Sustainable Software Ecosystems for Open Science:
15 Years of Practice and Experience at Kitware

Marcus D. Hanwell, Amitha Perera, Wes Turner, Patrick O’Leary, Katie Osterdahl, Bill Hoffman, and Will Schroeder

Kitware, Inc., 28 Corporate Drive, Clifton Park, NY 12065 USA.
http://www.kitware.com/

May 11, 2014

Introduction

Mathematics is the core language of science, and for centuries it was necessary to show the mathematical underpinnings of new research as part of scientific explorations. This lingua franca provided an essential level of understandability and precision; providing for unambiguous communication and rigorous verification of scientific claims beyond the inaccuracies of spoken languages. However, the last few decades have seen an erosion in this paradigm. The increased reliance of science on complex computational codes and large data makes the description of all but the most basic research error prone, impenetrable, and unverifiable.

This issue is not restricted to just one field of science, but is endemic throughout the broader scientific community and the consequences of opaque processes and lack of reproducibility are not trivial. Cases of irreproducible studies and clinical trials have been making headlines, from Bayer Health Care stopping nearly two-thirds of its target-validation projects because of inconsistencies with the initially published claims, to global economic policy being based on a single fundamentally flawed study by Harvard economists. These costly mistakes can be remedied much earlier, and before key decisions are made, simply by returning transparency and precision to the process of publication and review.

The question we must address is how best to reinstate a common language and what that language should be. We believe that the only practical choice is to require that disclosures of scientific research based on complex codes and data use the very same complex codes and data as the common language of publication. This means that as new studies and new scientific explorations are undertaken, the data, methods, and software used by the researchers to arrive at their conclusions must be made available and accessible to other researchers and the general populace. If this goal is to be realized then the standard of software engineering in science must be improved, and sustainable software ecosystems with meaningful credit must be realized. This is not simply limited to teaching scientists to write code; if sustainable software projects are to be established in science then issues such as testing, licensing, and collaboration must be addressed. Sufficient engineering discipline is required to realize robust foundations that can be extended through the use of code review, regression testing and proper citation and attribution of software used in research.

Vision

Kitware has been developing open-source solutions and laying the building blocks for open science for over a decade. We contribute to a wide and varied range of open-source projects in the scientific domain across many disciplines including supercomputing, scientific data visualization, large data management and informatics, computational fluid dynamics, medical imaging, chemistry and computer vision. Kitware’s specific expertise in this area, including business practices, collaboration patterns, and growth strategies, are discussed. Based on this experience, we believe practical frameworks for science revolve around well-defined and open application programming interfaces (APIs) between key steps in the analysis workflow from raw data to final figures in published manuscripts.

Although not directly related to the scientific goals, it is important to consider licensing in the context of scientific communities. It is not enough to simply make code and data available for free if we wish to see communities flourish—shared ownership and access must be provided under permissive licenses wherever possible. These should encourage reuse, derivatives, and allow those products to be shared. Permissive licenses such as MIT, BSD, and Apache 2 for software; and CC0 or CC-BY for data should be strongly encouraged over copyleft, non-commercial and no derivative clauses that can hamper further reuse of code or data. When a wealth of data and code is available under permissive licenses
that encourage reuse it is much easier to grow sustainable software ecosystems—suddenly the method a student developed in their research can be incorporated into a larger framework even after a student has moved on to the next challenge. This relies upon the code being published and made available under permissive licenses allowing for reuse in other contexts. The same path can be considered for data, where individual findings can be combined into larger collections and analyses performed on aggregate data to make new discoveries outside the scope of the original research in many cases.

**Practice and Experience**

Kitware started as an experiment in open source education beginning when three General Electric research employees wanted to author a book on visualization using a new programming language called C++. The book included code, and in order to encourage reuse and improve the general standard in the field they were granted authorization by GE to retain copyright and publish the code with the book. This would later become the Visualization Toolkit (VTK). In 1998 two of the authors left GE and with several others founded a small company in upstate New York named Kitware. Fifteen years later the adventure continues, with over 100 employees and sustained year-on-year growth.

**Baseline Implementations**

As noted, VTK began life as code to support a book. The goal was to improve the state-of-the-art in the visualization community by putting tested and verified implementations of important visualization and analysis algorithms into a software library that was permissively licensed and available for use by a broad and open community. The intent was to provide these implementations as a concrete instantiation of complex algorithms so that researchers around the world did not have to do this from the papers of the time, with varying degrees of success and different levels of verification. This same goal lies at the heart of the Insight Toolkit in medical imaging for image segmentation and registration. Over the years things such as the Insight Journal were added so that new algorithms could be proposed in formal publications that included code, data, and baselines demonstrating the algorithm. If accepted, the algorithm would be merged into the main codebase and made available to the wider community.

**Business Model**

The majority of well-known software companies use a licensing and intellectual property model in order to derive revenue from their development activity. In the sciences this is often bolstered by funding from major agencies as well. Kitware generates no intellectual property, and has moved away from the licensing model to a large extent—focusing our business activity on a services model. This is an extremely effective strategy when working in high-performance computing, and addresses one of the major flaws in many open-source projects where support is difficult to find. Services make up a larger share of the industry sector, with companies such as IBM and Red Hat deriving most of their income from services rather than licensing. This model enables us to work with academics, national laboratories, and industry as partners often with joint funding streams to develop new features and make headway in different avenues of research and development. Through the use of permissive licensing models, rigorous software processes and agile development methodologies we have been able to make significant progress and received recognition for major projects such as VTK and ParaView.

**Developing Communities**

One of our core focus areas at Kitware is software process and developing robust communities around software projects that can grow beyond individual contracts. This process is shown at a high level in Figure 1 where developers commit code, it is automatically tested, dashboards gather testing information and disseminate that information. This process is powered by CMake, which began as a build system for ITK when existing build systems proved inadequate, with the simple goal of building C++ code on all major platforms. This was later augmented with CTest that would run and report the results of automated testing to Dart, and later CDash. Packaging was addressed using CPack, enabling some degree of abstraction when creating binary installers which are now routinely generated each night so that non-developers can install the latest build of a software project to see if a bug has been fixed.

![Figure 1: Overview of the Kitware software process.](image)
the software using automated repository hooks, continuous integration, and advanced testing capabilities such as image-based regression images to verify that visualization algorithms produce consistent and correct output on a large number of platforms beyond the capability of any individual contributor.

Any community needs to establish a strong process to remain viable over the long term. This requires a mixture of technical and social resources to facilitate productive engagement and growth. Scientific projects often have limited resources, with a high turnover of developers/engineers as they move through their academic careers. This means that it is essential to establish procedures to help new community members get up to speed, and to retain group knowledge as people move on to new positions. Some will maintain long-term ties through different positions, as is normal in more mainstream open-source projects, others will not and it is important to ensure the parts of the project they developed do not atrophy.

**Open Software Process**

Kitware engineers and researchers have experimented with a number of techniques to improve induction of new community members and employees into our company and software communities, to support open-source development, and the growth of our projects. Most importantly, these experiments are more than just an academic exercise. All of the techniques are applied as part of our ongoing, commercial, software business. The techniques that offer pragmatic benefits to our business and open-source communities survive. Figure 2 shows a more detailed view of the software process used by the Visualization Toolkit (VTK).

Recently we started using Gerrit to conduct online code reviews, and added automated triggers so that proposed changes are built on all major operating systems. This simple modification allows us to highlight potential platform-specific issues before engineers review code, saving scarce engineering time. Our software projects are developed using test-driven development methodologies, and require the submission of tests for new code or features ensuring that these features are automatically tested and verified before they are merged.

We have a strong commitment to testing. We run nightly dashboards to provide wider coverage, ensuring that any problems are normally highlighted within 24 hours of merging them into the repository and allowing developers to review and remedy regressions while the changes are still fresh in their mind. All of these processes are learning opportunities, enabling developers to quickly discover what will and won’t work with different environments as new features are developed. These advantages were only made possible in recent years by migrating to distributed version control systems that enable development outside of the main repository and for changes to be pushed to staging locations before being merged into the main development branches.

We have worked hard to close the gap between developers of the frameworks and applications and their users by automatically generating binary installers. This enables them to download the latest nightly binary of any given project to check if their bug still exists, or work more closely with developers on exercising new features before the final release is made. Underlying all of this are multiple communication mediums including mailing lists, wikis, and bug trackers to offer a comprehensive set of community tools. Having a commercial company backing up these projects also offers the ability to provide books, webinars, and on-site courses.

**Mature Communities**

Kitware hosts or plays a leading role in the maintenance and engineering on a number of projects, and over the years has learned to be adaptable. The oldest Kitware-led community is VTK, which also has one of the longest running version histories of any project whose history is publicly available. This is a community that grew up organically around the VTK book, and many pieces of the code were experimented with and added as the community grew. According to Ohloh the project has had nearly 55,000 commits made by over 200 contributors and includes more than 3.5 million lines of code. The first recorded VTK commit occurred nearly 20 years ago and development remains active. Even when looking at the last 12 months the project has seen over 3,000 commits from 66 contributors under a permissive

![Figure 2: VTK’s software process incorporating online code review, automated testing of topic branches, and nightly testing with distributed mirrors.](image-url)
Figure 3: Statistics generated by Ohloh showing lines of code, and commit rates for VTK.

BSD license. Figure 3 shows a graphical overview of the project’s activity from 1994 to present.

Even so, these numbers understate the total significance. For instance, they do not count the number of commercial contracts where Kitware supported the toolkit by providing engineers to extend VTK, or create/augment focused applications that leverage VTK, or research conducted using VTK. The development is also funded by several ongoing contracts with established groups, and funding streams from various federal agencies such as the DOE, NIH, DOD, DARPA, and NSF. Due to VTK’s importance to researchers in the medical area, it was granted a rare R01 maintenance grant from the NIH. Under this contract a consortium of companies and universities led by Kitware is working to update and overhaul aspects of the VTK rendering subsystems and to make other improvements over the next four years. VTK was able to garner a large number of support letters from the community of users and developers making use of VTK in their research, applications and products.

After the success of VTK, the ITK project was, at least in part, founded to emulate the success of VTK in the medical segmentation and registration field. ITK receives ongoing funding from the National Library of Medicine, initially to provide algorithms that could operate on and make sense of the data from the Visible Human project. It is a little younger, with its first commit in 2000, and is interesting as it was one of the first major projects that began after Kitware’s founding and was designed from the ground up as an open-source project. It has seen nearly 45,000 commits in that time from over 200 contributors with over 1.5 million lines of code. Over the last year more than 1300 commits were made by 67 contributors under a permissive Apache 2 license. The ITK project also has an associated non-profit organization that is used to coordinate community efforts and manage some of the funding and development.

The history of some of these older projects that have seen one or two decades of development effort should be contrasted with younger projects at different stages of development. Experimentation is encouraged, and not all of the projects that are started will achieve the critical mass required to become successful open source projects, but our established processes seek to make experimentation easy and the permissive open-source licensing means that even “failed” projects will often live on in other forms if the code developed for the project is useful.

A brief summary of some of these projects include Arbor/Avatol—an NSF funded project where Kitware is an engineering subcontractor in a larger project led by the University of Idaho. The goals of this project are to provide tools for the analysis and exploration of the Tree of Life. The XDATA project is a new project funded by DARPA with a large consortium (led by Kitware as the prime contractor) tasked with creating open-source technology to address big data analytics. The Open Chemistry project was funded by a DOD SBIR awarded to Kitware, with the aim of creating a suite of desktop applications for computational chemists.

In addition to creating, growing and shepherding our own communities Kitware has more recently begun helping other organizations to build successful communities. This includes the VA with the OSEHRA project, NA-MIC, and caBIG, all of whom use Kitware’s expertise to assist them in growing vibrant and successful communities around their projects.

Concluding Remarks
Sustainable software ecosystems are difficult to build, and require concerted effort, community norms and collaborations. In science it is especially important to establish communities in which faculty, staff, students and open-source professionals work together and treat software as a first-class product of scientific investigation—just as mathematics is treated in the physical sciences. Kitware has a rich history of establishing collaborative projects in the science, engineering and medical research fields, and continues to work on improving that model as new technologies and approaches become available. This approach closely follows and is enhanced by the movement towards practicing open, reproducible research in the sciences where data, source code, methodology and approach are all available so that complex experiments can be independently reproduced and verified.

License
This document is released under the Creative Commons Attribution 3.0 license (CC-BY), see http://creativecommons.org/licenses/by/3.0/.