Experiments in Sustainable Software Practices for Future Architectures

Charles R. Ferenbaugh *
HPC-1, Scientific Software Engineering
Los Alamos National Laboratory

Since its beginnings during World War II, the nuclear weapons program at Los Alamos National Laboratory has relied heavily on scientific computation. Large codes have been written over many years, and significant efforts have been made to develop and implement cutting-edge physics methods. However, relatively little attention has been given to the computer science and software engineering aspects of the codes. While some modern software development practices have been adopted by the code teams (version control, regression testing, automated builds and tests), much more remains to be done.

In recent years, the code projects have given increased attention to modern software development practices, due to a combination of factors. Scientists who started out writing small, temporary research tools for use by a few people are now working on large, long-lived production codes with teams of developers and dozens of users; this leads to an increased need for their code to be maintainable and extensible. Computational results that in the past were mainly used to inform experiment design and analyze results are now considered as deliverables in their own right; this places the code that produced them under much greater scrutiny. Projects that once could count on being well-funded now find their budgets shrinking; this drives managers to try and use their software development funds more efficiently. All of these factors are leading LANL and many other scientific computing centers to try to improve software development practices.

However, another driver has also arisen that is perhaps more specific to LANL: the need to deploy our codes on future architectures such as many-core, GPU, Intel MIC, and so on. The Roadrunner cluster was deployed at LANL in 2008. It was the first petaflop cluster, and also the first large-scale hybrid architecture, containing both traditional x86_64 CPUs and new IBM Cell processors as accelerators. Much effort was spent figuring out how to rewrite our existing algorithms to perform well on this system. Similar efforts are ongoing to prepare our codes for other current and future architectures. During this process, we have found a number of areas in which sustainable software practices can provide significant advantages.

Advantages of Sustainable Practices for Future Architectures

In the area of code development, we found that many of our traditional practices were not well suited to new architectures. Our usual coding style, best summarized as “just get the physics working,” led to code that

* Mailing address: Los Alamos National Laboratory, Mail Stop B295, Los Alamos, NM 87544, USA. Email: cferenba@lanl.gov.

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Los Alamos National Security LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396.

The author gratefully acknowledges the support of the NNSA Advanced Simulation and Computing (ASC) Program, SWIFT project, for this work. Thanks to Tim Kelley and Bryan Lally (project leads for Exa11 and Exa12, respectively) for helpful conversations. This document is released internally at LANL as LA-UR-13-26936.
was difficult to understand and modify. In particular, there was often heavy coupling between the physics algorithms themselves and the infrastructure needed for performance (memory management, database access, MPI calls, etc.); this made it hard to change the infrastructure to support new architectures while leaving the physics intact. Also, our data structures were often designed using the “giant common block” mentality, assuming that all data was accessible directly from anywhere in the code (even if the implementation didn’t actually use common blocks). This meant that the data structures themselves were the interface, so that we couldn’t restructure the data without touching all of the code that uses it. It also meant that we couldn’t easily determine which data was used where, for purposes of managing data movement between different memory spaces. We hope that use of modern language features and better software design techniques in our existing code bases will address these issues and ease the transition to the newer architectures.

Similarly, when we considered code maintenance for the new codes we were developing, we faced the prospect of having to maintain distinct versions of large sections of the code for each new architecture we were asked to support. This would lead to nightmares in trying to maintain consistency between an ever-increasing number of implementations of similar algorithms. Instead, we are trying to minimize this problem and reuse as much code as possible on new architectures by improving the design of the software, introducing appropriate abstractions, and using advanced language features such as templating and function inlining.

Finally, we discovered several challenges related to software testing. Most noticeably, we found that the increasing amount of concurrency in the new architectures led to non-reproducible results on a scale we had never experienced before. For many years we had been able to have consistent results as long as the hardware and software environment remained constant; some variation could occur when hardware, compilers, or library versions changed, but these changes were infrequent and manageable. On the new architectures, however, variations could (and did) easily occur between one run and the next, in ways that our usual testing methodologies weren’t designed to handle.

To further complicate matters, we found that many of our legacy algorithms were numerically unstable: the smallest change to the inputs could lead to large changes in outputs. In the past developers did not pay much attention to this issue, as it wasn’t a problem; the small input changes that exposed it were few and far between. On new architectures, however, the unstable algorithms would only amplify the frequent small variations described above. We found that we would need to add numerical stability to our list of considerations in any new code we developed; and worse yet, we would have to go back through thousands of lines of legacy algorithms to determine their stability as well.

As a consequence of the non-reproducibility and non-stability we discovered, our traditional testing methodology (create a reproducer, rerun in the debugger, track down the error) would in many cases be inadequate for future architectures. We’d need to find other ways of eliminating bugs from our code. The good news was that modern software practice provided a number of possible tools, such as:

- extensive unit testing, with particular attention to corner cases;
- static and dynamic analysis tools; and
- inspection techniques such as code reviews and pair programming.

The challenge, then, was to find ways to incorporate practices like these into our current and future code projects.

Given all of these connections, it made sense for us to include a focus on software practices as we continued our work on moving codes to future architectures.
Two Experiments

In the past few years, LANL has run two small experimental projects as initial attempts to raise awareness of new software practices and programming approaches for new architectures.

First, starting in the fall of 2010, the “Exascale Tutorial” series was launched. This was a year-long, part-time “boot camp” for experienced code developers from our large multi-physics code projects, intended to help them become more familiar with advanced architectures and with modern software practices. Four developers participated in each of the fiscal years 2011 and 2012, with a few computer scientists working alongside. Work was done using C++ to program CPUs, and CUDA or OpenCL for GPUs; most participants had little or no experience in these languages. Attempts were made to practice requirements gathering, unit and integrated testing, and documentation where appropriate. The Exa11 group developed a small molecular dynamics mini-app, first in a reference CPU version, then in several GPU versions using various strategies and programming models. The Exa12 group did similar work on other smaller codes and code fragments. The participants generally described the tutorial as a useful educational experience, and went on to use what they learned in other efforts; many moved on to the SWIFT project described below.

Next, we launched the Software Infrastructure for Future Technologies (SWIFT) project in the fall of 2011. SWIFT started with seven developers, representing a mix of domain science and CS backgrounds, working half-time; this number increased to ten in the second year. The project goal was to use modern software practices to produce, in four years, a prototype multi-physics code suitable to run on future architectures. (A much-repeated piece of folklore at LANL states that “it takes 15 years to develop a weapons code”; thus, the four-year schedule for SWIFT was considered to be quite ambitious.)

Modern software tools and techniques used on the SWIFT project included:

- C++ language for writing (nearly) all code;
- Mercurial for distributed version control;
- Eclipse for an integrated development environment;
- cmake for a build system; and
- CppUTest for a unit test harness.

No team member had used all of these before, and some had used few or none of them. In addition, the group used agile development practices adapted from Alistair Cockburn’s “Crystal Clear” [1], including co-location, pair programming, short (two-week) iterations, and daily stand-up meetings.

The SWIFT project was terminated at the end of its second year, due to tightening budgets and to pressing needs elsewhere in the program. At that point, we had not made as much progress as we had hoped toward the four-year goal (some reasons will be explored below). However, we had developed some design ideas that were demonstrated in several prototype codes, and learned useful lessons in a number of areas along the way. The SWIFT team members are now being deployed to other code projects to help with modernization efforts, in hopes that the lessons learned in SWIFT can be applied to those projects.

Lessons Learned

Participants in both of the experimental projects gained valuable experience with new techniques and tools. We found some of these to be helpful and applicable to LANL projects; others were perhaps helpful in principle, but had enough problems and limitations that we would recommend alternatives for future projects. We also had our first experiences at LANL with the disciplined development practices that are common in the software industry. Since these were new to us, we understandably encountered many rough spots,
and our execution could have been better. Still, we gained enough positive experience to agree we should continue in this direction, learning more about these practices and finding ways to use them at LANL.

In addition to the technical knowledge we gained, we benefitted from the increased interaction between domain scientists and computer scientists. Historically, these two communities at LANL have for the most part operated in isolation. The projects gave us good opportunities to learn from each other, and to build working relationships that are continuing into other efforts. It also helped team members from each of the groups (domain science and CS) to realize that the other group had something important to contribute to the scientific code development process.

There were issues, though, that kept these projects from being as productive as they perhaps could have been. One disadvantage, noted by several participants in both projects, is that it’s difficult for a learner to stretch in several different directions simultaneously. The domain scientists in particular were often learning a new language, new tools, new kinds of architectures, and in some cases even a new problem domain, all at the same time; this was sometimes too much to take in at once.

Another disadvantage to both projects was their dual nature: were we supposed to be experimenting and free to fail, so we could learn from our failures? Or were we working toward a normal deliverable with a hard deadline? Often we tried to do both, and as a result we didn’t do either very well. This caused some difficulty in particular with our use of agile development methods, which are designed for “real” projects; we couldn’t always see how to make these fit in “experimental” mode. Even so, we generally agreed that the basic agile ideas were better suited to the LANL development environment than the more formal, structured project lifecycles that some team members had used elsewhere.

We also discovered some larger cultural issues at LANL that made it hard to fully implement our agile development ideas. Since all of the experimental projects were only part-time efforts, we attempted to co-locate for whatever fraction of time we were working, to allow for things like pair programming, group design reviews, and extended brainstorming sessions. We found this to be a useful practice. However, the LANL culture tends to be very much interrupt-driven: it’s expected that people, especially key people, are available on demand. There was a common perception that our experimental work didn’t have “real” deadlines, so that other deliverables and milestones took precedence. This made it hard to protect our co-location time against interruptions, and our productivity suffered as a result.

**Next Steps**

Efforts are underway in several of our large code projects to modernize the code base and prepare for future architectures. As noted earlier, the SWIFT project members will be deployed to help in these efforts, bringing with them the lessons they have learned related to sustainable software practices. Some higher-level discussions with management will be needed to try and address larger cultural issues that were exposed in the tutorials and the SWIFT project.

In the past couple of years we have also started sharing our experiences with the other NNSA labs (Sandia and Livermore) as they have ramped up on advanced architecture work. As more labs and universities begin to deal with these architectures, we hope to expand our level of collaboration with them in this area.

**References**

[1] Cockburn, Alistair. *Crystal Clear: A Human-Powered Methodology for Small Teams*, Addison-Wesley, Boston, 2005.