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Developing open source scientific practice

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Dedicated to the memory of John D. Hunter III, 1968-2012.

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1.1 Introduction

Computational tools are at the core of modern research. In addition to experiment and theory, the notions of simulation and data-intensive discovery are often referred to as "third and fourth pillars" of science [12]. It is probably more realistic to simply accept that computing is now inextricably woven into the DNA of science, as today, even theory and experiment are computational. Experimental work requires computing (whether in data collection, preprocessing, or analysis) and theoretical work requires symbolic manipulation and numerical exploration to develop and refine models. Scanning the pages of any recent scientific journal, one is hard-pressed to find an article that does not depend on computing for its findings.

Yet, for all its importance, computing receives perfunctory attention in the training of new scientists and in the conduct of everyday research. It is treated as an inconsequential task that students and researchers learn "on the go" with little consideration for ensuring computational results are trustworthy, comprehensible, and ultimately a secure foundation for reproducible outcomes. Software and data are stored with poor organization, little documentation, and few tests. A haphazard patchwork of software tools is used with limited attention paid to capturing the complex workflows that emerge. The evolution of code is not tracked over time, making it difficult to understand what iteration of the code was used to obtain any specific result. Finally, many of the software packages used by scientists in research are proprietary and closed-source, preventing complete understanding and control of the final scientific results.

We argue that these considerations must play a more central role in how scientists are trained and conduct their research. Our approach grows out of our experience as part of both the research and the open source scientific Python communities. We begin (§ 1.2) by outlining our vision for the scientific software development in everyday research. In the remaining sections, we provide specific recommendations for computational work. First, we describe the routine practices (§ 1.3) that should be part of the daily conduct of computational work. We next discuss tools and practices developed by open source communities to enable and streamline collaboration (§ 1.4). Finally, we present an approach to developing and communicating computational work that we call literate computing in contrast to the traditional approach of literate programming (§ 1.5).

1.2 Computational research

Consider a researcher using Matlab for prototyping a new analysis method, developing high-performance code in C, post-processing by twiddling controls in a graphical user interface, importing data back into Matlab for generating plots, polishing the resulting plots by hand in Adobe Illustrator, and finally pasting the plots into a publication manuscript or PowerPoint presentation. What if months later they realize there is a problem with the results? Will they will be able to remember what buttons they clicked to reproduce the workflow to generate updated plots, manuscript, and presentation? Can they validate that their programs and overall workflow is free of errors? Will other researchers or students be able to reproduce these steps to learn how a new method works or understand how the presented results were obtained?

The pressure to publish encourages us to charge forward chasing the goal of an accepted manuscript, but the term "reproducibility" implies repetition and thus a requirement to also move *back*—to retrace one's steps, question or change assumptions, and move forward again. Unfortunately, the all-too-common way scientists conduct computational work makes this necessary part of the research process difficult at best, often impossible.

The open source software development community[1] has cultivated tools and practices that, if embraced and adapted by the scientific community, will greatly enhance our ability to achieve reproducible outcomes. Open source software development uses public forums for most discussion and systems for sharing code and data. There is a strong culture of public disclosure, tracking and fixing of bugs, and development often includes exhaustive validation tests that are executed automatically whenever changes are made to the software and whose output is publicly available on the Internet. This detects problems early, mitigates their recurrence, and ensures that the state and quality of the software is known under a wide variety of situations (operating systems, inputs, parameter ranges, etc). The same systems used for sharing code also track the authorship of contributions. All of this ensures an open collaboration that recognizes the work of individual developers and allows for a meritocracy to emerge.

As we learn from the open source process how to improve our scientific practice, we recognize that the ideal of scientific reproducibility is by necessity a reality of shades. We see a gradation from a pure mathematical result whose proof should be accessible to any person skilled in the necessary specialty to one-of-a-kind experiments such as the Large Hadron Collider or the Hubble Space Telescope, that cannot be reproduced in any realistic sense. However, it is always possible to improve our confidence in the results: whether we reexamine the same unique datasets with independently developed packages run by separate groups or we reacquire partial sampling of critical data multiple times.

Similarly, in computational research we also have certain areas where complete reproducibility is more challenging than others. Some projects require computations carried on the largest supercomputers, and these are expensive resources that cannot be arbitrarily allocated for repeated executions of the same problem. Others may require access to enormous datasets that cannot easily be transferred to the desktop of any researcher wishing to re-execute an analysis. But again, alternatives exist: it is possible to partially validate scaled versions of the largest problems against smaller runs created on the same supercomputing environments. Similarly, coarse resolution datasets can be used to conduct an analysis that may provide insights into the reliability of the full analysis. While not every quantity can be studied in this manner and there are deep research questions embedded in this problem, we should not consider this to be a paralyzing impediment to the quest for better computational reproducibility. Fortunately, the vast majority of research is conducted in smaller, simpler environments where full replication is feasible.

1.2.1 Computational research life cycle

We advocate an integrated approach to computing where the entire life cycle of scientific research is considered, from the initial exploration of ideas and data to the presentation of final results. Schematically, this life cycle can be broken down into the following phases:

- **Individual exploration:** a single investigator tests an idea, algorithm, or question, likely with a small-scale test data set or simulation.

- **Collaboration:** if the initial exploration appears promising, more often than not some

[1]We take it as a forgone conclusion (see [16]) that to share our research code with one another, we must use open source tools. Instead of discussing the need for using open source software, we focus on adopting development practices used by open source communities.

kind of collaborative effort ensues to bring together complementary expertise from colleagues.

- **Production-scale execution:** large data sets and complex simulations often require the use of clusters, supercomputers, or cloud resources in parallel.
- **Publication:** whether as a paper or an internal report for discussion with colleagues, results need to be presented to others in a coherent form.
- **Education:** ultimately, research results become part of the corpus of a discipline that is shared with students and colleagues, thus seeding the next iteration in the cycle of research.

Before presenting our approach, we examine the typical patchwork of tools and approaches that researchers use to navigate these phases and discuss how the standard approach makes the goal of reproducibility nearly unattainable.

For **individual work**, researchers use various interactive computing environments: Microsoft Excel, Matlab, Mathematica, Sage, and more specialized systems like R, SPSS, SAS, and STATA for statistics. These environments combine interactive, high-level programming languages with a rich set of numerical and visualization libraries. The impact of these environments cannot be overstated; researchers use them for rapid prototyping, interactive exploration and data analysis, as well as visualization. However, they have limitations: (a) some of them are proprietary and/or expensive (Excel, Matlab, Mathematica), (b) most (except for Sage) are focused on coding in a single, relatively slow, programming language and (c) most (except for Sage and Mathematica) do not have a document format that is rich, i.e., that can include text, equations, images, and video in addition to source code. While the use of proprietary tools is not a problem *per se* and may be a good solution in industry, it is a barrier to scientific collaboration and to the construction of a common scientific heritage where anyone can validate the work of others and build upon it. Scientists cannot share work unless all colleagues can purchase the same package; students are forced to work with black boxes they are legally prevented from inspecting. Furthermore, because of their limitations in performance and handling large, complex code bases, these tools are mostly used for prototyping: researchers eventually have to switch tools for building production systems.

For **collaboration**, researchers tend to use a mix of email, version control systems and shared network folders (Dropbox, etc.). Version control systems (see § 1.3.1) are critically important in making research collaborative and reproducible. They allow groups to work collaboratively on documents and track how they evolve over time. Ideally, all aspects of computational research would be hosted on publicly available version control repositories, such GitHub or Google Code. Unfortunately, the common approach is for researchers to email documents to each other with *ad hoc* naming conventions that provide a poor man's version control (and are the source of endless confusion and frequent mistakes). This form of collaboration makes it nearly impossible to track the development of a large project and establish reproducible and testable workflows. While a small group can make it work, this approach most certainly does not scale beyond a few collaborators, as painfully experienced by anyone who has participated in the madness of a flurry of email attachments with oddly-named files such as `paper-final-v2-REALLY-FINAL-john-ACT9.doc`.

For **production-scale execution**, researchers typically turn away from the convenience of interactive computing environments to compiled code (C, C++, Fortran) and parallel computing libraries (MPI, Hadoop), as most interactive systems do not provide the performance necessary for large-scale work and have limited support for distributed and parallel computing. These tools are specialized enough that their mastery requires a substantial investment of time. We emphasize, that before production-scale computations begin, the researchers already have a working prototype in an interactive computing environment. Therefore, turning to new parallel tools means starting over and maintaining at least two versions of the code moving forward. Furthermore, data produced by the compiled version is often imported back into the interactive environment for visualization and analysis. The resulting back-and-forth workflow is nearly impossible to capture and put into version control systems, making the computational research difficult to reproduce. Obviously the alternative, taken by many, is simply to run the slow serial code for as long as it takes. This is hardly a solution to the reproducibility problem, as runtimes in the weeks or months become in practice single-shot efforts that no one will replicate.

For **publications** and **education**, researchers use tools such as LaTeX, Google Docs, or Microsoft Word and PowerPoint. The most important attribute of these tools in this context is that, LaTeX excepted, they integrate poorly with version control systems and are ill-suited for workflow automation. Digital artifacts (code, data, and visualizations) are often manually pasted into these documents, which easily leads to a divergence between the computational outcomes and the publication. The lack of automated integration requires manual updating, something that is error-prone and easy to forget.

From this perspective, we now draw a few lessons:

1. The common approaches and tools used today introduce discontinuities between the different stages of the scientific workflow. Forcing researchers to switch tools at each stage, which in turn makes it difficult to move fluidly back and forth. Driven by the pressure to publish, it is natural to charge *forward*, pressing on to assemble results in pursuit of an accepted manuscript but rarely going back to question assumptions, replicate earlier experiments with updated versions of code or parameter tweaks, etc. Because reproducing results effectively requires going *back* to the beginning of the pipeline, a workflow that from the onset makes this inherently difficult will likely result in outcomes that not even the original authors can reliably reproduce.
2. A key element of the problem is the gap that exists between what we view as “final outcomes” of the scientific effort (papers and presentations that contain artifacts such as figures, tables, and other outcomes of the computation) and the pipeline that feeds these outcomes. Because most workflows involve a manual transfer of information (often with unrecorded manual changes along the way), the chances that these final outcomes match what the computational pipeline actually produces at any given time are low.
3. The problems listed above are *both* technical and social. While we largely focus on the tools aspect in this chapter, it is critical to understand that at the end of the day, only when researchers make a conscious decision to adopt improved work habits will we see substantial improvements on this problem. Obviously higher quality tools will make it easier and more appealing to adopt such changes; but other factors—from the inertia of ingrained habits to the pressure applied by the incentive models of modern research—are also at play.

Asking about reproducibility by the time a manuscript is ready for submission to a journal is simply too late: this problem must be tackled from the start, not as an afterthought tacked-on at publication time. We must therefore look for approaches that allow researchers to fluidly move back and forth between the above stages and that integrate naturally into their everyday practices of research, collaboration, and publishing, so that we can simultaneous address the technical and social aspects of this issue.

1.2.2 Open source ecosystem

With the above in mind, our approach to the problem of reproducibility in computational research focuses on the need for tools and practices that enable researchers to naturally consider the entire cycle of research as a continuum, and where "doing the right thing" is the easy and natural path rather than an awkward and cumbersome one. Rather than the haphazard patchwork of tools and processes described above, we promote the development and adoption of a robust, open source ecosystem that makes reproducible research a central aim.

To illustrate our point, we briefly describe the scientific Python ecosystem [25, 22, 29] and introduce a few core projects, which serve as examples throughout the chapter. While strong proponents of Python for scientific computing, we understand Python is not the only choice for scientific computing or reproducible research. Rather we consider the scientific Python ecosystem as a case study for the type of community-developed software stack that we believe necessary for improving the reliability and reproducibility of our computational results.

Initially written for teaching, the Python programming language has a simple, expressive, and accessible syntax that emphasizes code readability (see § 1.3.4). Rather than imposing a single programming paradigm, it allows one to code at many levels of sophistication, including the procedural programming style familiar to many scientists. Python is available in an easily installable form for almost every platform and, therefore, ideal for a heterogeneous computing environment. It is also powerful enough to manage the complexity of large applications, supporting functional programming, object-oriented programming, generic programming, and metaprogramming. Due to excellent support for scripting tools written in other languages (including C, C++, Fortran, and R), Python is often used as an *integration language* for calling routines from a wide array of high-quality scientific libraries. Finally, it has an extensive standard library that provides built-in functionality for many tasks including database access, Internet protocols, data compression, and operating system services.

Importantly, from our perspective, Python is not specifically designed for scientific computing. So it is extremely capable at a diverse set of none science-specific tasks. This benefits the scientific community, by providing an assortment of useful functionality and features while we focus on extending them with the specific features necessary for our research. While there are numerous libraries and extensions for scientific computing in Python, the three most widely used are NumPy,[2] SciPy,[3] and matplotlib.[4] NumPy [34] provides a high-level multidimensional array object and basic operations to manipulate them. SciPy is a collection of common numerical operations used in scientific computing. Matplotlib [14, 15] is the standard 2D plotting library. In addition to these tools, there are even more specialized packages to provide advanced support and algorithms for machine learning, image processing, graph theory, symbolic mathematics, etc. On top of these general scientific libraries, there are even more domain specific projects developed by those scientific communities. For instance, we are both members of the Neuroimaging in Python [23] community in addition to participating in the more general parts of the scientific Python software stack. The ability to participate and contribute at multiple levels of the tool chain is possible because of the adoption of common tools, standards, and procedures—many of which we discuss in this chapter.

In addition to this stack of scientific software packages, we briefly introduce IPython,[5] a

[2]`http://numpy.org`
[3]`http://scipy.org`
[4]`http://matplotlib.org`
[5]`http://ipython.org`

system for interactive and parallel computing that has become the *de facto* standard environment for scientific computing and data analysis in the Python community. It was created by one of us (FP) in 2001 as an interactive command-line shell for Python, and has evolved into a large collaborative open-source project with contributions from a broad team of scientists [28]. We call special attention to it as the natural focus of our integrated approach to the computational life cycle. As such, it will serve as a primary example throughout the chapter and will be discussed in detail in § 1.5.3.

1.2.3 Communities of practice

While the case can be made for the use of open source software in science, even more important is the benefit that comes with open source community-driven development practices. In community-developed projects, the distinction between users and developers is more fluid than it is in proprietary software projects where this distinction is not just expected, but often rigorously enforced by legal mechanisms. This does not mean that everyone must become a *core developer*. There are still differing levels of contribution, which includes reporting issues, suggesting functionality, contributing enhancements, discussing use cases, answering questions, and much more.

Communities of practice must drive the development of our scientific software [32]. A participatory community of active researchers using and contributing to the development of the code we depend on for our scientific output is necessary for robust software ecosystems where we can share and verify our work. As this work becomes more reliant on computational tools and techniques the questions we can ask will be constrained by what our software can do and how easy it is to extend. Hence moving a field forward will increasingly require scientists to be computationally literate, part of which includes embracing the tools and practices widely adopted by the open source community.

There are real concerns that arise when attempting to transplant the practices of open source development directly to computational research. The open source development model is one where, in practice, the copyright and authorship of any large collaborative project is spread among many authors, possibly thousands. While the source control tools in use allow for a precise provenance analysis to be performed, this is rarely done and its success is contingent on the community having followed certain steps rigorously to ensure that attribution was correctly recorded during development.

This is not a major issue in open source, as the rewards mechanisms tend to be more informal and based on the overall recognition of any one contributor in the community. Sometimes people contribute to open source projects as part of their official work responsibilities, and in that case a company can enact whatever policies it deems necessary; often contributions are made by volunteers for whom acknowledgment in the project's credits is sufficient recognition.

In the academic world, the authorship of scholarly articles in scientific journals and conference proceedings is currently the main driver of professional advancement and reward. In this system, the order of authorship matters enormously (with the many unpleasant consequences familiar to all of us), and so does the total number of authors in a publication. While in certain communities papers with thousands of authors do exist (experimental high-energy physics being the classic example), most scientists need the prominent visibility they can achieve in a short author list. The dilution of authorship resulting from a largely open collaborative development model is an important issue that must be addressed.

Furthermore, the notion of a fully open development model typical of open source projects is at odds with another aspect of the scientific publication and reward system: the "first to publish" race. Many scientists are, understandably, leery of exposing their projects on an openly accessible website when in their embryonic stages. The fear of being scooped by others is real, and again we must properly address it as we consider how to apply the lessons of open source development to the scientific context.

1.3 Routine practice

The practices recommended in this section are distilled from writing and maintaining software, teaching programming courses to students and scientists, as well as extensive interaction and discussion with a diverse group of scientists and engineers. Whole books have been dedicated to best practices in software development with highly specialized tools and habits for individual programming languages and methodologies. In this short section, we highlight the practices and tools essential to any computational work. For a more detailed discussion, we recommend [17, 13, 1].

We begin by discussing practices and tools that should be applied to even exploratory, individual research. These practices are so essential to efficient and productive use of computational resources that we routinely use them whenever we use a computer. In § 1.4, we discuss how these practices and tools extend to collaborative work.

1.3.1 Version control

When collecting data, running analyses, or writing papers, you inevitably need to keep track of the various versions of your work: data is augmented and curated; code is adapted and improved; and writing is revised and expanded. While only keeping the most recent version of your work is possible, this is seldom sufficient. There are tentative new directions, detours, and dead ends.

We have witnessed numerous researchers attempting to manage different versions of their work using manual and laborious kludges. The most common patterns include using *ad hoc* naming schemes (e.g., `file.txt.bak`, `file.txt.1st`, etc.), emailing different versions to yourself, or using the application specific functionality such as Microsoft Word's "Track Changes" feature. While these approaches are partial solutions to the problem, they are also cumbersome, prone to failure, or limited to a specific applications. More importantly, they are unsustainable beyond simple scenarios with only one or two files and do not scale to any kind of sensible collaboration workflow.

Because tracking and managing how work evolves over time is so fundamental to the workflow of software development, programmers have created specialized software tools to do exactly this. These tools are called *version control* systems. Several open source version control systems (VCS) have been developed over the years, the most well known being CVS, SVN, Git, and Mercurial.

While there are notable differences among these tools, they all share some basic concepts. All project files (code, text, figures, etc.) are stored in a *repository* (often represented on disk in a directory hierarchy). There are commands to add and remove files to a repository. To track changes to a file, it must be *committed* to the repository, ideally with a meaningful *commit message*. The repository and commit mechanism provide a complete historical log of the project from inception to current state, including every change made along with timestamps, author, comments, and other metadata for each modification.

Code changes may follow a linear progression of commits. However it is more common for projects to include alternate development paths.[6] Given the exploratory nature of re-

[6]This tendency becomes more pronounced in collaborative projects (see § 1.4).

search, several approaches to a problem are often pursued simultaneously. In such cases, commits will resemble a tree with several *branches* diverging from a common base or trunk. When exploring these alternative approaches on different branches, several branches may eventually converge and need to be *merged* back together. If the changes in each of these branches do not overlap with one another, the VCS can merge them together in a completely automated fashion. When there are *conflicting* changes in different branches (e.g., edits to the same line of code), then manual intervention is required. But in all cases, a VCS is the only reasonable solution for managing the evolution of multiple branches of parallel development in a set of files (whether written documents, computer code, or data).

In the design of more modern VCS such as Git,[7] an important consideration is woven into the core of the system: built-in *data integrity verification* via cryptographically robust fingerprinting of all content. The basic idea is that at every commit, the VCS computes a "fingerprint" of the content being committed as well as the data it depended on.[8] This makes it possible to establish the integrity of the entire history of a repository at any point, by computing these fingerprints and comparing them against the stored one. By the nature of hash functions, even small changes will result in new hashes. This key design idea is used by VCS for all kinds of internal operations; but it also means that when a scientist gets a copy of a repository, he or she can be confident the content (including every recorded change) has not been tampered with in any way.

Strong guarantees on data integrity are a necessary condition of any reproducible workflow, and one of the reasons why we emphasize so much the pervasive use of modern version control systems as the foundation of a reproducible research environment.

It is important to note that VCS were developed for the management of human-generated content such as computer source code or text documents, not for the handling of large binary data that is common in science. By virtue of their design, they tend to be somewhat inefficient if you attempt to store all the changes in a project with many frequently changing large binary files, which somewhat limits their use for the tracking of all assets in a research project. But new efforts exist to mitigate these limitations, such as the git-annex[9] project, which uses Git for storing all metadata about large binary assets, along with a static (configurable) storage resource external to Git for the assets themselves. This approach makes it possible to smoothly integrate the management of binary data within a VCS workflow, without creating an explosion in the size of the VCS storage area.

The use of version control should become second nature; we routinely use it for everything—including the writing of this document.[10] We suggest researchers adopt a practice of pervasive version control: research codes, teaching materials, manuscripts, and data analysis projects should be developed, from the beginning, *always* using version control systems that track the actual history of everyone's contributions.

1.3.2 Execution automation

Just as it is impossible to reproduce old results if you don't have access to the code and data that created them (hence the need for version control), it is equally impossible if you did not record somewhere how the code and data were used. You could write everything down and manually follow these instructions again later on, but a more sensible approach is to record

[7]From this point on, we will mainly focus on Git, which is our preferred VCS. It is also the one that is mostly widely used in the scientific Python community.

[8]More precisely, a hash function is evaluated on the content of the commit and the hash of all commits it depends on, which creates a directed acyclic graph of hash values that signs the entire repository. Today these systems employ the SHA1 hash function, but other hashes could be equally used if necessary.

[9]`http://git-annex.branchable.com`

[10]`http://github.com/fperez/repro-chapter-oss`

them in a machine-readable way so that the computer can execute them. Furthermore, since most computational processes are a chain of executions where each step depends on the previous or on inputs that may have been modified, ideally you should be able to understand the structure of these dependencies and only run things when necessary.

Since building complex software with many source files is repetitive, full of detail, and time-consuming, this is another task for which the software development world has developed powerful, automated solutions. The venerable `make` system is the workhorse of process automation [30]. It has a declarative syntax for expressing dependencies between sources and targets and a simple (timestamp-based) mechanism for resolving when dependencies need to be rebuilt. To get an idea how this works consider the situation where a plot is created by a script, which reads a data file. In the parlance of `make`, the output `plot` is a *target* that depends on two *sources*—the data file and the script. If you type `make plot`, for example, `make` checks whether the script or data has been modified after the current plot was generated; if so, it calls the script on the data to generate an updated plot. In this simple scenario, using `make` does not offer much more than just running the script by hand. However, if the data this script consumes is generated by a chain of other scripts and data files, then the benefit of `make` becomes apparent.

More modern systems also exist, and a detailed review of the options is beyond our scope. But whether running a sequence of scripts to produce some figures, compiling your software, or creating the final PDFs for a grant proposal, you should be able to do so by typing `make results` or the equivalent syntax in your system of choice. Once things are automated in this way, it becomes possible for others (humans or machines, and even yourself on a new system or months later) to reliably repeat the process.

1.3.3 Testing

Computing is error-prone. While there is no foolproof way to rid computing of error, there are ways to limit and reduce it. One of the most successful and widely used techniques involves comprehensive testing, so that bugs (i.e., errors) are found quickly. Finding bugs as soon as possible in the development process is extremely valuable. Depending on the nature of the bug, it may reveal a fundamental problem with the overall design of your code requiring months more of coding. Even small errors that are easily fixed may require rerunning months of analysis. To reduce the amount of time it takes to uncover bugs and to ease the pain of debugging your code, it is essential to adopt a rigorous testing practice up front.[11]

Testing should be performed on multiple levels and begun as early as possible in the development process. For programs that accept input either from a user or file, it is important that the code validates the input is what it expects to receive. Tests that ensure individual code elements (e.g., functions, classes, and class methods) behave correctly are called *unit tests*. Writing unit tests early in the process of implementing new functionality helps you think about what you want a piece of code to do, rather than just how it does it. This practice improves code quality by focusing your attention on use cases rather than getting lost in implementation details. By thinking about the test at the outset, you can avoid finding that the code you just wrote is a huge, untestable mess. It also improves documentation because an example (i.e., the test case) is often better than an explanation. And if you regularly run the test, you will quickly know when your code no longer works for the example (something you may never notice in the case of explanatory text). Finally,

[11]While testing is an extremely useful practice, we should also point out that it is often more interesting work than debugging.

unit testing leads to more robust code as you will more quickly isolate bugs, which makes them easier to fix [26].

Testing is mainly a language-specific pursuit (as it must be implemented in the programming language of a given project to be most effective). The authors are most familiar with the Python-based world, and [4] is a good hands-on starting point for the tool most widely used in scientific Python projects, namely the nose[12] testing framework.

1.3.4 Readability

While writing code that is well tested and systematically managed by a modern VCS is important, code that is not easy to read will be difficult to understand, correct, and modify. Readable code is written with explanatory names, clear logical structure, and comprehensive documentation where necessary. There is an extensive and growing literature on stylistic aspects of good programming [3, 9, 17, 13, 21]. Because scientific papers and grant submissions have become the currency of the scientific realm, many scientists have read classics such as Strunk & White's *Elements of Style*. Yet, even as an increasing amount of our work is produced in lines of code, there is a paucity of scientists paying the same attention to the elements of good programming style. The emphasis on readability is included in this section because even when you are the only one using or working on your code, the chance that you will need to read your own code is high. Even when your code is widely used and shared, you will still often be the one most frequently reading it.

Self-documenting code, as the name implies, reduces the need for external documentation by placing an emphasis on clear, well-written code that is easy to read and understand. In mathematics, it is accepted practice to follow established naming conventions (e.g., capital letters for sets and lower case letter for set elements). It is equally expected that when making a mathematical argument, one shouldn't arbitrarily switch from functional to relational notation. Similarly, using consistent and uniform naming conventions when programming should be standard practice. Brevity in naming should be balanced against explicit and descriptive words. For example, you might use the term `download` rather than `get` in a function call to download a specific dataset from the Internet. Expressions are the next block to readability. While mathematical manipulation (e.g., De Morgan's laws) can be used to great effect in making your expressions more easily understood, it is often important to use the right level of abstraction. Higher-level programming languages (e.g., Python and R) provide data structures (such as n-dimensional vectors or statistical formulas) that enable the code to be more readily understood at the level of the mathematical ideas they implement. Finally, the overall control flow of your code must be clear and easy to follow. Finding the best control flow requires a deep understanding of your problem and an in-depth knowledge of programming methodology and the specifics of the language you are using. Like good writing, good coding is achieved through deliberate practice.

Inspired by the idea of self-documenting code, some argue that good code does not need comments. Indeed, liberally commenting your program to compensate for poorly written, obscure code is counterproductive. Comments that merely explain how a piece of code works add limited benefit. If code is so obscure to need explanation, it is better to revise or rewrite it. Another limitation of comments (as with many types of documentation) is that it is often uncoupled from the actual code. This means that there is no way to ensure that the two do not diverge. And, if they diverge, it may not be obvious which is correct.

To illustrate how comments and documentation *can* enhance readability of your code, we discuss the commenting and documentation system that has been developed by NumPy and is used by other scientific Python projects. While this section is specific to the tools

[12]`http://nose.readthedocs.org`

and processes put in place in the scientific Python community, the general ideas are more broadly applicable.

In 2007, NumPy lacked good reference information for the various functions, classes, and modules it provided. Users and developers had access to the source code, a nearly 400 page "Guide to NumPy", and an active mailing list. Yet, it was clear that this level of documentation was not enough. To address this, the community began a yearlong effort to develop a *documentation string standard*.[13] In Python, a documentation string (or docstring) is any string in the first line in an object's (e.g., function, class, etc.) definition. Since docstrings are embedded in the source code, they are readily available to anyone directly viewing the source. When the code is executed this string is associated with the object and can be programmatically accessed and used by introspection tools such as IPython. Docstrings can also be accessed for autogenerating documentation. Similar functionality exists in other programming languages such as R. Even in languages that don't include this functionality, it is common practice to include comments at the beginning of object definitions that are used similarly.

Given our desire for better documentation and wanting to leverage Python docstrings, the discussion focused on what they should include. Besides the information such as a brief statement of purpose as well as input and output parameters, we identified several issues with particular relevance for scientific applications. For instance, many algorithms had simple mathematical expressions that were not immediately obvious from their implementation in Python, but which a few equations written in LaTeX make clear. Often, our code implemented functionality described in peer-reviewed academic journals that could be referenced. Finally, we could provide short mini-examples of how to use the code. Since Python makes it easy to include examples in the docstrings as part of the test suite, this also improves test coverage and helps ensure that the documentation doesn't get out of sync with the actual code. These types of standards encourage contributors to explicitly think about input, output, equations, examples, and references. This, in turn, helps promote more deliberate and rigorous coding practices. And when reviewing code already written, having these details recorded aids in understanding whether the code is performing as expected.

1.3.5 Infrastructure

For small projects, managing everything by hand may be straightforward. But as your research project (code, data, and text) evolves, the burden of running your tests, building your project, and generating reports will become overwhelming. Eventually you will need tools and procedures in place to take care of these details for you. Even when the project is small enough that you can manually manage things, automating these tasks can be extremely beneficial [7].

We have often seen colleagues shy away from adopting certain practices related to the infrastructure that supports their computational research with claims of not having enough time or energy to invest in learning how to use them. This is a good example of being penny wise and pound foolish: a small initial investment in learning best practices pays off manyfold over time in increased productivity and smoother workflows that can support collaboration and scale to complex scenarios. The manual execution and repetition of common computational tasks may appear like an easy solution, but it is error-prone and impossible to apply reliably in collaborative settings beyond two or three people.

In the next section we will discuss collaborative scenarios, but we want to address first how certain tools and practices have enormous value even for the individual researcher.

[13]`http://github.com/numpy/numpy/blob/master/doc/HOWTO_DOCUMENT.rst.txt`

And these are precisely the foundation that will then make it possible to naturally evolve a project from a single-person effort into a collaboration without a breakdown of complexity.

Hosted version control. While Git can be used purely locally, there are many advantages to having your repositories replicated on a server that is externally accessible. Git's design allows it to simultaneously keep track of multiple repositories tied to a single project, and it can synchronize and merge work between these multiple sources. Each of these sources is denoted a *remote* in Git lingo, and while a remote can be simply another location in your hard drive, the most useful kind of remotes are those that are physically in other computers. By synchronizing your local repository with an external remote you simultaneously have an automatic backup of your entire project's history. But more importantly, this external remote is now available to synchronize with *other* computers, so you can cleanly and robustly sync multiple machines, even if you do independent development on each of them at some point.

There are many services online that host repositories from Git and other version control systems; in recent years GitHub[14] has gained wide adoption among the community of scientists who write open source software in Python and R. As we discuss in § 1.4.2, these systems truly shine once you use them to *collaborate* with others, since collaboration hinges on the ability of multiple parties to synchronize their work.

Continuous integration. Once your computational code is stored in version control repositories, has tests and scripts that automate the execution of these tests, then it becomes possible to have a machine do this for you, all the time, bugging you only when something goes wrong. This is known as *continuous integration* (CI). CI systems are servers that grab the most recent version of a project from version control, execute the test suite, and gather statistics of this process. They are typically configured to log and summarize these results, and to only produce alerts when something goes wrong (typically by email, but more aggressive options such as SMS are possible). The amount of data collected during the test execution can be configured, so it is possible to have setups that range from a basic summary of success and failure to a detailed collection of metrics on the performance evolution of a codebase.

These systems are called *continuous* because they are meant to be used all the time: as the codebase evolves (typically when changes are committed to an official version control repository), the system fires automatically and collects its data. Therefore, these systems can also fulfill an important role: over time they accumulate a *historical retrospective* of a project's evolution. And this is where the importance of collecting detailed metrics is realized: a CI system configured to do a fairly detailed analysis of a project when it runs becomes an invaluable tool to analyze what is happening over time. Is performance degrading in subtle ways that are not evident from day to day? Is the fraction of code that is tested (known as the *test coverage*) going down over time, indicating that new contributions are not being tested as thoroughly as the older code? Questions like these are impossible to answer in a manually managed workflow, yet they come *for free* once a few tools are set up, and can be an extremely important part of managing a healthy computational pipeline. A more detailed discussion of Continuous Integration can be found in [5].

While a number of these tools exist, one of the most widely used by projects from many different programming languages and communities is called *Jenkins*.[15] Jenkins is a highly configurable CI system that can be run on a personal laptop or internal server and that is available hosted in the cloud as a service from a variety of sources. *Travis CI*[16]

[14]`http://github.com`
[15]`http://jenkins-ci.org`
[16]`http://travis-ci.org`

is a purely hosted CI system that, while not as configurable for fine-grained statistics as Jenkins, requires minimal setup, is free for open-source projects, and is tightly integrated with the version control hosting service GitHub.

Documentation generation systems. We have already discussed the importance of documenting your code, and in recent years a number of systems have been developed that allow you to easily produce complex documentation that combines hand-written narrative sections with parts that are automatically extracted from the code. While the ability to automatically extract and generate documentation is valuable and important, we stress that it is critical that your projects have at least a modicum of *narrative* explaining the purpose of your tools, their scope, how to use them—with examples, and how the various concepts fit together. This kind of information cannot be gleaned from automatically extracted fragments that refer to individual function calls, and without it, your tools will be much less useful as a building block of robust scientific practice.

A number of tools exist for the generation of documentation, from the well-known LaTeX to systems focused on the generation of source-based documentation such as Doxygen[17] and newer ones designed for a combination of narrative and automatic documentation, like Sphinx.[18] There are other such systems, but Doxygen and Sphinx are widely used in the software world, actively developed and with rich toolkits that support complex documentation tasks.

Before discussing these tools, it is important to note that in recent years, new formats for *authoring* documentation have emerged, in particular reStructuredText[19] (often abbreviated as reST) and Markdown.[20] These formats have slightly different philosophies, but they both aim at being more friendly to manual authoring and reading than LaTeX, while supporting more convenient integration with HTML output. They both share the basic philosophy of looking like plaintext with simple visual markup for commonly used tasks, for example marking emphasis and boldface with asterisks (e.g., `*italics*` → *italics* and `**boldface**` → **boldface**). Markdown is aimed at the production of HTML and is a strict subset of HTML; it defines only a few special markup rules and leaves more complex tasks to be done by hand in pure HTML. In contrast, reST is a highly extensible format, where new commands (called "roles" and "directives") can be created and where the user can define entire new output pipelines by adding plugins written in Python to the processing stream. For example, the SciPy Conference Proceedings[21] are written in reST and the PDF version is generated by a custom LaTeX translator written in Python.

So while Markdown is simple and easy for the production of simple HTML, it is not well suited to the generation of complex multipart documents with rich internal cross-referencing, bibliographic support, etc. Both Markdown and reST support LaTeX for mathematical expressions, and with the right toolchain for rendering the output they can generate a final PDF document that has been typeset by LaTeX. In talking about new documentation formats it is important to mention the universal document converter, pandoc.[22] Pandoc is capable of translating between many document formats, including taking Markdown or reST input and producing HTML, LaTeX, and many other formats. It is an invaluable tool in managing a modern documentation workflow.

Returning our attention to systems that produce final output based on these formats, Doxygen has its own syntax that combines HTML with special commands for many tasks

[17]http://doxygen.org
[18]http://sphinx-doc.org
[19]http://docutils.sourceforge.net/rst.html
[20]http://daringfireball.net/projects/markdown/syntax
[21]http://github.com/scipy/scipy_proceedings
[22]http://johnmacfarlane.net/pandoc

specific to computer source code, such as the specification of variable types, function arguments, and return values, etc. It also supports Markdown, allowing users to use this more readable and concise syntax for the generation of common HTML markup. Sphinx, on the other hand, is designed around reStructuredText: it supports the basic format and provides a number of additional extensions aimed at the documentation of software projects. Sphinx was originally developed to produce the official documentation for the Python programming language, but has become much more widely used. For instance, the SciPy community has developed an online wiki-like documentation editing system [33] on top of Sphinx that leverages the documentation standard discussed in § 1.3.4, dramatically increasing the extent and quality of the NumPy and SciPy documentation.[23] Today most Python projects use Sphinx as their documentation system, and because of the flexibility and extensibility of reST, it has also become widely used as a way of creating rich, complex documents with a strong computational base even beyond Python. There are even some statistics courses taught in R, which use Sphinx to create web-based notes with embedded R code and automatically generated output.[24]

We note that all the formats we have discussed here, LaTeX, HTML, Markdown, and reST, share one critical feature: they can be hand-written in a plain text editor and they are stored in files amenable to version control with the tools described earlier. This stands in contrast to the binary formats of Microsoft Word and similar tools that lead to a terrible version control experience and which we avoid in computational workflows.

1.4 Collaboration

Open source developers build on one another's work just as scientists build on each other's work. Since development communities are geographically spread and often dependent on contributions from volunteers, there has been careful attention paid to efficient and productive tools and processes for managing collaborations. As scientific practice becomes increasingly computational, it is imperative that we learn from the collaborative practices used in the open source world.

1.4.1 Distributed version control

Earlier we discussed how version control system (VCS) should be the foundation of a reproducible research workflow, even for a single investigator working in isolation. But the true power of these systems comes into its own when considering the need to collaborate with others. Modern systems such as Git and Mercurial were designed from the ground up for large-scale distributed collaboration: Git was written by Linus Torvalds, the creator of the Linux kernel, to coordinate its development. The Linux kernel is arguably the largest and most complex open source development project today: version 3.7 of the kernel included roughly 12,000 distinct sets of changes affecting over 1,100,000 lines of code by nearly 1,300 individual contributors.[25] Git's entire design aims to make collaboration on this scale smooth and efficient, and it succeeds admirably. Scientists can benefit from this power as well for any project that requires collaboration, whether it is the development of

[23]`http://docs.scipy.org/doc`
[24]`http://www.stanford.edu/class/stats191`
[25]`http://lwn.net/Articles/526748`

an open source research code or the writing of a manuscript or grant proposal with multiple authors.

Git and other tools like it are called *distributed* version control systems (DVCS) because they don't depend on a central server for their functioning, instead maintaining the entire history of a project inside every repository. This is in contrast to legacy systems such as CVS and SVN, that made a distinction between the "working copy" that users would work on and which contained only the most recent version of files, and a special repository hosted on a central server that had the entire project history. The centralized model does enable collaboration, but it also creates a number of problems that the distributed model addresses. In a DVCS there is no single point of failure, as every repository carries all the project history and therefore serves as an automatic backup.

More importantly, a DVCS enables anyone who can *clone* a repository (the term used to indicate getting a full copy of an existing repository to start new work off of it) to develop their own history with new commits, even if they don't have write permission to the original source from where the repository was cloned. This means that once you have a clone of a repository (which could be someone else's or yours from a different computer), you can start working on that copy and building new history even if you are disconnected from the original system, such as when working on a plane or train without network access. If at a later stage you decide to merge your new history with the original repository, the merge capabilities in all DVCS make this straightforward.

This model of cloning an existing repository, building new history in isolation and then merging it back into a common history, is the basis for how these systems enable a fluid workflow for collaboration. When the time comes for a merge operation, DVCS can communicate the necessary changes even via email attachments, but the simplest way to do so is to have a special repository[26] in a common location that all parties have access to and where the changes are *pushed*. Pushing, as the term suggests, means sending the set of changes from one repository into another; once the changes have been put into this central repository, all parties can *pull* them into their personal copies to synchronize their states and continue working again. So in practice, the simplest and most common collaboration workflow with a DVCS is one where each person has a copy they develop on, and they all connect in a star topology to a central node where a shared copy exists that is used for synchronization.

1.4.2 Code review

In recent years, a number of web services have appeared that play the role of this central node; the most popular of them by far is GitHub,[27] but others such as BitBucket[28] and Gitorious[29] play similar roles. GitHub has had a tremendous impact in the open source community, reaching in a few years millions of active users and gaining rapidly popularity in scientific circles. We can attest to the power of this platform with our own experience: IPython moved its development to GitHub in early 2010 and immediately saw a rapid uptick in the pace of contributions. The workflow for collaboration enabled by GitHub was so much smoother than all previously available tools that many people were more willing to send

[26]We note that this central repository does not change the distributed nature of the process: while it plays a special role for purposes of *synchronization*, the central repository is otherwise completely symmetrical to everyone's personal copy in the information it holds, and can be replaced at any time in case it is lost or damaged from anyone's copy.

[27]`http://github.com`

[28]`http://bitbucket.org`

[29]`http://gitorious.org`

contributions, while the core team was able to review and integrate these contributions at a much more rapid pace.

The core element of the collaborative process on GitHub is known as a *pull request*, and it is something akin to a public peer review of a set of changes to a manuscript. Let us illustrate how it works with a simple example: Alice wants to contribute to IPython, a project available on GitHub[30] but to which she does not have write access. She can do so by getting her own personal copy of the IPython Git repository where she makes all the changes she wants, and once she is ready to share them with the IPython team she can publish them on her GitHub user account.[31] At that point, she can click on a button to create a pull request for these changes: this contacts the IPython developers and creates a special page on the website that summarizes her changes as well as allowing everyone to begin a discussion about the changes. This discussion page allows the developers to ask Alice questions (even making comments on specific lines of her new code), and she can respond to these questions, update her code with new commits in order to address any required improvements, etc. Once the IPython developers are satisfied with this review and discussion (which may happen immediately or may require a lengthy back-and-forth process, depending on the changes), they can apply the changes to the official IPython repository with a click of a button. Once the changes are merged, they become part of the official project source and every individual commit that was merged is credited to Alice from the time she made it while she was working on her personal copy. Furthermore, even closed pull requests remain available on the website to inform future discussions, making the entire collaboration process an open one.[32]

The pull request process allows for a dynamic and open peer review process of all proposed changes to a project. The only special role that the official project authors have is the ability to approve the final merging of new changes, but otherwise everyone participates on an equal footing in terms of access to tools. This highly symmetrical structure proves to be extremely beneficial in encouraging a meritocratic process of contribution and review, where there are few points of special authority and where the discussions can remain focused around the contribution that initiated the pull request. Paraphrasing how some of the GitHub employees describe the process in public presentations: "a pull request is a conversation that starts with code."

From a scientific research perspective, we should consider these ideas in a broader context that goes beyond code: while peer review is one of the pillars of how the scientific community moves forward, in practice modern scientific peer review is often an opaque, arbitrary, and limited process. The open, dynamic, and ongoing process of peer review enabled by the GitHub pull request system (or the equivalent ones that exist on other similar services) stands in sharp contrast to some of our institutional traditions, and our community could benefit significantly from adopting these ideas in a in our own review practices [11].

It is worth noting that by using a DVCS, authors can maintain private branches in the context of a publicly available project; this can be useful if new work needs to be developed in private prior to publication and subsequent public release. By tracking the public repository but keeping a private branch, they can maintain exclusive access to their new work until it is published, while continuing to develop the openly accessible code with the rest of the scientific community. Once the code is ready to be made public, the new contributions can be seamlessly merged with the public version and their entire provenance (including information such as time of invention and individual credit within the lab) becomes available for inspection. This simple observation shows how these tools can be used to balance the

[30] `http://github.com/ipython`

[31] `http://gitub.com/alice/ipython` if her GitHub user name is `alice` for example

[32] `http://github.com/ipython/ipython/pull/1732` is an example pull request and the entire, recorded review process

sometimes valid requests for privacy that may exist in a research environment with the desire for subsequent disclosure and publication, without losing any of the benefits of version control with regard to attribution and provenance tracking.

1.4.3 Infrastructure redux

Once we have adopted tools that allow for distributed collaboration (e.g., Git and GitHub) and our computational machinery has tests and scripts that allow for automated installation and execution of the test suite, we achieve a number of important benefits that we can think of as *machine collaboration.* That is, once we have described in a standard way how our software must be installed or tested, then not only can our colleagues do that as they start collaborating with us, but so can machines. The Travis CI system, for example, can be configured to automatically run a project's test suite on every pull request created on GitHub. This means that when the humans come to review the proposed code, a report is already attached to the pull request that indicates whether the test suite passed or not (and provides details of any failures). This can save enormous amounts of time and make the collaboration much smoother, as reviewers don't need to wait before starting a new review for the tests to complete on their system, and may even review when they are away from a development machine capable of actually running the tests. In the IPython project we have seen the value of having this information always ready, as it reduces the small but persistent amount of 'friction' we had before when each reviewer was responsible for running all tests first locally for each new pull request. While we still have tools for that and occasionally run tests beyond what Travis does (as Travis doesn't install every optional library we require), saving even five minutes for each review can make a huge difference for a project that sometimes has to process multiple pull requests in a day.

In a similar vein, the ReadTheDocs[33] project does for documentation what Travis does for CI. ReadTheDocs hosts documentation built with Sphinx, but more importantly, can be configured to automatically build it when new commits are made to the project at GitHub. In this way, users can always find a fully updated build of the project documentation without developers having to spend time on this.

Automated CI testing and documentation building are only two aspects of the benefits that can be gained from building on a foundation of distributed version control, well automated processes, integrated test suites, and documentation generation. Once all these elements come together, a virtuous cycle can be sustained where the focus of the scientists or developers can be on producing new results (be they text, code, or computational outputs) and this machinery ensures that everything is validated and documented along the way.

While some of these points are more easily applied in the context of pure software development, the critical thing is how these ideas and tools work in concert to produce an environment of robust, reproducible results. Adopting this viewpoint, it is always possible to adapt to the specifics of any given project and apply only what is relevant. We conclude noting that the practices, tools, and ideas described in the previous two sections (§ 1.3 and § 1.4) may be put to use relatively quickly, but writing high-quality, trustworthy, scientific code is not easy. Mastery and expertise in developing reliable code that can be trusted to provide valid results takes sustained focus and deliberate practice.[34]

[33]`http://readthedocs.org`
[34]`http://norvig.com/21-days.html` is recommend reading

1.5 Communication

Instead of imagining that our main task is to instruct a *computer* what to do, let us concentrate rather on explaining to *human beings* what we want a computer to do.

Literate programming (1984)
Donald Knuth

Whether engaging colleagues in data analysis, educating students about numerical algorithms, or publishing computational results, scientist need to ultimately convey their computational work to others—not just the artifacts of that work, but the specific details of how those artifacts arose. We begin with a brief description of some existing tools for literate programming as a backdrop to present a more recent approach we refer to as literate computing. Again, our view is shaped by the desire to tackle the life cycle of computational research described in § 1.2.1 in an integrated way. From this perspective, we argue that the literate computing approach is a better fit to the needs of reproducibility in computational research than traditional literate programming tools, and will present the IPython notebook as an example implementation.

1.5.1 Literate programming

Donald Knuth proposed *literate programming* in the early 1980s and a complete description of this approach to computer programming can be found in his later book of the same title [19]. Knuth's concern was the development of a better approach to documenting computer software; he devised a process whereby programmers would write literate source files that describe in full prose the ideas underlying a given program, interspersed with the code fragments implementing the actual computations. Knuth developed tools that can process these input files to produce two different representations: a *tangled* code file meant for compilation and execution by a computer, and a *woven* file containing the formatted documentation. Knuth's original implementation, the WEB system [18], was focused on producing Pascal code and LaTeX documentation, but this basic idea has been extended to many other programming languages and documentation systems.

The R community has embraced the ideas behind literate programming, and a mature implementation of the concept exists for R in the Sweave system [20]. Sweave is one of the central elements of the Bioconductor system [10, 8] for computational biology and bioinformatics. All Bioconductor packages must be accompanied by at least one *vignette*, a literate program that contains executable code illustrating the tasks the package is meant to perform. Vignettes can be read in PDF format, but functions exist to automatically extract all the R code for immediate execution. The journal Biostatistics encourages authors to use literate programming tools such as LaTeX and Sweave when submitting articles they wish to be designated reproducible [27].

A new entrant to the R community that is gaining rapid adoption is the knitr package.[35] Knitr can be seen as a highly evolved Sweave with a number of improvements, but still within the conceptual lineage of literate programming tools. The use of literate programming tools are gaining increasing traction in statistical education as well. For instance, at UC Berkeley, students taking computational classes in both the Statistics Department and the Division of Biostatistics are encouraged to use LaTeX with Sweave or LaTeX (or R Markdown) with knitr.

As the above examples suggest, literate programming has been most commonly adopted

[35]`http://yihui.name/knitr`

when the desired final document is intend primarily for human consumption. Few, if any, large software libraries are written this way. In fact, the most prevalent use of literate programming has been among scientists to communicate computational ideas and results to one another. These ideas have also influenced open source software projects where tools have been developed to automatically generate project documentation based on source files and to create *live documentation* containing the output from embedded code run during document generation (see § 1.3.5).

1.5.2 Literate computing

Tools described in the previous section for literate programming are mature and have been used to great effect to improve the quality of documentation in scientific programs and data analysis, especially in the R community. But they remain rooted in the original model proposed by Knuth, of authoring a literate file that is then post-processed by various tools to produce either documentation or executable code.

In this section, we present an alternate approach to improving the connection between code and documentation that we refer to as *literate computing.* Our choice of terminology emphasizes the act of computing itself rather than the writing of code, as the systems we describe are all centered around *interactive environments* where the user can enter code for immediate execution, obtain results, and continue with more commands that produce new results based on the previous ones. A literate computing environment is one that allows users not only to execute commands but also to store in a literate document format the results of these commands along with figures and free-form text that can include formatted mathematical expressions. In practice it can be seen as a blend of a command-line environment such as the Unix shell with a word processor, since the resulting documents can be read like text, but contain blocks of code that were executed by the underlying computational system.

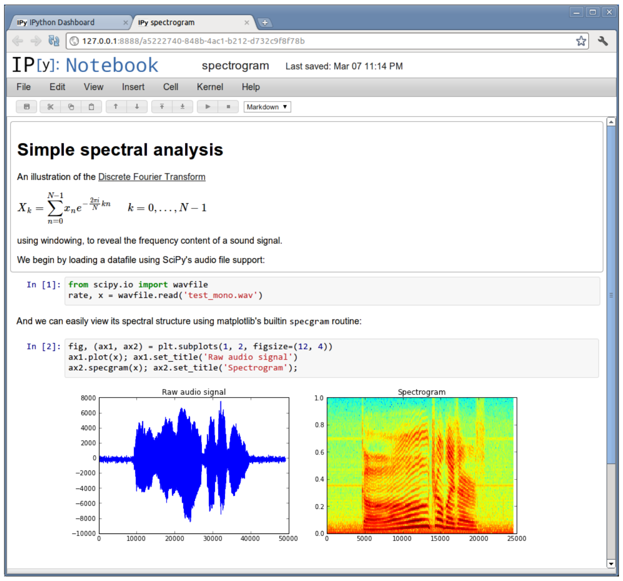
The earliest full-fledged implementation of these ideas is the graphical user interface of the Mathematica *Notebook* system, which dates back to early versions of Mathematica on the NeXT computer platform and took advantage of the superior graphical capabilities of NeXT. Today a number of other systems (both open source and proprietary) provide similar capabilities; on the open-source front we notably mention the Maxima[36] symbolic computing package, the Sage[37] mathematical computing system, and the interactive computing project IPython, on which we will focus the rest of our discussion.

1.5.3 IPython notebook

In 2011, a web-based notebook was developed in IPython that connects to the same interactive core as the original command-line shell, but does so using a web browser as the user interface, automatically enabling either local or remote use as the system running the web browser can be different from that executing the code, with all communication happening over the network. Fig. 1.1 shows a typical notebook session with code, text, mathematics, and figures.

The driving idea behind the IPython Notebook is to enable researchers to move fluidly between all the phases of the research life cycle described in § 1.2.1. If the environment where we conduct our exploratory research can also support all subsequent stages of this cycle, and does so while smoothly integrating with the version control and process practices we've previously espoused, the likelihood that a final published result will be reproducible

[36] `http://maxima.sourceforge.net`
[37] `http://www.sagemath.org`



Simple spectral analysis

An illustration of the Discrete Fourier Transform

$$X_k = \sum_{n=0}^{N-1} x_n e^{-\frac{2\pi i}{N} kn} \qquad k = 0, \ldots, N-1$$

using windowing, to reveal the frequency content of a sound signal.

We begin by loading a datafile using SciPy's audio file support:

```
In [1]: from scipy.io import wavfile
        rate, x = wavfile.read('test_mono.wav')
```

And we can easily view its spectral structure using matplotlib's builtin `specgram` routine:

```
In [2]: fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(12, 4))
        ax1.plot(x); ax1.set_title('Raw audio signal')
        ax2.specgram(x); ax2.set_title('Spectrogram');
```

FIGURE 1.1
The web-based IPython Notebook combines explanatory text, mathematics, multimedia, code and the results from executing the code.

increases significantly. The Notebook system is designed around two central ideas: (a) an openly specified protocol to control an interactive computational engine, and (b) an equally open format to record these interactions between the user and the computational engine, including the results produced by the computations.

Before diving into the specifics of these two ideas, we note that the above design is independent of the Python language: while IPython started its life as a Python-specific project, the vision of the Notebook system is language-agnostic. First, while working in Python, users can mark entire code blocks for execution via a separate language by using a special syntax on the block's first line: a user can for example start a block `%%R`, `%%octave`, `%%bash` or `%%ruby` and IPython will execute the entire block with the respective system. The development community is also busy implementing similar support for new and experimental scientific languages such as Julia, enabling a user to control from a single IPython notebook a workflow that combines the most commonly used high-level languages in modern scientific computing. Second, an *entire notebook* can be executed in a different language if a remote engine (referred to as a *kernel*) exists that implements the interaction protocol. As of this writing, prototype kernels are being developed for Ruby, JavaScript, R, and Julia.

The IPython architecture provides a way to capture, version control, re-execute, and convert into other output formats, any computational session. Notebooks can be shared with colleagues in their native form for re-execution or converted into HTML, LaTeX, or PDF formats for reading and dissemination. They can be used in slideshow mode to give presentations that remain connected to a live computation and can be exported into plain scripts for traditional execution outside of the IPython framework.

The IPython protocol consists of messages in JSON (JavaScript Object Notation) format that encode all actions that an interactive user can request of a computational kernel, such as executing code, transferring data, or sending results, among many others. While this protocol is implemented in IPython, it can be independently implemented to provide new kernels also able to interact with the notebook interface and clients. The notebook file format is a simple JSON data structure that contains a series of one or more worksheets, each of which is a list of cells. A cell can contain either text or code, and code cells can also have the output corresponding to the execution. All sub-structures in the notebook format (the entire notebook, the worksheets, and the individual cells) have attached flexible metadata containers; this metadata can be used by post-processing tools. The file format stores the communication protocol's payloads unmodified, so it can be thought of as a structured and filtered log (since the user chooses what to keep while working interactively) of the computation.

The IPython project has taken elements pioneered by the Mathematica and Sage notebooks and created a generic protocol and file format to control and record literate computing sessions in any programming language. This was a deliberate choice in contrast to the literate programming approach: by providing a tool that operates close to the live workflow of research computing (in contrast to the batch-processing mode encouraged by classic literate programming tools), the resulting documents are immediately reproducible sessions that can be published in their own right or as companion materials to a traditional manuscript. Given how IPython also includes support for parallel computing, which we don't discuss here in the interest of conciseness, the system provides an end-to-end environment for the creation of reproducible research.

The real-world possibilities this offers were demonstrated during a collaboration in 2012 between the IPython team, a microbiology team led by Rob Knight from the University of Colorado and Greg Caporaso from the University of Northern Arizona, and Justin Riley from MIT who created the StarCluster[38] system for deployment and control of parallel resources on Amazon's EC2 cloud platform. As part of an NIH-funded workshop to explore the future of genomics data analysis in the cloud, this combined team collaborated on creating a fully parallelized analysis comparing the predictive behavior of different sizes and locations of gene sequence reads when reconstructing phylogenetic trees. The microbiologists had developed a serial prototype of this idea using their Qiime libraries [6], but a large-scale analysis with a full dataset would require roughly a month of CPU time on a single workstation. By locating the IPython Notebook server on Amazon cloud instances, the entire team was able to log into a single instance and by editing the code directly in the cloud, in a single day turn this prototype into a set of production notebooks that would execute the analysis in parallel using multiple Amazon servers. Once the parallel code was tested, it became evident that there was not only an interesting example of using cloud technologies for rapid development of research ideas but also a biologically relevant finding; within a week the team had completed a more extensive run using 24 hours of execution on 32 nodes and submitted a manuscript for publication [31]. This paper is now accompanied by all of the IPython notebooks that enable any reader to fully reproduce our analysis, change parameters and question our assumptions, without having to re-implement anything or be hampered by lack of access to the code and data. We have made available not only the final notebooks, but also the Amazon Virtual Machine Images (data files that represent a virtual computer on Amazon's cloud platform), so that the entire analysis can literally be re-executed under identical conditions by anyone with an Amazon account.

This example, anecdotal as it may be, indicates the validity of the vision we propose here: that by providing tools that encompass the entire cycle of research, from exploration to large-scale parallel production and publication, we can provide the scientific community with results that are immediately accessible to others and reproducible, seeding the continued evolution of the research process.

The IPython project has also developed tools to make it easy to share and disseminate

[38]`http://star.mit.edu/cluster`

content created as notebooks in a variety of forms. The Notebook Viewer[39] is an online service that renders *any* publicly available IPython notebook as a web page. This enables users to share notebooks by simply putting them online and pointing colleagues to the rendered webpage. The same technology that powers the notebook viewer service can also generate HTML files suitable for inclusion in other websites, in particular, blogs. Since a lot of rapid technical communication is happening today on the Internet via blogs, this is an important aspect of linking reproducible research to the rapid feedback cycle of web-based discussion. With a single command, a user can convert a notebook file into HTML ready for posting to a blog, and this is already being used by scientists to write both short technical posts and also more complex materials: Jose Unpingco, a researcher with the US Department of Defense, is currently working on a book titled *Python for Signal Processing*, and this book is available during writing as a GitHub repository.[40] This repository contains a series of IPython notebooks so that readers can directly execute the code in the book, and they are also being published as a series of blog posts as they become available,[41] so readers can comment and discuss with the author throughout the process of book development, and they can do so based directly on the actual code that creates all the examples in the book.

The signal processing book is, to our knowledge, the first example of a full book being written as a collection of executable IPython notebooks, but this follows a tradition created by Mathematica, whose documentation is itself a collection of executable Notebooks. Furthermore, in recent years Rob Beezer, from the University of Puget Sound, has developed a popular Introductory Linear Algebra book [2] that is based on the Sage system and also combines the mathematics and text with code that can be directly executed and modified by the readers. This ability to "close the loop" between what the authors had on their screens and what their readers can execute themselves is an important element of the movement towards reproducibility in research.

As a concrete implementation of the ideas of reproducible research using the tools we've described in this chapter, during the ongoing process of research itself, we can point to work being carried by a collaboration where one of us (FP) is a member, on novel ways to model the mathematical structure of the signal generated by MRI devices in the imaging of water diffusion in the brain. This work, as yet unpublished, is being developed as an open repository on GitHub[42] where all code for our research is posted during writing, all computational experiments are created as IPython notebooks, and submitted manuscripts are created directly from the code and notebooks (along with additional narrative written by hand).

The above tools are also playing a central role in the last stage of the computational research life cycle, education. We will increase our chance that the next generation of scientists adopts improved reproducibility practices if we educate them with the same tools that we use for everyday research, and a couple of modern efforts that aim to bring improved computational literacy to scientific research have adopted the IPython notebook. Software Carpentry[43] is a project funded by the Alfred P. Sloan Foundation and led by Greg Wilson at the Mozilla Foundation whose motto is Richard Feynman's famous "What I cannot create, I do not understand." They produce, with rigorous follow-up and assessment, workshops aimed at working scientists (typically graduate students and postdoctoral researchers, but always open to broad audiences) and whose purpose is to instill in them a collection of skills and best practices for effectively using computing as a daily research tool. The Software Carpentry workshops cover topics ranging from the basics of the Unix

[39]`http://nbviewer.org`
[40]`http://github.com/unpingco/Python-for-Signal-Processing`
[41]`http://python-for-signal-processing.blogspot.com`
[42]`http://github.com/fperez/spheredwi`
[43]`http://software-carpentry.org`

shell to version control, Makefile automation of processes and basics of scientific Python including data analysis and visualization. They have recently adopted the IPython Notebook as the base system for teaching the scientific Python parts of their curricula, and provide the IPython team with direct feedback on its strengths and weaknesses as an educational tool. In a similar vein, Josh Bloom from the astronomy department at UC Berkeley has led, for a number of years, 3-day workshops on the use of Python as a tool for scientific computing.[44] These are open to the entire campus community and followed by an optional for-credit seminar where students learn more advanced skills for using Python as a research tool. F. Pérez and other members of the IPython team at UC Berkeley regularly lecture in the bootcamps and courses, where the notebook is the means for delivery of course materials and interactive lecturing. While we have identified a number of weaknesses and areas for improvement, we have also found this environment to be markedly superior to all previous tools we had used in the past for teaching in similar contexts.

As these capabilities in IPython reach wider usage, with scientists now developing complete books and lecture series based on the system, we are considering a number of new challenges and questions introduced by these capabilities. The interactive computing model is a fluid and natural one, but we need to find ways to extend it into the development of longer-term production codes that are robust, documented, tested and integrated into reusable libraries. This means bridging the gap between a *scripting* mentality and a *developer* one, and while we have already made progress on that front in IPython, many questions remain open for the future.

1.6 Conclusion

As research grows increasingly dependent on computing, it becomes critical for our computational resources to be developed with the same rigor, review, and access, as the results they support. In particular, we believe that reproducibility in computational research requires: (1) sharing of scientific software, data, and knowledge necessary for reproducible research; (2) readable, tested, validated, and documented software as the basis for reliable scientific outcomes; (3) high standards of computational literacy in the education of mathematicians, scientists, and engineers; and (4) open source software developed by collaborative, meritocratic communities of practice.

Achieving these goals won't be easy. It requires changing the educational process for new scientists, the incentive models for promotions and rewards, the publication system [24], and more. In this chapter, we focused on the need for an open source ecosystem for scientific computing developed by communities of practice. We then introduced several tools and practices necessary—but not sufficient—for reliable code that can be the basis of reproducible research. We illustrated these ideas with examples of how they have been applied and advanced in the open source scientific Python community. Finally, we presented the IPython project's powerful combination of interactivity, distributed and remote computing features, and literate computing functionality as a natural integration point for the computational research life cycle in order to make it more fluid, efficient, and reproducible.

We emphasize that the mechanical reproduction of computational results is not an end in itself. The ultimate goal is to bring the rigor, openness, culture of validation and collaboration, as well as other aspects of reproducible research to our everyday computational

[44] `http://pythonbootcamp.info`

practices. This is not a goal we will happily attain one day and then move on to pursue another; it must become and remain an ongoing part of our scientific practice.

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