Towards Long-term and Archivable Reproducibility

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Abstract—Reproducible workflow solutions commonly use high-level technologies that were popular when they were created, providing an immediate solution which is unlikely to be sustainable in the long term. We therefore introduce a set of criteria to address this problem and demonstrate their practicality and implementation. The criteria have been tested in several research publications and can be summarized as: completeness (no dependency beyond a POSIX-compatible operating system, no administrator privileges, no network connection and storage primarily in plain text); modular design; minimal complexity; scalability; verifiable inputs and outputs; temporal provenance; linking analysis with narrative; and free-and-open-source software. As a proof of concept, we have implemented “Maneage”, a solution which stores the project in machine-actionable and human-readable plain-text, enables version-control, cheap archiving, automatic parsing to extract data provenance, and peer-reviewable verification. We show that requiring longevity of a reproducible workflow solution is realistic, without sacrificing immediate or short-term reproducibility and discuss the benefits of the criteria for scientific progress. This paper has itself been written in Maneage, with snapshot 1637c6e.

Reproducible supplement — Necessary software, workflow and output data are published in Zenodo.3872248.

Index Terms—Data Lineage, Provenance, Reproducibility, Scientific Pipelines, Workflows

I. INTRODUCTION

Reproducible research has been discussed in the sciences for at least 30 years [1], [2]. Many reproducible workflow solutions (hereafter, “solutions”) have been proposed, mostly relying on the common technology of the day: starting with Make and Matlab libraries in the 1990s, to Java in the 2000s and mostly shifting to Python during the last decade.

However, these technologies develop fast, e.g., Python 2 code 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 technology of their tools, because it determines their results and interpretations. Decades later, scientists are still held accountable for their results and therefore the evolving technology landscape creates generational gaps in the scientific community, preventing previous generations from sharing valuable experience.

II. COMMONLY USED TOOLS AND THEIR LONGEVITY

Longevity is as important in science as in some fields of industry, but this is not always the case, e.g., fast-evolving tools can be appropriate in short-term commercial projects. To highlight the necessity of longevity, some of the most commonly-used tools are reviewed here from this perspective.

A common set of third-party tools that are commonly used can be categorized as: (1) environment isolators – virtual machines (VMs) or containers; (2) package managers (PMs) – Conda, Nix, or Spack; (3) job management – shell scripts, Make, SCons, or CGAT-core; (4) notebooks – such as Jupyter.

To isolate the environment, VMs have sometimes been used, e.g., in SHARE (which was awarded second prize in the Elsevier Executable Paper Grand Challenge of 2011 but was discontinued in 2019). However, containers (in particular, Docker, and to a lesser degree, Singularity) are currently the most widely-used solution, we will thus focus on Docker here.

Ideally, it is possible to precisely identify the Docker “images” that are imported with their checksums, but that is rarely practiced in most solutions that we have surveyed. Usually, images are imported with generic operating system (OS) names e.g. [3] uses ‘FROM ubuntu:16.04’. The extracted tarball (from https://partner-images.canonical.com/core/xenial) is updated almost monthly and only the most recent five are archived. Hence, if the Dockerfile is run in different months, its output image will contain different OS components. In the year 2024, when long-term support for this version of Ubuntu will expire, the image will be unavailable at the expected URL. Other OSes have similar issues because pre-built binary files are large and expensive to maintain and archive. Furthermore, Docker requires root permissions, and only supports recent (“long-term-support”) versions of the host kernel, so older Docker images may not be executable.

Once the host OS is ready, PMs are used to install the software, or environment. Usually the OS’s PM, like ‘apt’ or ‘yum’, is used first and higher-level software are built with generic PMs. The former suffers from the same longevity problem as the OS, while some of the latter (like Conda and Spack) are written in high-level languages like Python, so the PM itself depends on the host’s Python installation. Nix and GNU Guix produce bit-wise identical programs, but they need root permissions and are primarily targeted at the Linux kernel. Generally, the exact version of each software’s dependencies is not precisely identified in the PM build instructions (although this could be implemented). Therefore, unless precise version identifiers of every software package are stored by project authors, a PM will use the most recent version. Furthermore, because each third-party PM introduces its own language and framework, this increases the project’s complexity.

With the software environment built, job management is the next component of a workflow. Visual workflow tools like Apache Taverna, GenePattern, Kepler or VisTrails (mostly introduced in the 2000s and using Java) encourage modularity and robust job management, but the more recent tools (mostly in Python) leave this to the authors of the project. Designing a modular project needs to be encouraged and facilitated because scientists (who are not usually trained in project or data...
management) will rarely apply best practices. This includes automatic verification: while it is possible in many solutions, it is rarely practiced, which leads to many inefficiencies in project cost and/or scientific accuracy (reusing, expanding or validating will be expensive).

Finally, to add narrative, computational notebooks [4], like Jupyter, are currently gaining popularity. However, due to their complex dependency trees, they are vulnerable to the passage of time, e.g., see Figure 1 of [5] for the dependencies of Matplotlib, one of the simpler Jupyter dependencies. It is important to remember that the longevity of a project is determined by its shortest-lived dependency. Further, as with job management, computational notebooks do not actively encourage good practices in programming or project management. Hence they can rarely deliver their promised potential [4] and can even hamper reproducibility [6].

An exceptional solution we encountered was the Image Processing Online Journal (IPOL, ipol.im). Submitted papers must be accompanied by an ISO C implementation of their algorithm (which is build-able on any widely used OS) with example images/data that can also be executed on their webpage. This is possible due to the focus on low-level algorithms with no dependencies beyond an ISO C compiler. However, many data-intensive projects commonly involve dozens of high-level dependencies, with large and complex data formats and analysis, and hence this solution is not scalable.

III. PROPOSED CRITERIA FOR LONGEVITY

The main premise is that starting a project with a robust data management strategy (or tools that provide it) is much more effective, for researchers and the community, than imposing it in the end [2], [7]. In this context, researchers play a critical role [7] in making their research more Findable, Accessible, Interoperable, and Reusable (the FAIR principles). Simply archiving a project workflow in a repository after the project is finished is, on its own, insufficient, and maintaining it by repository staff is often either practically infeasible or unscaleable. We argue and propose that workflows satisfying the following criteria can not only improve researcher flexibility during a research project, but can also increase the FAIRness of the deliverables for future researchers:

Criterion 1: Completeness. A project that is complete (self-contained) has the following properties. (1) It has no dependency beyond the Portable Operating System Interface: POSIX. IEEE defined POSIX (a minimal Unix-like environment) and many OSes have complied. (2) “No dependency” requires that the project itself must be primarily stored in plain text, not needing specialized software to open, parse or execute. (3) It does not affect the host OS (its libraries, programs, or environment). (4) It does not require root or administrator privileges. (5) It builds its own controlled software for an independent environment. (6) It can run locally (without an internet connection). (7) It contains the full project’s analysis, visualization and narrative: from access to raw inputs to doing the analysis, producing final data products and its final published report with figures as output, e.g., PDF or HTML. (8) It can run automatically, with no human interaction.

Criterion 2: Modularity. A modular project enables and encourages the analysis to be broken into independent modules with well-defined inputs/outputs and minimal side effects. Explicit communication between various modules enables optimizations on many levels: (1) Execution in parallel and avoiding redundancies (when a dependency of a module has not changed, it will not be re-run). (2) Usage in other projects. (3) Easy debugging and improvements. (4) Modular citation of specific parts. (5) Provenance extraction.

Criterion 3: Minimal complexity. Minimal complexity can be interpreted as: (1) Avoiding the language or framework that is currently in vogue (for the workflow, not necessarily the high-level analysis). A popular framework typically falls out of fashion and requires significant resources to translate or rewrite every few years. More stable/basic tools can be used with less long-term maintenance. (2) Avoiding too many different languages and frameworks, e.g., when the workflow’s PM and analysis are orchestrated in the same framework, it becomes easier to adopt and encourages good practices.

Criterion 4: Scalability. A scalable project can easily be used in arbitrarily large and/or complex projects. On a small scale, the criteria here are trivial to implement, but can rapidly become unsustainable.

Criterion 5: Verifiable inputs and outputs. The project should verify its inputs (software source code and data) and outputs. Reproduction should be straightforward enough such that “a clerk can do it” [1] (with no expert knowledge).

Criterion 6: History and temporal provenance. No exploratory research project is done in a single, first attempt. Projects evolve as they are being completed. It is natural that earlier phases of a project are redesigned/optimized only after later phases have been completed. Research papers often report this with statements such as “we [first] tried method [or parameter] X, but Y is used here because it gave lower random error”. The derivation “history” of a result is thus not any less valuable as itself.

Criterion 7: Including narrative, linked to analysis. A project is not just its computational analysis. A raw plot, figure or table is hardly meaningful alone, even when accompanied by the code that generated it. A narrative description must also be part of the deliverables (defined as “data article” in [7]): describing the purpose of the computations, and interpretations of the result, and the context in relation to other projects/papers. This is related to longevity, because if a workflow only contains the steps to do the analysis or generate the plots, in time it may get separated from its accompanying published paper.

Criterion 8: Free and open source software: Reproducibility (defined in [2]) can be achieved with a black box (non-free or non-open-source software), this criterion is thus necessary because nature is already a black box. A project that is free software (as formally defined), allows others to learn from, modify, and build upon it. When the software used by the project is itself also free, the lineage can be traced to the core algorithms, possibly enabling optimizations on that level and it can be modified for future hardware. In contrast, a non-free tools typically cannot be distributed or modified by others, making it reliant on a single supplier (even without payments).
IV. PROOF OF CONCEPT: MANEAGE

With the longevity problems of existing tools outlined above, a proof-of-concept tool is presented here via an implementation that has been tested in published papers [8], [9]. It was in fact awarded a Research Data Alliance (RDA) adoption grant for implementing the recommendations of the joint RDA and World Data System (WDS) working group on Publishing Data Workflows [7], from the researchers’ perspective.

The tool is called Maneage, for Managing data Lineage (the ending is pronounced as in “lineage”), hosted at https://maneage.org. It was developed as a parallel research project over five years of publishing reproducible workflows of our research. The original implementation was published in [10], and evolved in zenodo.1163746 and zenodo.1164774.

Technically, the hardest criterion to implement was the first one (completeness) and, in particular, avoiding non-POSIX dependencies. One solution we considered was GNU Guix and Guix Workflow Language (GWL). However, because Guix requires root access to install, and only works with the Linux kernel, it failed the completeness criterion. Inspired by GWL+Guix, a single job management tool was implemented for both installing software and the analysis workflow: Make.

Make is not an analysis language, it is a job manager, deciding when and how to call analysis programs (in any language like Python, R, Julia, Shell or C). Make is standardized in POSIX and is used in almost all core OS components. It is thus mature, actively maintained, highly optimized, efficient in managing exact provenance, and even recommended by the pioneers of reproducible research [1], [11]. Researchers using free software tools have also already had some exposure to it.

Linking the analysis and narrative (criterion 7) was historically our first design element. To avoid the problems with computational notebooks mentioned above, our implementation follows a more abstract linkage, providing a more direct and precise, yet modular, connection. Assuming that the narrative is typeset in \LaTeX, the connection between the analysis and narrative (usually as numbers) is through automatically-created \LaTeX macros, during the analysis. For example, [8] writes ‘... detect the outer wings of M51 down to S/N of 0.25 ...’. The \LaTeX source of the quote above is: ‘detect the outer wings of M51 down to S/N of $0.25$ ...’. The \LaTeX source of the quote above is: ‘detect the outer wings of M51 down to S/N of $\S$\demosfoptimizeds$\$’. The macro ‘\demosfoptimizeds’ is generated during the analysis, and expands to the value ‘$0.25$’ when the PDF output is built. Since values like this depend on the analysis, they should also be reproducible, along with figures and tables.

These macros act as a quantifiable link between the narrative and analysis, with the granularity of a word in a sentence and a particular analysis command. This allows accurate post-publication provenance and automatic updates to the embedded numbers during a project. Through the latter, manual updates by authors are by-passed, which are prone to errors, thus discouraging improvements after writing the first draft.

Acting as a link, the macro files build the core skeleton of Maneage. For example, during the software building phase, each software package is identified by a \LaTeX file, containing its official name, version and possible citation. These are combined at the end to generate precise software acknowledgment and citation (see [8], [9]), which are excluded here due to the strict word limit.

The macro files also act as Make targets and prerequisites to allow accurate dependency tracking and optimized execution (in parallel, no redundancies), for any level of complexity (e.g., Maneage builds Matplotlib if requested; see Figure 1 of [5]). All software dependencies are built down to precise versions of every tool, including the shell, POSIX tools (e.g., GNU Coreutils) or \TeXLive, providing the same environment. On GNU/Linux distributions, even the GNU Compiler Collection (GCC) and GNU Binutils are built from source and the GNU C library is being added (task 15390). Temporary relocation of a project, without building from source, can be done by building the project in a container or VM.

The analysis phase of the project however is naturally different from one project to another at a low-level. It was thus necessary to design a generic framework to comfortably host any project, while still satisfying the criteria of modularity, scalability and minimal complexity. We demonstrate this design by replicating Figure IC of [12] in Figure 1 (top). Figure 1 (bottom) is the data lineage graph that produced it (including this complete paper).

Listing 1

This project’s simplified top-make.mk, also see Figure 1

```
# Default target/goal of project.
all: paper.pdf

# Define subMakefiles to load in order.
makesrc = initialize \ # General
download \ # General
format \ # Project-specific
demo-plot \ # Project-specific
verify \ # General
paper \ # General

# Load all the configuration files.
include reproduce/analysis/config/*.conf

# Load the subMakefiles in the defined order
include $(foreach s,$(makesrc), \ reproduce/analysis/make/$s.mk)
```

The analysis is orchestrated through a single point of entry (top-make.mk, which is a Makefile; see Listing 1). It is only responsible for including the modular subMakefiles of the analysis, in the desired order, without doing any analysis itself. This is visualized in Figure 1 (bottom) where no built (blue) file is placed directly over top-make.mk (they are produced by the subMakefiles under them). A visual inspection of this file is sufficient for a non-expert to understand the high-level steps of the project (irrespective of the low-level implementation details), provided that the subMakefile names are descriptive (thus encouraging good practice). A human-friendly design that is also optimized for execution is a critical component for the FAIRness of reproducible research.

All projects first load initialize.mk and download.mk, and finish with verify.mk and paper.mk (Listing 1). Project authors add their modular subMakefiles in between. Except for paper.mk (which builds the ultimate target: paper.pdf), all subMakefiles build a macro file with the same base-name (the .tex file in each subMakefile of Figure 1). Other built
Fig. 1. Top: an enhanced replica of Figure 1C in [12], shown here for demonstrating Maneage. It shows the ratio of the number of papers mentioning software tools (green line, left vertical axis) to the total number of papers studied in that year (light red bars, right vertical axis on a log scale). Bottom: Schematic representation of the data lineage, or workflow, to generate the plot above. Each colored box is a file in the project and the arrows show the dependencies between them. Green files/boxes are plain-text files that are under version control and in the project source directory. Blue files/boxes are output files in the build directory, shown within the Makefile (*.mk) where they are defined as a target. For example, paper.pdf depends on project.tex (in the build directory; generated automatically) and paper.tex (in the source directory; written manually). The solid arrows and full-opacity built boxes correspond to this paper. The dashed arrows and low-opacity built boxes show the scalability by adding hypothetical steps to the project. The underlying data of the top plot is available at zenodo.3872248/tools-per-year.txt.

files (intermediate analysis steps) cascade down in the lineage to one of these macro files, possibly through other files.

Just before reaching the ultimate target (paper.pdf), the lineage reaches a bottleneck in verify.mk, to satisfy the verification criteria (this step was yet not available in [8], [9]). All project deliverables (macro files, plot or table data and other datasets) are verified at this stage, with their checksums, to automatically ensure exact reproducibility. Where exact reproducibility is not possible, values can be verified by any statistical means, specified by the project authors.

To further minimize complexity, the low-level implementation can be further separated from the high-level execution through configuration files. By convention in Maneage, the subMakefiles (and the programs they call for number crunching) do not contain any fixed numbers, settings or parameters. Parameters are set as Make variables in “configuration files” (with a .conf suffix) and passed to the respective program by Make. For example, in Figure 1 (bottom), INPUTS.conf contains URLs and checksums for all imported datasets, enabling exact verification before usage. To illustrate this, we report that [12] studied 53 papers in 1996 (which is not in their original plot). The number 1996 is stored in demo-year.conf and the result (53) was calculated after generating columns.txt. Both numbers are expanded as \LaTeX{} macros when creating this PDF file. An interested reader can change the value in demo-year.conf to automatically update the result in the PDF, without necessarily knowing the underlying low-level implementation. Furthermore, the configuration files are a prerequisite of the targets that use them. If changed, Make will only re-execute the dependent recipe and all its descendants, with no modification to the project’s source or other built products. This fast and cheap testing encourages experimentation
(without necessarily knowing the implementation details, e.g., by co-authors or future readers), and ensures self-consistency.

Finally, to satisfy the temporal provenance criterion, version control (currently implemented in Git) is another component of Maneage (see Figure 2). Maneage is a Git branch that contains the shared components (infrastructure) of all projects (e.g., software tarball URLs, build recipes, common subMakefiles and interface script). Derived project start by branching off, and customizing it (e.g., adding a title, data links, narrative, and subMakefiles for its particular analysis, see Listing 2, there is customization checklist in README-hacking.md).

| Listing 2 |
| --- |
| **STARTING A NEW PROJECT WITH MANEGE, AND BUILDING IT** |
| # Cloning main Maneage branch and branching off it. |
| $ git clone https://git.maneage.org/project.git |
| $ cd project |
| $ git remote rename origin origin-maneage |
| $ git checkout -b master |
| # Build the raw Maneage skeleton in two phases. |
| $ ./project configure # Build software environment. |
| $ ./project make # Do analysis, build PDF paper. |
| # Start editing, test-building and committing |
| $ emacs paper.tex # e.g., add project title. |
| $ ./project make # Re-build to see effect. |
| $ git add -u && git commit # Commit changes |

The branch-based design of Figure 2) allows projects to re-import Maneage at a later time (technically: merge), thus improving its low-level infrastructure: in (a) authors do the merge during an ongoing project; in (b) readers do it after publication, e.g., the project remains reproducible but the infrastructure is outdated, or a bug is fixed in Maneage. Low-level improvements in Maneage can thus propagate to all projects, greatly reducing the cost of curation and maintenance of each individual project, before and after publication.

Finally, the complete project source is usually ~100 kilobytes. It can thus easily be published or archived in many servers, for example it can be uploaded to arXiv (with the \TeX\ source, see the arXiv source in \cite{8,10}), published on Zenodo and archived in SoftwareHeritage.

V. DISCUSSION

We have shown that it is possible to build workflows satisfying all the proposed criteria, and we comment here on our experience in testing them through this proof-of-concept tool. With the support of RDA, Maneage user-base grew, underscoring some difficulties for a widespread adoption.

Firstly, while most researchers are generally familiar with them, the necessary low-level tools (e.g., Git, \LaTeX, the command-line and Make) are not widely used. Fortunately, we have noticed that after witnessing the improvements in their research, many, especially early-career researchers, have started mastering these tools. Scientists are rarely trained sufficiently in data management or software development, and the plethora of high-level tools that change every few years discourages them. Indeed the fast-evolving tools are primarily targeted at software developers, who are paid to learn and use them effectively for short-term projects before moving on to the next technology.

Scientists, on the other hand, need to focus on their own research fields, and need to consider longevity. Hence, arguably the most important feature of these criteria (as implemented in Maneage) is that they provide a fully working template, using mature and time-tested tools, for blending version control, the research paper’s narrative, the software management and a robust data carpentry. We have noticed that providing a complete and customizable template with a clear checklist of the initial steps is much more effective in encouraging mastery of these modern scientific tools than having abstract, isolated tutorials on each tool individually.

Secondly, to satisfy the completeness criterion, all the required software of the project must be built on various POSIX-compatible systems (Maneage is actively tested on different GNU/Linux distributions, macOS, and is being ported to FreeBSD also). This requires maintenance by our core team and consumes time and energy. However, because the PM and analysis components share the same job manager (Make) and design principles, we have already noticed some early users adding, or fixing, their required software alone. They later share their low-level commits on the core branch, thus propagating it to all derived projects.

A related caveat is that, POSIX is a fuzzy standard, not guaranteeing the bit-wise reproducibility of programs. It has been chosen here, however, as the underlying platform because our focus on reproducing the results (data) which doesn’t always need that bit-wise identical software. POSIX is ubiquitous and low-level software (e.g., core GNU tools) are install-able on most; each internally corrects for differences affecting its functionality (partly as part of the GNU portability library). On GNU/Linux hosts, Maneage builds precise versions of the compilation tool chain, but glibc is not install-able on some POSIX OSs (e.g., macOS). The C library is linked with all programs, and this dependence can hypothetically hinder exact reproducibility of results, but we have not encountered this so far. With everything else under precise control, the effect of differing Kernel and C libraries on high-level science can now be systematically studied with Maneage in followup research.

Other implementations of the criteria, or future improvements in Maneage, may solve some of the caveats above, but this proof of concept already shows their many advantages. For example, publication of projects meeting these criteria on a wide scale will allow automatic workflow generation, optimized for desired characteristics of the results (e.g., via machine learning). The completeness criteria implies that algorithms and data selection can be included in the optimizations.

Furthermore, through elements like the macros, natural language processing can also be included, automatically analyzing the connection between an analysis with the resulting narrative and the history of that analysis+narrative. Parsers can be written over projects for meta-research and provenance studies, e.g., to generate “research objects”. Likewise, when a bug is found in one science software, affected projects can be detected and the scale of the effect can be measured. Combined with SoftwareHeritage, precise high-level science components of the analysis can be accurately cited (e.g.,
Fig. 2. Maneage is a Git branch. Projects using Maneage are branched off it and apply their customizations. (a) A hypothetical project’s history prior to publication. The low-level structure (in Maneage, shared between all projects) can be updated by merging with Maneage. (b) A finished/published project can be revitalized for new technologies by merging with the core branch. Each Git “commit” is shown on its branch as a colored ellipse, with its commit hash shown. The commits are colored to identify their branch. The collaboration and two paper icons are respectively made by ‘mynamepong’ and ‘iconixar’ from www.flaticon.com.

even failed/abandoned tests at any historical point). Many components of “machine-actionable” data management plans can also be automatically completed as a byproduct, useful for project PIs and grant funders.

From the data repository perspective, these criteria can also be useful, e.g., the challenges mentioned in [7]: (1) The burden of curation is shared among all project authors and readers (the latter may find a bug and fix it), not just by database curators, improving sustainability. (2) Automated and persistent bidirectional linking of data and publication can be established through the published and complete data lineage that is under version control. (3) Software management: with these criteria, each project comes with its unique and complete software management. It does not use a third-party PM that needs to be maintained by the data center (and the many versions of the PM). Hence enabling robust software management, preservation, publishing and citation. For example, see zenodo.3524937, zenodo.3408481, zenodo.1163746, where we have exploited the free-software criterion to distribute the tarballs of all the software used with each project’s source as deliverables. (4) “Linkages between documentation, code, data, and journal articles in an integrated environment”, which effectively summarizes the whole purpose of these criteria.

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