 Ld Journa J.O. Journa J.O. navets J. 554, newty J. 554. pef 3.1.2, pef 3.1.2, pefplots 1.16, pefplots 1.16, preprint 2011, premaint 2011 setunace 6.7a setunace 6.7a tex 3.14159265 tex 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 referes 2016-06-24 when 2016-06-24 when 2016-06-24 scolor 2.12, scolor 2.12, skeward 2.7a and skeward 2.7a. We are very grateful to all their creators for freely providing this necessary infrastructure. This research (and many others) would not he possible 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-

### 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, (b) Histogram 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 contex of your research for cristing 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, Matglothb 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, txfonts 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-

### Software citation automatically generated in paper (only GNU Astronomy Utilities)

#### Appendix A: Software acknowledgement

The reproducible paper template that is customized for this project automatically installs all the necessary software. Directly listing all the high-level software and their versions is done with two primary motives: 1) software citation and acknowledgetzent of the hard work (as part of different software projects) that this project utilized. 2) reproducibility for (future) readers.

This recannels was done with the following the software temperature.

grams and libraries: Bzip2 1.0.6, CFITSIO 3.47, CMalor 3.14.2. cURL 7.63.0. Discoteu flock 0.23. File 5.36. Git 2.22.0. GNU Astronomy Utilities 0.9.170-bffc (Akhlaghi and Ichikawa 2015), GNU AWK 5.0.0 GNU Bash 5.0.7 GNU Bingils 2.32 GNU Compiler Collection (GCC) 9.1.0. GNU Coroutils 8.31. GNU Diffutils 3.7. GNU Findutils 4.6.0.199-e3fc. GNU Gree 3.3 GNU Grin 1 10 GNU lateour Set Library 0 18 GNU Library 2.4.6 GNU M4.1.4.18 GNU Make 4.2.90 GNU Makinla Procision Arithmetic Library 6.1.2. GNU Multiple Precision Comoles library, GNU Multiple Precision Floating-Point Reliable 4.0.2. GNU NCURSES 6.1. GNU Readline 8.0. GNU Scientific Library 2.5, GNU Sed 4.7, GNU Tar 1.32, GNU Wget 1.20.3 GNU Which 2.21, GPL Ghostscript 9.26, Libbsd 0.9.1, Libgit2 0.28.2. Libipeg v9b, Libtiff 4.0.10, Lzip 1.20, Metastore (forked) Lingpag von, Librill 4 J. H., Lisp L. M., Shelastone (Orlead)
 L12-23-fa9170b, OpenSSL 1.1.1a, ParchELF 0.9, pkg-config
 Q29.2, Unzip 6.0, WCSLIB 6.2, XZ Utils 5.2.4, Zip 3.0 and Zlih 1.2.11. The PfleX source of the rarser was correlated to make the PDF using the following rackages: hiber 2.12, hibitates 3.12. caption 2018-10-05, charter 2016-06-24, courier 2016-06-24 counter \$ 24 determs 2.60 or 1.0 aminos 0.1 stocker 2.66 extrices 1.4a, fancybdr 3.10, fintcount 3.05, fortunes 1.04, footmisc 5 5h fo 2 Ld Jedustic 2016-05-24 Jineno 4 41 Joesso I 0 newtx 1.554, pgf 3.1.2, pgfplots 1.16, preprint 2011, setspace times 2016-06-24. fiffesec 2.10.2. trimspaces 1.1, txSonts 2016 06-24, ulem 2016-06-24, xcolor 2.12 and xkeyval 2.7a. We are very grateful to all their creators for freely providing this necesvary infrastructure. This properly (and many others) would not be possible without them.

Article number, page 5 of 5

### Software citation automatically generated in paper (only GNU Astronomy Utilities)

#### Appendix A: Software acknowledgement

The reproducible paper template that is customized for this project automatically installis all the necessary software. Directly issting all the high-level software and their versions is done with two primary motives: 1) software citation and acknowledgement of the hard work as part of different software projects that this project utilized. 2) reproducibility for (future) readers.

That removals was also see with the olderings for earlier are per SIGIL 78.4.1 December 40.2.3. Feb. 3.5. (e. 12.22.0. CMI)

CMI 20.4.5. December 40.2.3. Feb. 3.5. (e. 12.22.0. CMI)

CMI 20.4.5. December 40.3. (e. 12.20.0. CMI)

CMI 20.4.5. 20.4.5. (e. 12.20.0. CMI)

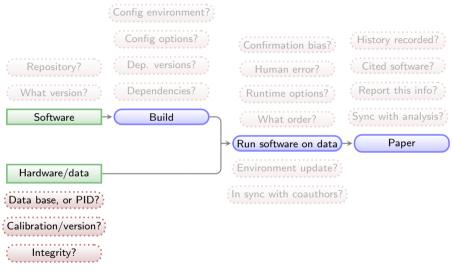
CMI 20.4.5. 20.4.5. (e. 12.20.0. CMI)

CMI 20.4.5. 20.4.5. (e. 12.20.0. CMI)

CMI 20.4.5. (e. 12.20.0.

Article number, muce 5 of 5

#### General outline of a project (after data collection)



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.



#### 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).





#### 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  $\frac{\text{downloaded}}{\text{during the analysis}}$ .

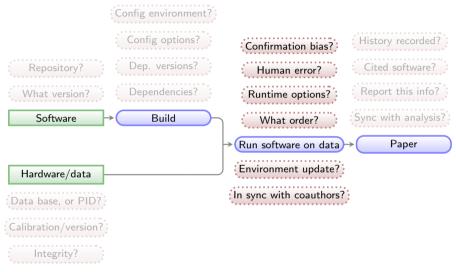
MD5-sums are checked to make sure the download was done properly or the file is the same (hasn't changed on the server/source).

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.

Blue boxes with rounded corners: *built* components.

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



#### 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).





### 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).





### Reproducible science: Maneage is managed through a Makefile

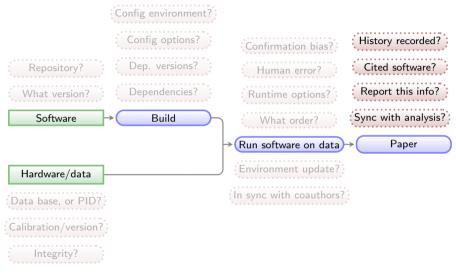
All steps (downloading and analysis) are managed by Makefiles (example from zenodo.1164774):

- 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.

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



#### 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{tsNeq} $$ \left( S_a \right) = \frac{S_a}{S_a}^2} = \frac{S_a}{S_a}^2} = \frac{S_a}{S_a}^2} . $$ \left( S_a \right)^2 + \frac{S_a}{S_a}^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  $\langle small \ S/N \rangle_{\tau} \rangle$  from the objects in  $\mathbb{R}_s$  for the three examples in Figure \ref{dettf} 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  $\{\mbox{\sc small } S/N\}$  of false detections in real, reduced/co-added images. A comparison of scales on the  $\{\mbox{\sc small } S/N\}$  histograms between the mock ((a.5.1) and (b.5.1)) and real (c.5.1) examples in Figure \ref{dettf}\$ shows the effect quantitatively. In the histograms of Figure \ref{dettf}\$, the bin with the largest number of false pseudo-detections respectively has an  $\{\mbox{\sc small } S/N\}$  of  $\{\mbox{\sc small } S/N\}$  of  $\{\mbox{\sc small } S/N\}$  of  $\{\mbox{\sc small } S/N\}$  and  $\{\mbox{\sc$ 

smaller than —detsminarea are removed from the analysis in both  $R_c$  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 pseudodetection,  $SN_T$  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 SNT from the objects in R<sub>s</sub> 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 S/N of false detections in real, reduced/co-added images. A comparison of scales on the S/N 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 S/N of 1.89, 2.37, and 4.77

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

#### 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{tsNeq} $$ \hat{t}Neq \\ \mathcal{S}Ne_{T}^{-NS_a}_{\sqrt{NF+N}sigma_s^2} \\ = \frac{s^2}{\sqrt{NF-S_a}}^{-2} \\ = \frac{s^2}{\sqrt{F-S_a}}^{-2}. \end{aligned}
```

#### \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 -detsnminarea are removed from the analysis in both  $R_c$  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,  $SN_T$  can be written as,

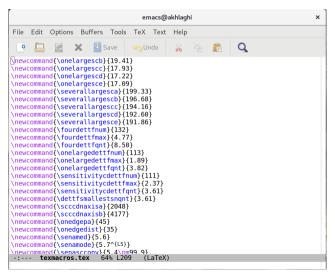
$$S/N_T = \frac{NF - NS_a}{\sqrt{NF + N\sigma_S^2}} = \frac{\sqrt{N}(F - S_a)}{\sqrt{F + \sigma_S^2}}.$$
 (3)

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 SNT from the objects in R<sub>s</sub> 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 S/N of false detections in real, reduced/co-added images. A comparison of scales on the S/N 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 S/N of 1.89, 2.37, and 4.77.

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

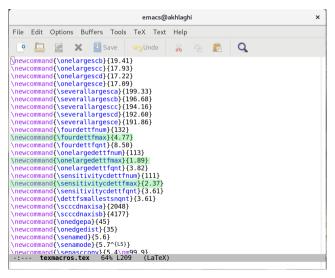
### Analysis step results/values concatenated into a single file.

All LATEX macros come from a single file.



### Analysis 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"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
```

#### Analysis results stored as LATEX macros

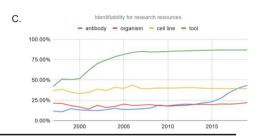
The analysis scripts write/update the LaTEX macro values automatically.

```
# 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 $\pm$ 2020 (DOI:10.1101/2020.01.15.908111)

#### **ORIGINAL PLOT**

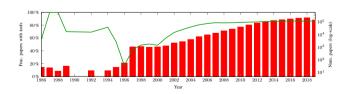
The Green plot shows the fraction of papers mentioning software tools from 1997 to 2019.



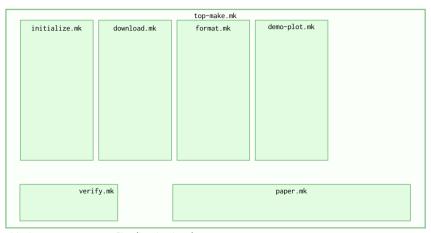
#### **OUR enhanced REPLICATION**

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

Red histogram is the number of papers studied in each year



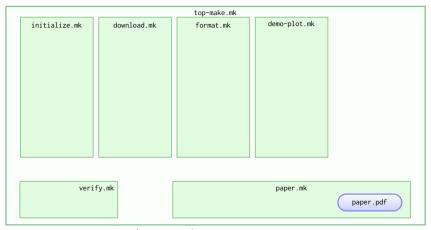
### Makefiles (.mk) keep contextually separate parts of the project, all imported into top-make.mk



Green boxes with sharp corners: source files (hand written).

Blue boxes with rounded corners: built files (automatically generated),

#### The ultimate purpose of the project is to produce a paper/report (in PDF).



Green boxes with sharp corners: source files (hand written).

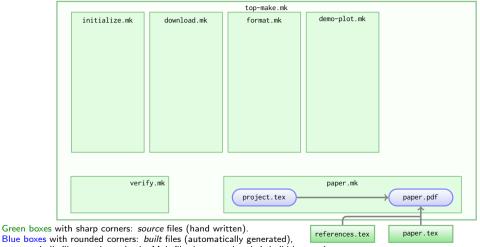
Blue boxes with rounded corners: built files (automatically generated),

### The narrative description, typography and references are in paper.tex & references.tex.

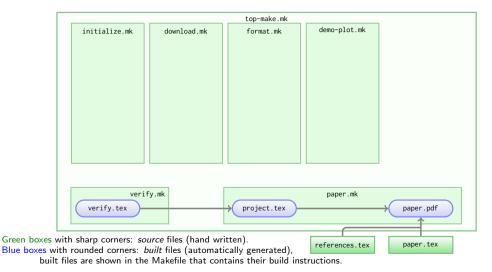


4□ > 4□ > 4□ > 4□ > 4□ > □

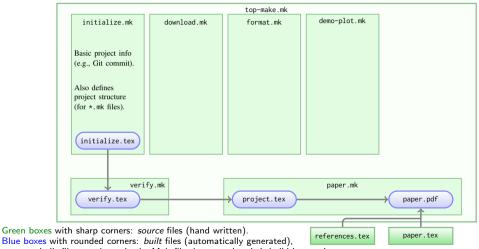
### Analysis outputs (blended into the PDF as LATEX macros) come from project.tex.



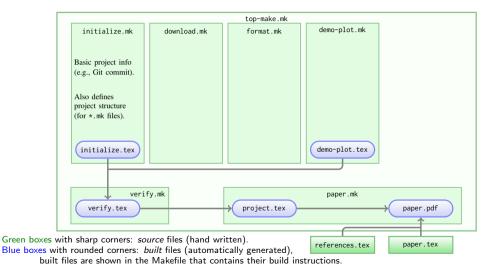
### But analysis outputs must first be *verified* (with checksums) before entering the report/paper.



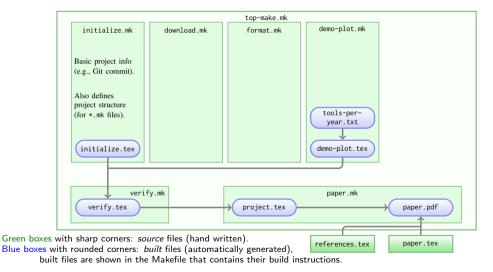
#### Basic project info comes from initialize.tex.



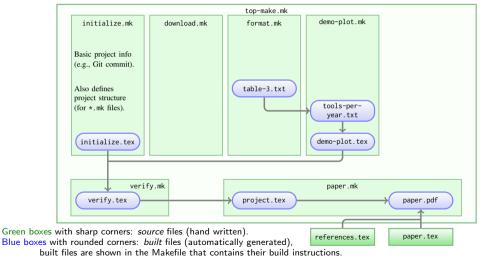
#### The paper includes some information about the plot.



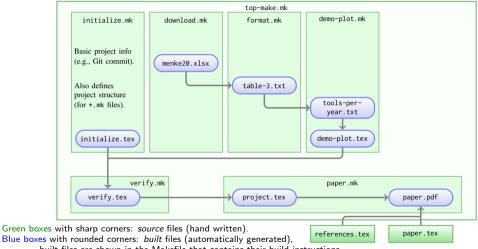
#### The final plotted data are calculated and stored in tools-per-year.txt.



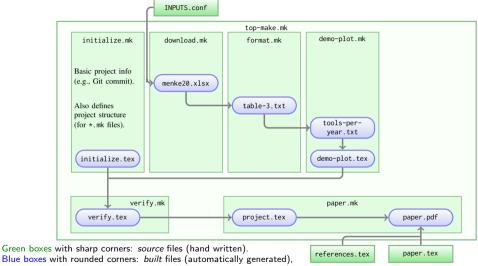
### The plot's calculation is done on a formatted sub-set of the raw input data.



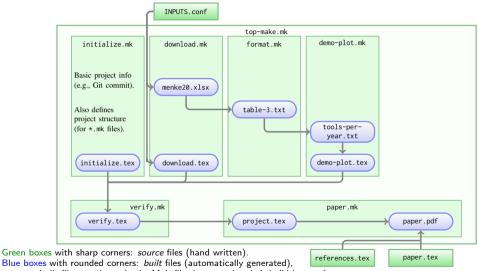
#### The raw data that were downloaded are stored in XLSX format.



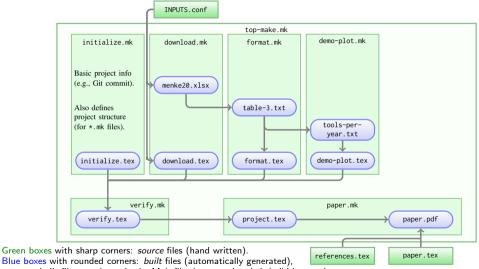
#### The download URL and a checksum to validate the raw inputs, are stored in INPUTS.conf.



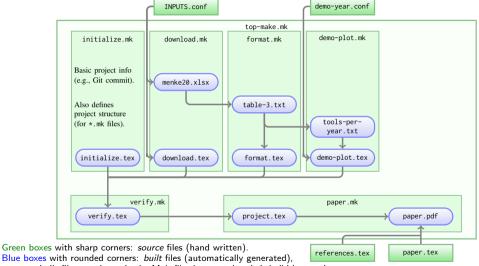
### We also need to report the URL in the paper...



### Some general info about the full dataset may also be reported.

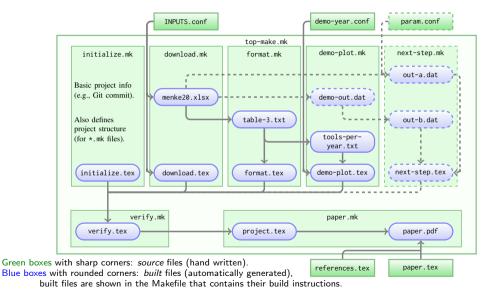


### We report the number of papers studied in a special year, desired year is stored in .conf file.



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)



# The whole project is a directed graph (codifying the data's lineage).

► Every file (source or built) is a node in the graph (connected to others). (The links/connections/dependencies between the nodes, defined by the Makefiles: \*.mk)

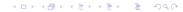
- ► There are two types of nodes/files:
  - Source nodes (\*.conf and paper.tex) only have an outward link.
  - ▶ Built files always have inward and (except paper.pdf) outward link(s).

► All built files ultimately originate from a \*.conf file, ... and ultimately conclude in paper.pdf.

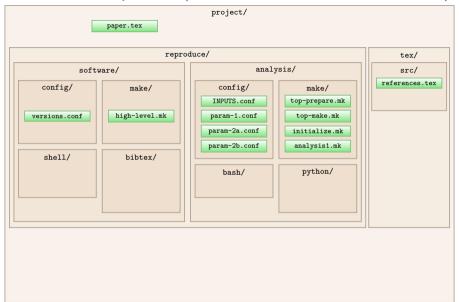
#### Benefits of using Make

- Make can parallelize the analysis: Make knows which steps are indepenent and will run them at the same time.
- ► Make can automatically detect a change and will re-do *only* the affected steps. (for example to change the multiple of sigma in a configuration file to see its effect)
- ► Easily backtrace any step (without needing to remember!). (very useful to find problems/improvements)
- ▶ The above will speed up your work, and encourage experimentation on methods.
- ▶ Make is available on any system: many people are already familiar with it.
- And again: its all in plain text!

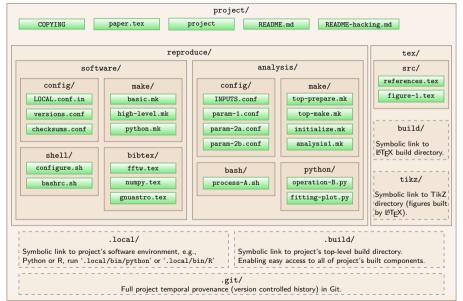
  (doesn't take much space, easy to read, distribute, parse automatically, or archive)
- ▶ Recall that the project's software installation was also managed in Make.



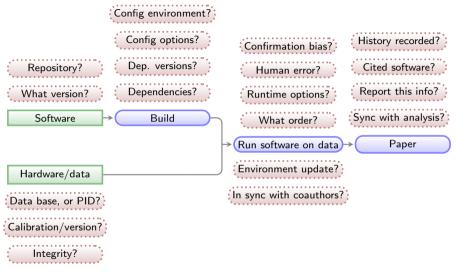
#### Files organized in directories by context (here are some of the files discussed before)



### Files organized in directories by context (now with other project files and symbolic links)



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



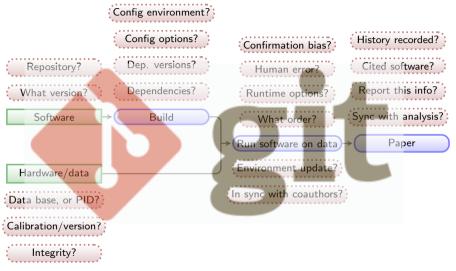
Green boxes with sharp corners: *source*/input components/files.

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.

Blue boxes with rounded corners: *built* components.

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



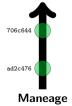
► The project (answers to questions above) will evolve.

► The project (answers to questions above) will evolve.





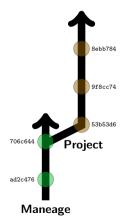
Each point of project's history is recorded with Git.



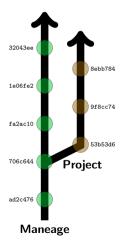
706c644 Project

Maneage

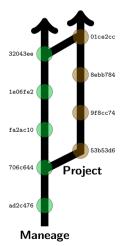
- Each point of project's history is recorded with Git.
- New project: a branch from the template. Every commit contains the following:
  - Instructions to download, verify and build software.
  - Instructions to download and verify input data.
  - Instructions to run software on data (do the analysis).
  - ► Narrative description of project's purpose/context.



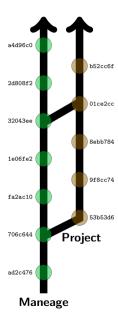
- Each point of project's history is recorded with Git.
- New project: a branch from the template. Every commit contains the following:
  - Instructions to download, verify and build software.
  - Instructions to download and verify input data.
  - Instructions to run software on data (do the analysis).
  - Narrative description of project's purpose/context.
- Research progresses in the project branch.



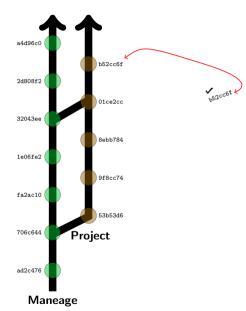
- Each point of project's history is recorded with Git.
- New project: a branch from the template. Every commit contains the following:
  - Instructions to download, verify and build software.
  - Instructions to download and verify input data.
  - Instructions to run software on data (do the analysis).
  - ► Narrative description of project's purpose/context.
- Research progresses in the project branch.
- Template will evolve (improved infrastructure).



- Each point of project's history is recorded with Git.
- New project: a branch from the template. 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.

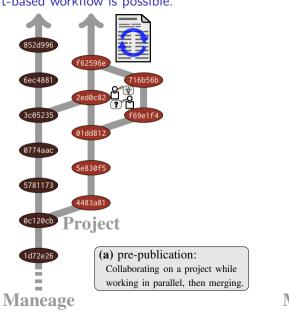


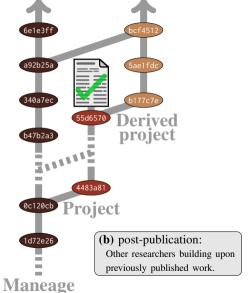
- ► Each point of project's history is recorded with Git.
- New project: a branch from the template. Every commit contains the following:
  - Instructions to download, verify and build software.
  - Instructions to download and verify input data.
  - Instructions to run software on data (do the analysis).
  - ► 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).



- Each point of project's history is recorded with Git.
- New project: a branch from the template. 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 commit ID identifies the peer-reviewed version of record (apart from journal typesetting, proofreading corrections).

### Any Git-based workflow is possible.





#### Publication of the project

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

- Makefiles.
- LATEX 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  $\sim 100$  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:2112.14174).
- Zenodo: Along with all the input datasets (many Gigabytes) and software (for example zenodo.6794222) and given a unique DOI.
  - ... and put links to data in paper! See the caption of Fig. 3 in Borkowska & Roukema (2022).
- Software Heritage: to archive the full version-controlled history of the project. (for example swh:1:dir:33fea87068c1612daf011f161b97787b9a0df39fk)
  - ... and put links to exact parts of the code! See caption of Listing 1 in the Maneage paper.



#### Project source and its execution

Programs [here: Scientific projects] must be written for people to read...

...and only *incidentally* for machines to *execute*.

Harold Abelson, Structure and Interpretation of Computer Programs

### General outline of using this system (e.g. arXiv:2112.14174)

```
$ git clone https://codeberg.org/boud/gevcurvtest
                                                    # Import the project.
$ cd gevcurvtest # Enter the directory.
$ ./project --help # RTFM. Skip if brave enough.
$ ./project configure
                         # You will specify the build directory on your system,
                         # and it will build all software (\sim2-3 hours on 4 cores).
$ ./project make
                             # Does all the analysis and makes final PDF.
```

#### Practical experience: peer-reviewed papers

- Roukema (2021), PeerJ, 9:e11856, "Anti-clustering in the national SARS-CoV-2 daily infection counts"
  - https://arXiv.org/abs/2007.11779
  - ▶ frozen record: https://zenodo.org/record/4765705
  - ▶ live git: https://codeberg.org/boud/subpoisson
  - archived git: swh:1:rev:72242ca8eade9659031ea00394a30e0cc5cc1c37
- Peper & Roukema (2021), MNRAS, 505, 1223, "The role of the elaphrocentre in void galaxy formation"
  - https://arXiv.org/abs/2010.03742
  - frozen record: https://zenodo.org/record/4699702
  - ▶ live git: https://codeberg.org/boud/elaphrocentre
  - archived git: swh:1:rev:a029edd32d5cd41dbdac145189d9b1a08421114e
- Borkowska & Roukema (2022), CQG, in press, "Does relativistic cosmology software handle emergent volume evolution?"
  - https://arXiv.org/abs/2112.14174
  - frozen record: https://doi.org/10.5281/zenodo.5806027
  - ▶ live git: https://codeberg.org/boud/gevcurvtest
  - archived git swh:1:rev:d9b47736f81aff9bb8f2f359d9f0331aa923f38d
- Was it a lot of work? Yes.
- ▶ Did we feed our variations and fixes upstream to Maneage? Some, yes.
- ▶ Overall feeling: was it worth it? Yes.



#### How can you contribute?

- Try to reproduce Borkowska & Roukema (2022), e.g. from SWH: swh:1:rev:d9b47736f81aff9bb8f2f359d9f0331aa923f38d (0.5 Mb; fits on a floppy disk)
  - Did it fully configure, run and verify? If not, then help with a task or a bug:
- ► Tasks: https://savannah.nongnu.org/tasks/?group=reproduce, e.g.
  - ▶ #15739 debian-verified sources (stable || testing)
  - ▶ #15363 file dates after git checkout
  - ▶ #15997 safe-rm
  - ▶ #15390 glibc within Maneage
- Bugs: https://savannah.nongnu.org/bugs/?group=reproduce, e.g.
  - ▶ #62879 Maneage handling of /dev/shm and required RAM
- Core Maneage: https://git.maneage.org/project.git
- ► Merge requests: any git server of your choice
- Description of implementation, how-to guide, recommendations: https://codeberg.org/boud/maneage\_dev/src/branch/maneage/README-hacking.md
- Interactive discussion: irc at https://libera.chat: channel ##maneage



#### Conclusion

Maneage is a customisable template that does the following — all in 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.
- Only those components that need to be re-done are re-done.
- Using LATEX macros, the paper's figures, tables and numbers will be Automatically updated.
- ▶ The whole project is under version control (Git) encouraging tests and experimentation.
- The Git commit hash of the project source is printed in the paper and on output data products.

this pdf – full of clickable links: https://cosmo.torun.pl/~boud/Roukema20220916TYG.pdf