BIG Data, BIG responsibility

Maneage: *Man*aging data lin*eage* for long-term and archivable reproducibility (Published in CiSE 23 (3), pp 82-91: DOI:10.1109/MCSE.2021.3072860, arXiv:2006.03018)

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Software Sustainability SIG, eScience Center, Netherlands (remote) 28th of November 2024

Most recent slides available in link below (this PDF is built from Git commit 125dd08): https://maneage.org/pdf/slides-intro.pdf









RESEARCH DATA ALLIANCE EUROPE



Let's start with this nice image of the Wirlpool galaxy (M51): https://i.redd.it/jfqgpqgOhfk11.jpg



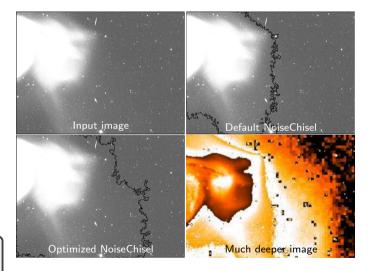
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Now, let's assume you want to study M51's outer structure, but you'll have to detect it first.

Example: Using a single exposure SDSS image with NoiseChisel (a program that is part of 'GNU Astronomy Utilities').

- When optimized, outskirts detected down to S/N =1/4, or 28.3 mag/arcsec². By default, it only reaches S/N > 1/2.
- Akhlaghi 2019 (arXiv:1909.11230) describes optimized result:
 - Run-time options/configuration.
 - Steps before/after NoiseChisel.
- Deep/orange image from Watkins+2015 (arXiv:1501.04599) shown for reference.
- Therefore:
 - Default settings not enough.
 - Final number not just from NoiseChisel (more software involved).

Simply reporting in your paper that "we used NoiseChise!" is not enough to reproduce, understand, or verify your result.



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Reproducibility crisis in the sciences/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).

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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).

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Schroedinger'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).



Original image from https://www.redbubble.com

This problem isn't just limited to astronomy

Repeatability of published microarray gene expression analyses

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

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

Chang&Li2015 were are able to replicate less than half of 67 papers in well-regarded journals. Even *with help* from the authors. They "assert that economics research is usually not replicable". DOI:10.17016/FEDS.2015.083

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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, DOI:10.1038/533452a)

1576 researchers participated in a survey by Nature, 90% believed in a crisis!

Status	% agreed
Yes, a significant crisis	52
Yes, a slight crisis	38
Don't know	7
No, there is no crisis	3

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Full PDF available at https://www.nature.com/articles/533452a.pdf

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

DITORS: Lorena A. Barba, laberbaggeu edu Sandra Gaalor, anorira malomierd ar

SPECIAL TRACK: REPRODUCIBLE RESEARCH

Toward Long-Term and Archivable Reproducibility

Muhammad Abhagh [®], Institute de Astrofacio de Contrais, La Loguno, Tenerifo, 2000, Spain Rad Istate Faiter [®], Universidad et la Lagana, La Logana, Parente, 2020, Spain Dondrafy P. Robana, P. Kolsonio, Capernio Muhamistry, Toras R. 200, Ruind Muhammadreza hielta [®], Mois Acqueros Muhammadreza hielta [®], Mois Acqueros Acqueros Anna A Dand Valle Glaada, Paris Glaevanter, Paris 7004, France Dande Vallenza Baneta R. Muhammadineza de La Mijol, Loganio 2000, Spain

Analysis pipelines commonly use high-level technologies that are popular when created. but are unlikely to be readable, executable, or sustainable in the long term. A set of criteria is introduced to address this problem: completeness (no execution requirement beyond a minimal Unix-like operating system, no administrator privileges, no network connection, and storage primarily in plain text); modular design; minimal complexity; scalability; verifiable inputs and outputs: version control: linking analysis with narrative: and free and open-source software. As a proof of concept, we introduce "Maneage" (managing data lineage), enabling cheap archiving, provenance extraction, and peer verification that has been tested in several research publications. We show that longevity is a realistic requirement that does not sacrifice immediate or short-term reproducibility. The caveats (with proposed solutions) are then discussed and we conclude with the benefits for the various stakeholders. This article is itself a Maneage'd project (project commit 313db0b). Appendices-Two comprehensive appendices that review the longevity of existing solutions are available as supplementary "Web extras," which are available in the IEEE Computer Society Digital Library at http://doi.ieeecomputersociety.org/10.1109/ MCSE 2021.3072860. Reproducibility-All products gyallable in zerodo, 4913277, the Git history of this paper's source is at git maneage.org/paper-concept.git, which is also archived in Software Heritage autotyle-23fee87068c3612def011f16156769778750e0df10f Clicking on the SWHIDs in the digital format will provide more "context" for same content.

Reproducible research has been discussed in the sciences for at least 30 years.¹² Many "solutions") have been proposed, which mostly rely on the common technology of the day, starting

This work is licensed under a Creative Commons Attribution 4.0 License. For more information, see https://oreativecommore.org/ficenses/by/4.0/ Digital Object Identifier 10.1103/MCSE.2021.3072860 Date of publication 13 April 2021; date of ourrent vension 15 June 2021. with Make and Matlab libraries in the 1990s, Java in the 2000s, and mostly shifting to Python during the past decade.

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 could of staying up to date within this rapidly exciving 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 technology of their tools because it determines their results.

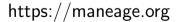
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Published by the IEEE Computer Society N

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Maneage is a framework for having full control over a project's data lineage (thus producing a reproducible result), Maneage is a recipient of the RDA Europe Adoption grant and was featured in a Nature Astronomy "News and Views" article (Kuttel 2021, free-to-read link). To learn more about its founding criteria and a basic introduction, see Akhitaghi et al. (2021), published in CISE (Gold Open Access), also available in arXiv:2006.03018 (with extended appendix in one PDF). You can also watch the short talk linked below or see this published FDA Adoption story (a short PDF).



Recognition 1: RDA adoption grant (2019) to IAC for Maneage



For Maneage, the IAC is selected as a Top European organization funded to adopt RDA Recommendations and Outputs.

Research Data Alliance was launched by the European Commission, NSF, National Institute of Standards and Technology, and the Australian Government's Department of Innovation.

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RDA Outputs are the technical and social infrastructure solutions developed by RDA Working Groups or Interest Groups that enable data sharing, exchange, and interoperability. Recognition 2: "News and Views" in Nature Astronomy (2021NatAs...5..986K)



REPRODUCIBILITY

No expiration date

The short lifespan of software puts a time limit on the reproducibility of computational research. To extend software longevity, guidelines and tools to preserve scientific workflows and analysis are helpful, but the challenge is to get researchers to use them.

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Michelle M. Kuttel

Free-to-read link: https://rdcu.be/cmYVx DOI: 10.1038/s41550-021-01402-3

Definitions & Clarification

Replicability (hardware/statistical)

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

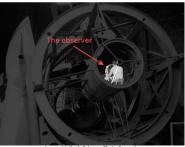


http://slittlefair.staff.shef.ac.uk

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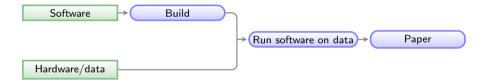
Reproducibility (Software/Deterministic)

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

DISCUSSED HERE.



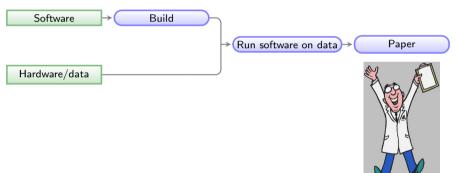
Wikimedia Commons



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.

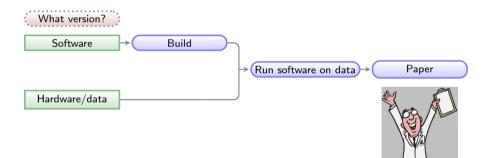


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https://heywhatwhatdidyousay.wordpress.com



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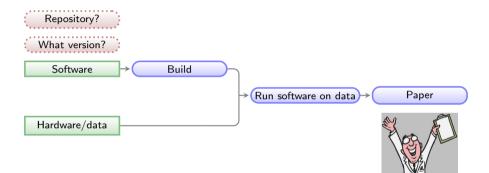
Different package managers have different versions of software (repology.org, 2021/12/02)

GNU Astrono	omy l	Jtilities (Gnuastro	b)
Packaging statu	s		
Debian 9			
Debian 10			
Debian 11			
Debian 12			
Debian Unstable			
Deepin			
Devuan 2.0			
Devuan 3.0			
Devuan 4.0			
Devuan Unstable			
DPorts			
FreeBSD Ports			
Gentoo			
GNU Guix		PureOS Amber	
Kali Linux Rolling		PureOS landing	
LiGurOS stable		Raspbian Oldstable	0.8
LiGurOS develop		Raspbian Stable	0.14
OpenBSD Ports		Raspbian Testing	0.16.1
openSUSE Leap 15.1		RPM Sphere	0.16.1
openSUSE Leap 15.2		Trisquel 9.0	0.5
openSUSE Leap 15.3		Trisquel 10.0	0.11
openSUSE Tumbleweed		Ubuntu 18.04	0.5
enSUSE Science Tumbleweed		Ubuntu 20.04	0.11
Pardus 17		Ubuntu 20.10	0.12
Pardus 19		Ubuntu 21.04	0.14
Pardus 21		Ubuntu 21.10	
Parrot		Ubuntu 22.04	0.14
PLD Linux	0.15	Ubuntu 22.04 Proposed	0.16.1

Astropy ekaning status

Packaging st	tatus
Debian 10	
Debian 11	
Debian 12	
Debian Unstable	
Debian Experimental	
Deepin	
Devuan 3.0	
Devuan 4.0	
Devuan Unstable	
Kali Linux Rolling	
Pardus 19	
Pardus 21	
Parrot	
PureOS Amber	
PureOS landing	
Raspbian Oldstable	
Raspbian Stable	
Raspbian Testing	
Trisquel 9.0	
Trisquel 10.0	
Ubuntu 18.04	
Ubuntu 20.04	
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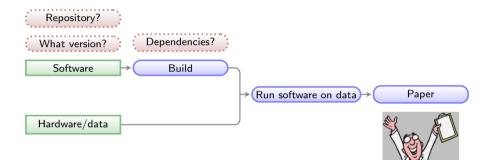


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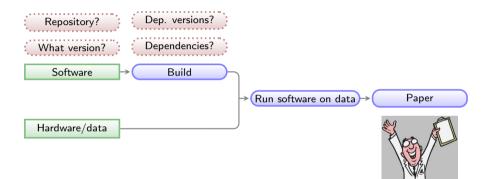
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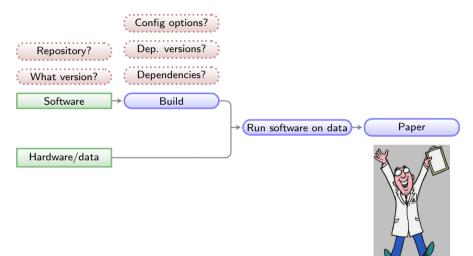


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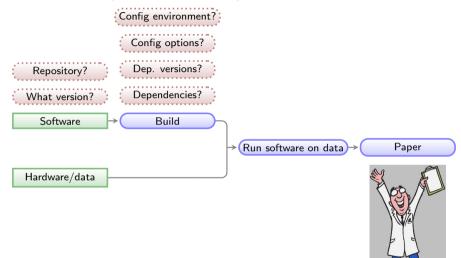
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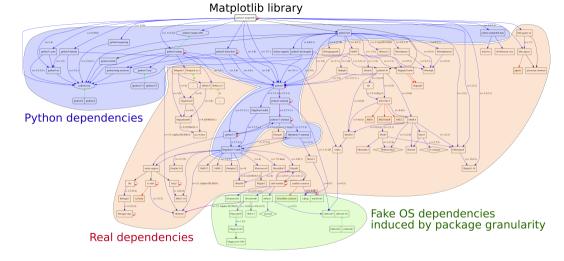
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Example: Matplotlib (a Python visualization library) build dependencies

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

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From "Attributing and Referencing (Research) Software: Best Practices and Outlook from Inria" (Alliez et al. 2020, CiSE, DOI:10.1109/MCSE.2019.2949413).

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



Tracker - Changelog - Bugs - packages.d.o - Source

Package(s):	astropy	Suite:	sid	~	Go
Compact mode	Co-maintainers				

Architecture	Version	Status	For	Buildd	State	Section	Logs	Actions
🗐 all	5.0.1	Installed	9d 9h 36m	x86-conova-01		misc	old all (1)	giveback
amd64	5.0-1	Installed	9d 9h 37m	x86-csail-01		misc	old all (1)	giveback
arm64	5.0-1	Installed	9d 9h 8m	arm-ubc-02		misc	old all (1)	giveback
🖩 armel	5.0-1	Installed	9d 6h 52m	antheil		misc	old all (1)	giveback
armhf	5.0-1	Installed	9d 8h 8m	hoiby		misc	old all (1)	giveback
🖬 i386	5.0.1	Installed	9d 9h 57m	x86-grnet-01		misc	old all (1)	giveback
🖬 mips64el 🕴	5.0-1	Build-Attempted	8d 18h 46m	mipsel-osuosl-04	out-of-date	misc	old all (3)	giveback
i mipsel	5.0-1	Installed	9d 9h 37m	mipsel-manda-05		misc	old all (1)	giveback
m ppc64el	5.0.1	Installed	9d 9h 37m	ppc64el-unicamp-01		misc	old all (1)	giveback
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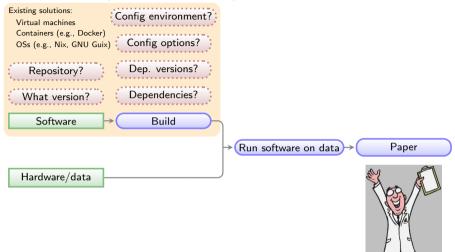
Astropy depends on Matplotlib



Debian Package Auto-Building

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Architecture	Version	Status	For	Buildd	State	Section	Logs	Actions
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amd64	$0.16.1 \cdot 1$	Installed	14d 6h 8m	x86-csail-01		misc	old all (1)	giveback
📾 arm64	0.16.1-1	Installed	14d 5h 56m	arm-ubc-03		misc	old all (1)	giveback
📾 armel	0.16.1-1	Installed	14d 5h 26m	henze		misc	old all (1)	giveback
📾 armhf	0.16.1 - 1	Installed	14d 5h 56m	arm-conova-02		misc	old all (1)	giveback
🖼 i386	0.16.1-1	Installed	14d 5h 56m	x86-ubc-01		misc	old all (1)	giveback
mips64el	0.16.1-1	Installed	14d 5h 26m	mipsel-aql-03		misc	old all (1)	giveback
i mipsel	0.16.1-1	Installed	11d 15h 26m	mipsel-osuosl-04		misc	old all (1)	giveback
ppc64el	0.16.1-1	Installed	14d 6h 8m	ppc64el-unicamp-01		misc	old all (1)	giveback
s390x	0.16.1-1	Installed	14d 6h 7m	zani		misc	old all (1)	giveback
🖬 alpha	0.16.1-1	Installed	7d 6h 11m	imago		misc	old all (2)	giveback
el hppa	0.16.1-1	Installed	14d 5h 31m	c8000b		misc	old all (1)	giveback
hurd-i386	0.16.1-1	Installed	12d 19h 21m	ironforge		misc	old all (1)	giveback
ia64	0.16.1-1	Installed	14d 5h 41m	lifshitz2		misc	old all (1)	giveback
kfreebsd-amd64	0.16.1-1	Installed	13d 22h 31m	kamp		misc	old all (1)	giveback
kfreebsd-i386	0.16.1-1	Installed	11d 11h 31m	kamp		misc	old all (1)	giveback
m68k	0.16.1-1	Installed	14d 4h 21m	vs92		misc	old all (1)	giveback
powerpc	0.16.1-1	Installed	14d 5h 31m	blaauw		misc	old all (1)	giveback
ppc64	0.16.1-1	Installed	14d 6h	blaauw2		misc	old all (1)	giveback
riscv64	0.16.1-1	Installed	14d 5h 30m	rv-osuosl-01		misc	old all (1)	giveback
🔤 sh4	0.16.1-1	Installed	14d 5h	sh4-do-02		misc	old all (1)	giveback
sparc64	0.16.1-1	Installed	14d 5h 10m	nvg5120b		misc	old all (1)	giveback
M x32	0.16.1-1	Installed	14d 6h	x32-do-02		misc	old all (1)	giveback

GNU Astronomy Utilities doesn't.

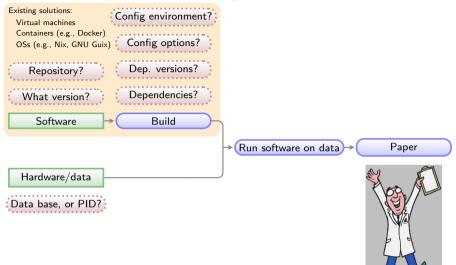


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Red boxes with dashed borders: questions that must be clarified for each phase.

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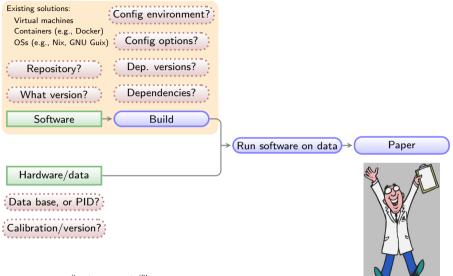
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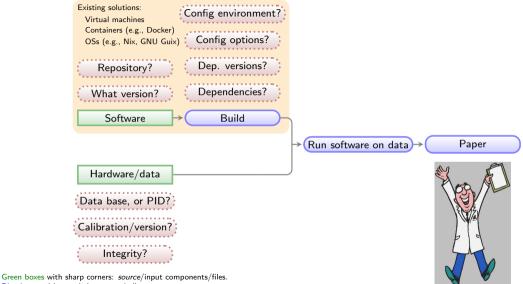
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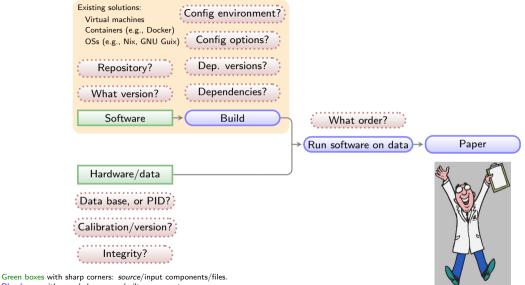
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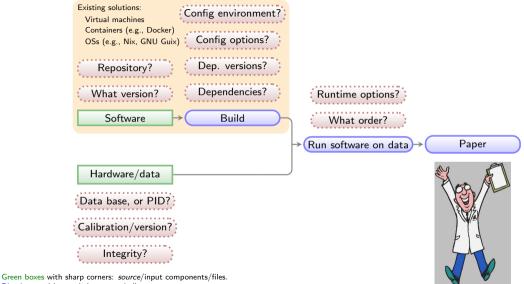


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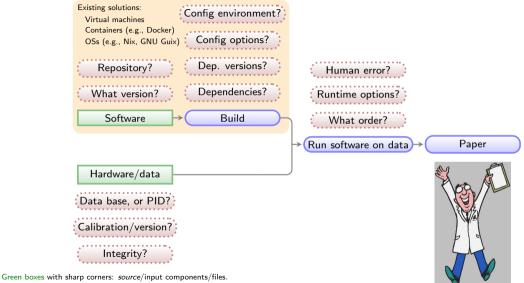


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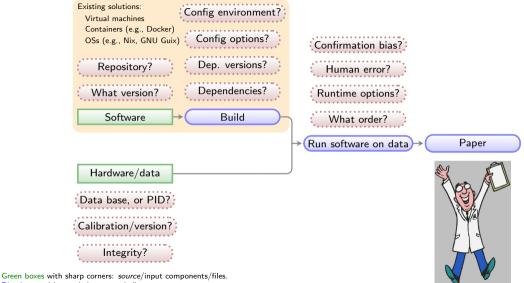
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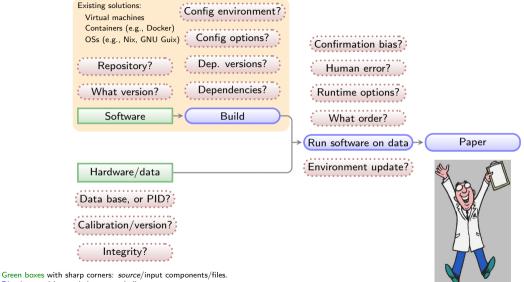
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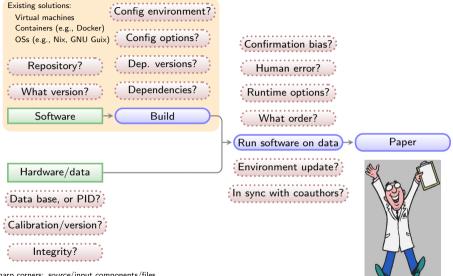
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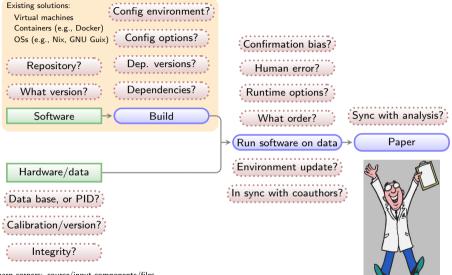


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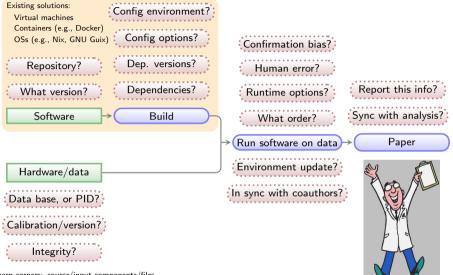


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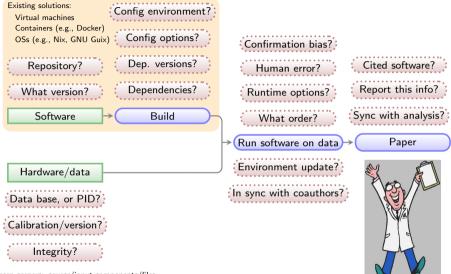


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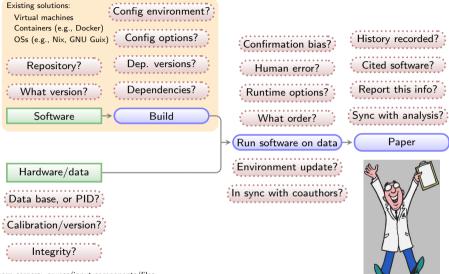
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Di Cosmo & Pellegrini (2019) Encouraging a wider usage of software derived from research

"**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)".

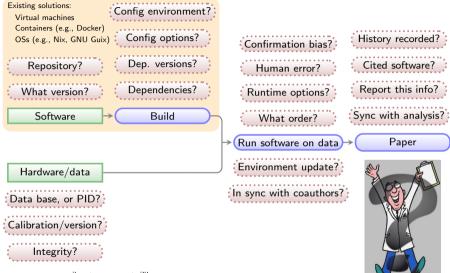


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https://heywhatwhatdidyousay.wordpress.com http://pngimages.net Data analysis [...] is a human behavior. Researchers who hunt hard enough will turn up a result that fits statistical criteria, but their discovery will probably be a false positive.

Five ways to fix statistics (Nature, 551, Nov 2017; DOI:10.1038/d41586-017-07522-z).

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**.

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

Basic/simple principle:

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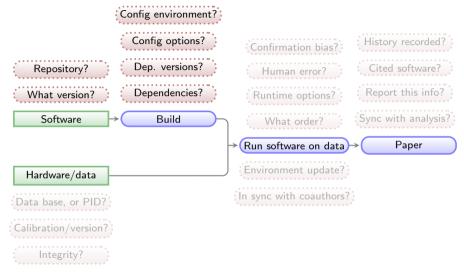
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- Free and open source software: Free software is essential: non-free software is not configurable, not distributable, and dependent on non-free provider (which may discontinue it in N years).



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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).

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Controlled environment and build instructions

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emacs@akhlaghi File Edit Options Buffers Tools Makefile Help 🛄 Save 👆 Undo 📈 p Q # not 'LIBS' # On Nac 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 (XX=clang++:) cd \$(ddir) \ && rn -rf cnake-\$(cnake-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 -lcrvpto -1z" VERBOSE=1 \ && make install \ && cd ... \ && rm -rf cmake-\$(cmake-version) \ A& echo "(Make Sicmake-version)" > 50 \$(ibidir)/ghostscript: \$(tdir)/ghostscript-\$(ghostscript-version).tar.gz \$(call obuild, \$<, obostscript-\$(obostscript-version)) \</pre> && echo "GPL Ghostscript \$(ghostscript-version)" > \$0 G(ibidir)/gnuastro: \$(tdir)/gnuastro-\$(gnuastro-version).tar.lz \ \$(ibidir)/ghostscript \ \$(ibidir)(libinen) \$(ibidir)/libtiff) \$(ibidir)/libnit2) \$(ibidir)/wcslib \ \$(ibidir)/asl ifen (\$(static build) ves) staticonts="--enable.staticsves --enable.shared=no": \$(call gbuild, \$<, gnuastro-\$(gnuastro-version), static, \</pre> \$\$staticopts. -i\$(punthreads). \ make check -i\$(numthreads)) \ A& on \$(dtexdir)/onuastro_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 gbuild, \$<, ImageMagick-\$(imagemagick-version), static, \</pre> --without-x --disable-openmp, V=1) \ && echo "ImageMagick \$(imagemagick-version)" > \$0

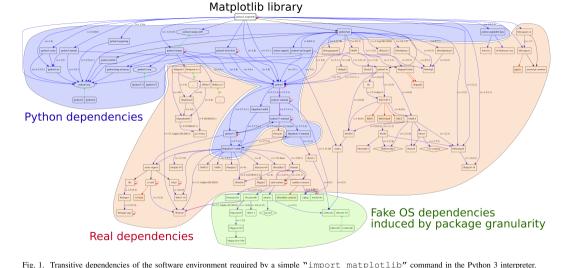
U:--- high-level.mk 67% L584 Git:master (Makefile)

Controlled environment and build instructions

emacs@akhlaghi File Edit Options Buffers Tools Makefile Help 0 Save 🥎 Undo 🐰 include reproduce/software/config/installation/texlive.mk # not 'LIBS' include reproduce/software/config/installation/versions.mk lockdir = \$(BDIR)/locks tdir = \$(BDIR)/software/tarballs ddir = \$(BDIR)/software/build-tmp export CC=clang: \ idir = \$(BDTR)/software/installed export (XX=clang++:) ibdir = \$(BDTR)/software/installed/bin 41 - 5 ildir = \$(BDIR)/software/installed/lib cd \$(ddir) \ dtexdir = \$(shell pwd)/reproduce/software/bibtex itidir = \$(BDIR)/software/installed/version-info/tex && tar xf \$< \ 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. && make install \ all: \$(foreach p, \$(top-level-programs), \$(ibidir)/\$(p)) \ && cd ... \ \$(foreach p. \$(top-level-python), \$(ipydir)/\$(p)) \ \$(itidir)/texlive # Other basic environment settings: We are only including the host # operating system's PATH environment variable (after our own!) for the Ø 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 ifen (\$(static build) ves) 2) Add '--noprofile --norc' to '.SHELLFLAGS' so doesn't load the uper's environment and if ONECHELLY CHELLEL ACC. := --noprofile --norc -ec export CCACHE DISABLE := 1 export PATH := \$(ibdir) export SHELL := \$(ibdir)/bash export CPPELAGS - . 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 := \$(rmath 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 Uters high-level mk 4% 181 Gittmaster (Makefile)

emacs@akhlaghi File Edit Options Buffers Tools Makefile Help 🛄 Save 👆 Undo 📈 p Q # On Nac 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 \ && rn -rf cnake-\$(cnake-version) \ && cd_cmake-\$(cmake-version) \ && ./bootstrap --prefix=\$(idir) --system-curl --system-zlib \ --system-bzip2 --system-liblzma --no-qt-gui \ && make -1\$(numthreads) LIBS="\$\$LIBS -1ssl -lcrvpto -1z" VERBOSE=1 \ && rm -rf cmake-\$(cmake-version) \ A& echo "(Make Sicmake-version)" > 50 \$(ibidir)/ghostscript: \$(tdir)/ghostscript-\$(ghostscript-version).tar.gz \$(call obuild, \$<, obostscript-\$(obostscript-version)) \</pre> && echo "GPL Ghostscript \$(ghostscript-version)" > \$0 [(ibidir)/gnuastro: \$(tdir)/gnuastro-\$(gnuastro-version).tar.lz \ \$(ibidir)/ghostscript \ \$(ibidir)(libinen) \$(ibidir)/libtiff) \$(ibidir)/libnit2) \$(ibidir)/wcslib \ \$(ibidir)/asl staticonts="--enable.staticsves --enable.shared=no": \$(call gbuild, \$<, gnuastro-\$(gnuastro-version), static, \</pre> \$\$staticopts. -i\$(punthreads). \ make check -i\$(numthreads)) \ A& on \$(dtexdir)/onuastro_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 gbuild, \$<, ImageMagick-\$(imagemagick-version), static, \</pre> --without-x --disable-openmp, V=1) \ && echo "ImageMagick \$(imagemagick-version)" > \$0

Utres high-level mk 67% 1584 Gittmaster (Makefile)



Example: Matplotlib (a Python visualization library) build dependencies

From "Attributing and Referencing (Research) Software: Best Practices and Outlook from Inria" (Alliez et al. 2019, hal-02135891)

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

GNU/Linux distribution

\$ ldd .local/bin/astnoisechisel

libgnuastro.so.7 => /PROJECT/libgnuastro.so.7 (0x00007f6745f39000) libgit2.so.26 => /PR0JECT/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 (0x00007f6745d12000) libwcs.so.6 => /PROJECT/libwcs.so.6 (0x00007f6745ba8000) libcfitsio.so.8 => /PR0JECT/libcfitsio.so.8 (0x00007f674588b000) libcurl.so.4 => /PR0JECT/libcurl.so.4 (0x00007f6745811000) $libssl.so.1.1 \Rightarrow /PR0JECT/libssl.so.1.1 (0x00007f6745777000)$ libcrypto.so.1.1 => /PR0JECT/libcrypto.so.1.1 (0x00007f6745491000) libz.so.1 => /PR0JECT/libz.so.1 (0x00007f6745474000) libgsl.so.23 => /PROJECT/libgsl.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) $/lib64/ld - linux - x86 - 64 \cdot so 2 => /usr/lib64/ld - linux - x86 - 64 \cdot so 2$

macOS

\$ 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/liblipme.5.dylib (comp ver 8.0.0, cur ver 8.4.0) /PROJECT/libgit2.26.2.dylib (comp ver 6.0.0, cur ver 12.0.0) /PROJECT/libcifisio.8.dylib (comp ver 6.0.0, cur ver 6.2.0) /PROJECT/libcifisio.8.dylib (comp ver 10.0.0, cur ver 13.47) /PROJECT/libcifisio.8.dylib (comp ver 10.0.0, cur ver 11.0) /PROJECT/libcifisio.8.dylib (comp ver 11.0, cur ver 11.0) /PROJECT/libcifisio.8.dylib (comp ver 11.0, cur ver 11.0) /PROJECT/libcifisio.8.dylib (comp ver 1.1.0, cur ver 11.0) /PROJECT/libcifisio.8.dylib (comp ver 1.0.0, cur ver 12.0.0) /PROJECT/libcifisio.8.dylib (comp ver 25.0.0, cur ver 25.0.0) /PROJECT/libgslcblas.0.dylib (comp ver 1.0.0, cur ver 1.0.0) /usr/lib/jibSystem.B.dylib (comp ver 1.0.0, cur ver 12.5.0.4)

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, LTEX, 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).



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Figure 21 (a) An example image of the Wide-Field Planetary Carners 2, or beaut the Habble Space Telescope from 1903 to 2009. This is one of the sample images freenthe FITS standard webpage, kept as examples for this (the format, (b) Habsgams of pilet solves in (a).

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References

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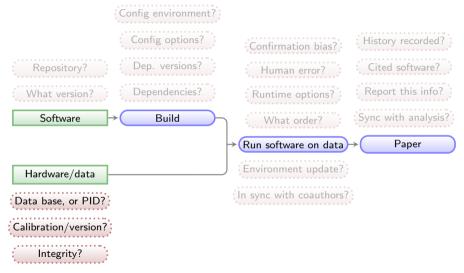
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Green boxes with sharp corners: source/input components/files.

Blue boxes with rounded corners: built components.

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

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Stored information about each input file:

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- Download URL.
- MD5-sum to check integrity.

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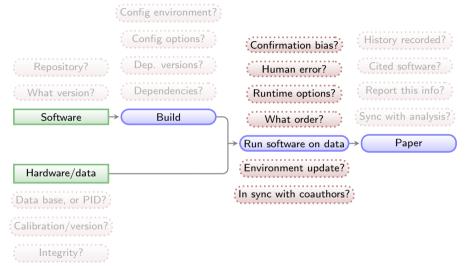
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UVUDFSEGINAGE = seg UVUDFSEGMDS = 29d	<pre>sb3e5311b77512b</pre>				
UVUDFSEGSIZE = 1.3			-		
					- 1
-: INPUTS.mk	All L1 G	it-master (GA	Waskofile)		

General outline of a project (after data collection)



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

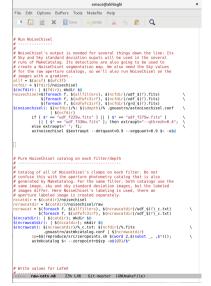
Blue boxes with rounded corners: built components.

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).



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Reproducible science: Maneage is managed through a Makefile

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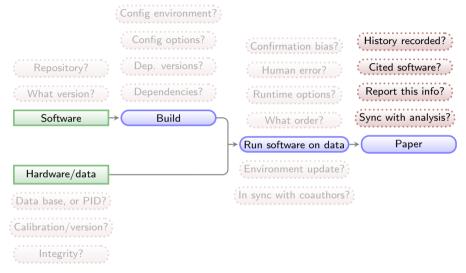
Reproducible science: Maneage is managed through a Makefile

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).

```
\begin{equation}
    \label{tSNeq}
    mathrm{5/N}_r=\frac{NF-NS_a}{\sqrt{NF+N\sigma_s^2}}
=\frac{\sqrt{N}(F-S_a)}{\sqrt{F+\sigma_s^2}}.
\end{equation}
```

\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 {\small S/N}s_T\$ from the objects in \$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 {\small S/N} of false detections in real, reduced/co-added images. A comparison of scales on the {\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 false detections respectively has an {\small S/N} of \$\conductfmax\$, \$\sensitivitycdettfmax\$, \$\]

smaller than --detsiminarea are removed from the analysis in both R_a 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, SNr 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 SN₇ from the objects in R_i 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-

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Analysis step results/values concatenated into a single file.

All LATEX macros come from a single file.

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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 ]: then
                         obase=four:
    elif [ $2 = sensitivity3 ]; then obase=sensitivityc;
    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 '/guantile 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 sobase"dettfnum" sdettfnum
    addtexmacro $obase"dettfmax" $dettfmax
    addtexmacro $obase"dettfont" $dettfont
    # Find the smallest S/N quantile:
    sqnt=$(echo " " | awk '{if('$dettfqnt'<'$sqnt') print '$dettfqnt'}')</pre>
for base in 4 onelarge sensitivity3
do dettfhist stexdir/dettf/ sbase: done
addtexmacro dettfsmallestsngnt $sgnt
```

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Analysis results stored as LATEX macros

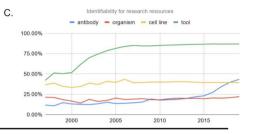
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                                       obase=$2;
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    if [ $2 == onelarge ]: then ind=" 7": else ind=" 12": fi
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for base in 4 onelarge sensitivity3
do dettfhist stexdir/dettf/ sbase: done
addtexmacro dettfsmallestsngnt $sgnt
```

Let's look at the data lineage to replicate Figure 1C (green/tool) of Menke+2020 (DOI:10.1101/2020.01.15.908111)

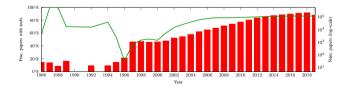
ORIGINAL PLOT

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

top-make.mk										
initialize.mk	download.mk	format.mk	demo-plot.mk							
verif	ŷ.mk	paper.mk								

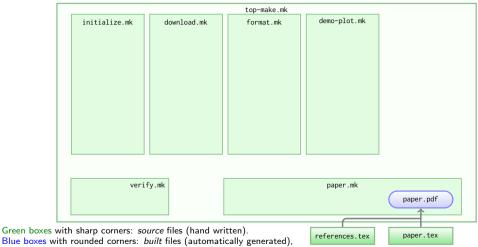
Green boxes with sharp corners: *source* files (hand written). Blue boxes with rounded corners: *built* files (automatically generated), built files are shown in the Makefile that contains their build instructions.

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

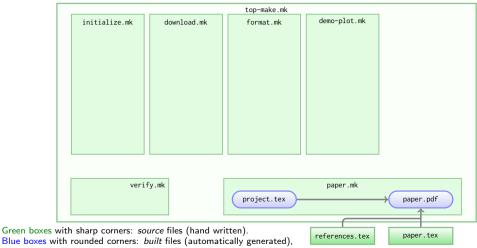
top-make.mk										
initialize.mk	download.mk	format.mk	demo-plot.mk							
veri	fy.mk		paper.mk	paper.pdf						

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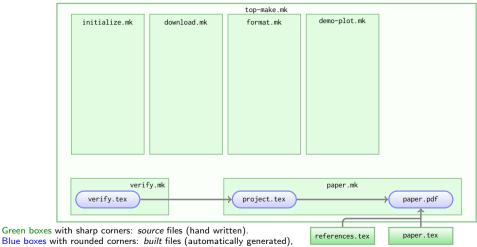
The narrative description, typography and references are in paper.tex & references.tex.



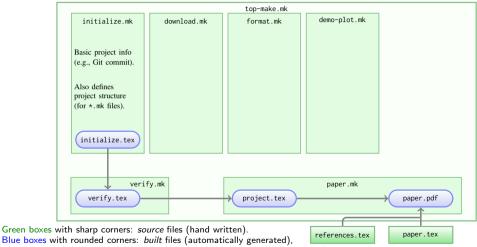
Analysis outputs (blended into the PDF as LATEX macros) come from project.tex.



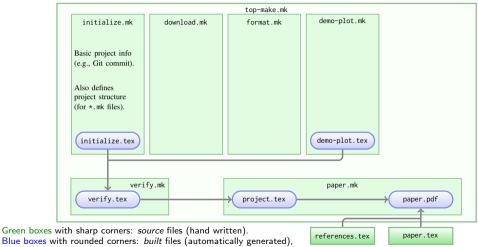
But analysis outputs must first be verified (with checksums) before entering the report/paper.



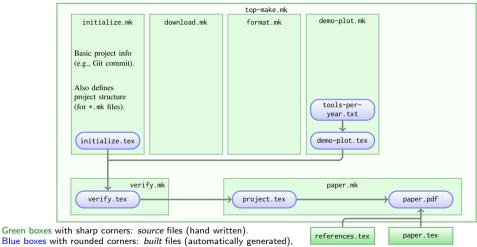
Basic project info comes from initialize.tex.



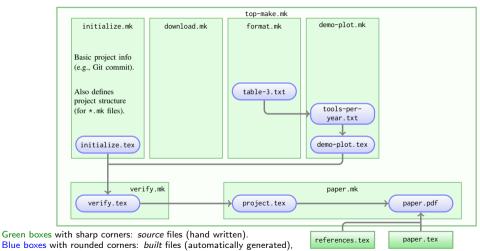
The paper includes some information about the plot.



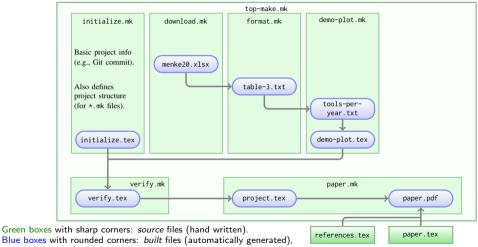
The final plotted data are calculated and stored in tools-per-year.txt.



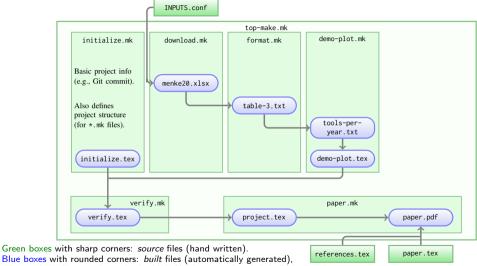
The plot's calculation is done on a formatted sub-set of the raw input data.



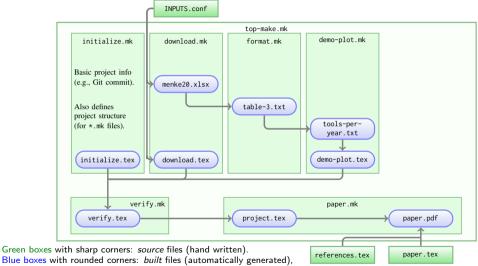
The raw data that were downloaded are stored in XLSX format.



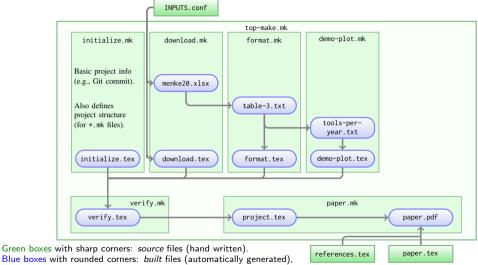
The download URL and a checksum to validate the raw inputs, are stored in INPUTS.conf.



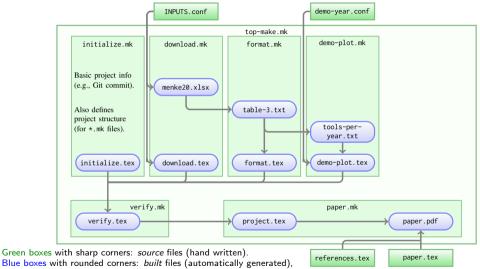
We also need to report the URL in the paper...



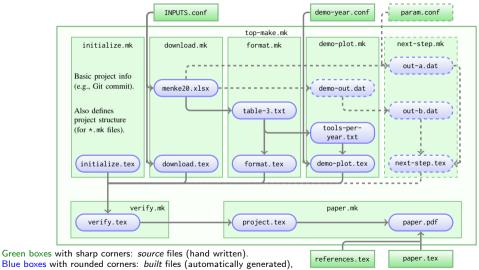
Some general info about the full dataset may also be reported.



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



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)

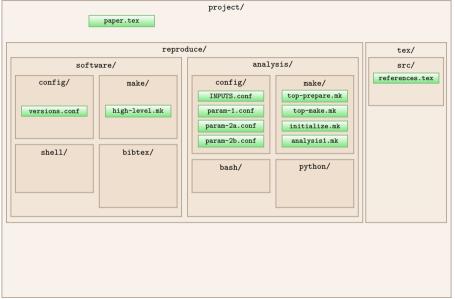
- There are two types of nodes/files:
 - Source nodes (*.conf and paper.tex) only have an outward link.
 - Built files always have inward and (except paper.pdf) outward link(s).

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

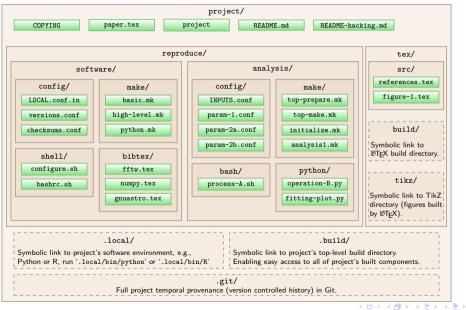
Benefits of using Make

- Make can parallelize the analysis: Make knows which steps are independent 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)

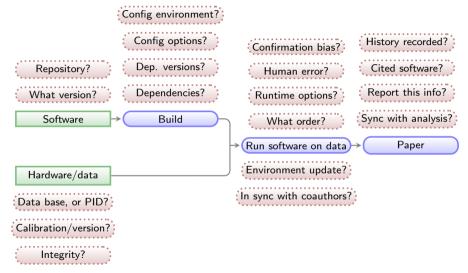


Files organized in directories by context (now with other project files and symbolic links)



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



A D > A B > A B > A B >

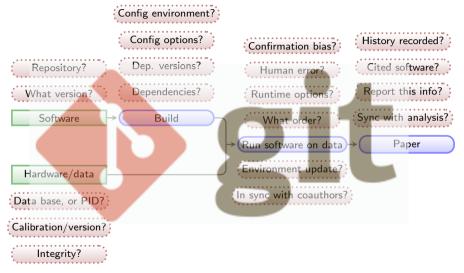
э.

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).



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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. New projects branch from Maneage

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



New projects branch from Maneage

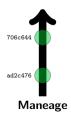
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Today

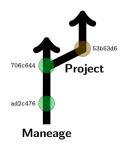
New projects branch from Maneage

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



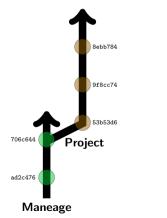
- Each point of project's history is recorded with Git.
- New project: a branch from the template. Recall that every commit contains the following:
 - Instructions to download, verify and build software.
 - Instructions to download and verify input data.
 - Instructions to run software on data (do the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

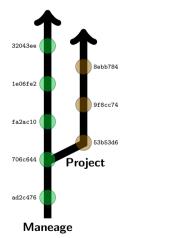
Narrative description of project's purpose/context.



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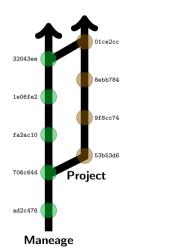
- Narrative description of project's purpose/context.
- Research progresses in the project branch.



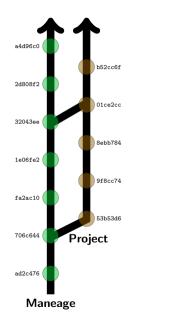


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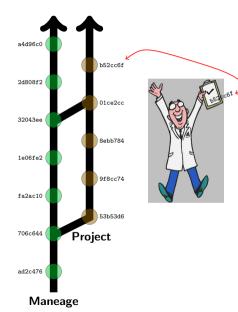
- Narrative description of project's purpose/context.
- Research progresses in the project branch.
- Template will evolve (improved infrastructure).



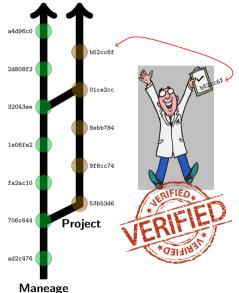
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- The template and project will evolve.
- During research this encourages creative tests (previous research states can easily be retrieved).
- Coauthors can work on same project in parallel (separate project branches).



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"Verified" image from vectorstock.com

Two recent examples (publishing Git checksum in abstract)

The Realm of the Low-Surface-Brightness Universe Proceedings IAU Symposium No. 355, 2019 D. Vallis-Gabuad, I. Trajillo & S. Okamoto, eds.

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Carving out the low surface brightness universe with NoiseChisel

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²Facultad de Física, Universidad de La Laguna, Avda. Astrofísico Fco. Sánchez s/n, 38200 La Laguna, Tenerife, Spain.

Abstract. Note:Cheft is a program to detext very for signal-noise rate (SUN) futures with minimal sampling on their marginglogy. The minimal rate of the signal strategies of the signal of the signal strategies of the signal strategies of the signal strategies of the signal Over the last two shalls release of Gramates, NoteCheff has a rightlendly improved determing removing the signal strategies of the signal strategies of the signal strategies of the line is signal strategies. The signal strategies are compared by the signal line is not program called Signates. Another may change in the final greetly strategies of the determinant strategies of the signal strategies of the signal strategies of the two therefore, here example. Marcheff at all not strets the outer specific strategies of Mitcheff at all strategies of the determinant strategies of the signal strategies of the signal strategies of the signal strategies of the strategies of the signal strategies of the signal strategies of the signal strategies of the signal strategies of the strategies of the signal strategies of the signal strategies of the signal strategies of the strategies of the signal s

Keywords. galaxies: halos, galaxies: photometry, galaxies: structure, methods: data analysis, methods: reproducible, techniques: image processing, techniques: photometric

1. Introduction

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Since its release, Nous-Gishe has been used in many studies. For example Boron et al. (2017) used it to identify deject has two emissed by Rabdek et al. (2016) interoferable (2017) used it to identify deject has two emissed by Rabdek et al. (2016) (neurophysical different configurations to avoid deibraching problems, but etill missed many sources with againtoni sugma, see Figure 1. Bordf et al. (2017), March et al. (2019), and Trijillo et al. (2019) used it for accurate flut field and Sky subtractions to create despress configuet al. (2019) used its for all controls that the state of the

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The Sloan Digital Sky Survey extended point spread functions

Raúl Infante-Sainz [•], ^{1,2}* Ignacio Trujillo [•], ^{1,2} and Javier Román [•], ^{1,2,3} ¹habas de Aurofínio de Canavia, el Via Lairea sis 6.8205 La Lapana, Everific, Spain ¹Departamente de Aurofínio, Detretridad de La Lapana, E-3205 La Lapana, Teverific, Spain

Accepted 2019 October 30. Received 2019 October 29; in original form 2019 September H

ABSTRACT

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1 INTRODUCTION

The point spread function (FSF), showshow the response of an imaging system to the light produced by point sources. Real FSFs have complex structures as their shapes depend on the optical point for tight takes as it mays the image. The structure, the respective structure is a structure is made the structure is the respective and the structure structure is the respective structure structure is the respective structure structure structure structure is the structure structu

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The operation of the most commonly used surveys for measuring photometric properties of astronomical objects is the Shan SAy Digital Survey (SDSS) York et al. 2006, covering 14 455 dag²⁴ on the sky (just over 35 per cent of the full sky) in five photometric bunds (u.g. r. i. and 2), Alhough SDSS is a realisively shallow survey compared

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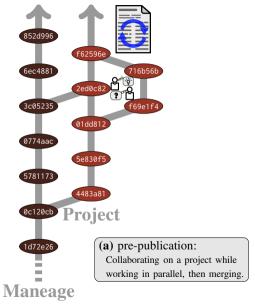
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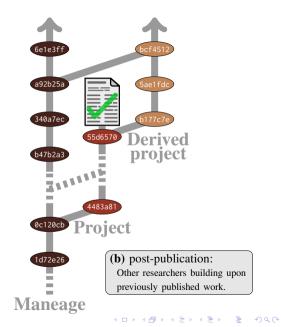
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Any Git-based workflow is possible.





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).

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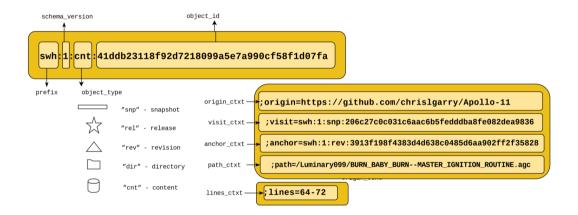
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The project's pipeline (customized Maneage) can be published in

- 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.3872247) and given a unique DOI.
 - ... and put links to data in paper! See ending of caption of Figure 1 in the Maneage paper.
- 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 or Table 1 of arXiv:1909.11230.

Software Heritage IDs (SWHID); persistent identifier for source code (or any text!)



For more details, see SoftwareHeritage FAQ (at https://www.softwareheritage.org/faq)

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

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General outline of using this system (for example arXiv:1909.11230)

\$ git clone http://gitlab.com/makhlaghi/iau-symposium-355 # Import the project.

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\$./project configure

You will specify the build directory on your system, # and it will build all software (about 1.5 hours).

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\$ git clone http://gitlab.com/makhlaghi/iau-symposium-355 # Import the project.

\$./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 is introduced as 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.
- Only parts affected by a modification are re-done.
- Using LaTeX macros, paper's figures, tables and numbers will be Automatically updated.
- ► The whole project is under version control (Git) encouraging tests/experimentation.
- ▶ The Git commit hash of the project source, is printed in the paper and on output data products.
- These 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

Feel free to contact me: mohammad@akhlaghi.org