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HEP Software Foundation Community White Paper Working Group – Software Development, Deployment and Validation

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Abstract: The High Energy Phyiscs community has developed and needs to maintain many tens of millions of lines of code and to integrate effectively the work of thousands of developers across large collaborations. Software needs to be built, validated, and deployed across hundreds of sites. Software also has a lifetime of many years, frequently beyond that of the original developer, it must be developed with sustainability in mind. Adequate recognition of software development as a critical task in the HEP community needs to be fostered and an appropriate publication and citation strategy needs to be developed. As part of the HEP Softare Foundation's Community White Paper process a working group on Software Development, Deployment and Validation was formed to examine all of these issues, identify best practice and to formulare recommendations for the next decade. Its report is presented here.

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1 Scope

As part of the process to layout the HEP Software Foundation's Community White Paper Roadmap [1] we formed a group to study issues around software development, deployment and validation. The starting point for the group was to recognise that modern High Energy Physics experiments are large distributed collaborations comprising up to a few hundred people actively writing software. It is therefore central that the processes and tools used for development are streamlined to ease the task of contributing code and to facilitate collaboration between geographically separated peers. At the same time we must properly manage the whole project, ensuring code quality, reproducibility and maintainability with the least effort possible. Making sure this happens is largely a continuous process, and shares a lot with non-HEP specific software industries.

The group is therefore interested in tracking and promoting solutions for the following areas:

- Distributed development of software components, including the tools and processes required to do so (code organisation, documentation, issue tracking, artifact building) and the best practices in terms of code and people management.
- Software quality, including aspects such as modularity and reusability of the developed components, sustainability of the development effort, architectural and performance best practices.
- Deployment of software and interaction with operations teams.
- Validation of the software both at small scales (e.g., best practices on how to write a unit test) and larger ones (large scale validation of data produced by an experiment).
- Software licensing and distribution, including their impact on software interoperability.
- Recognition of the significant contribution that software makes to High Energy Physics as a field.

The goal of this document is to highlight the challenges the field will face in the next 5 to 10 years, and to provide a strategy on how address them. Adopting best practices from non-HEP communities and adapting them to HEP-specific needs will be key for the success of the effort.

2 Main challenges in the next 5-10 years

The challenges can be divided into two broad categories: those generic to large-scale distributed software development and those specific to the HEP environment.

The HEP-specific challenges are those derived from the fact that HEP is a large, inhomogeneous community with multiple sources of funding, mostly formed of people belonging to small university groups and some larger laboratories. Software development effort within an experiment usually encompasses a huge range of experience and skills, from a few more or less full time experts to many physicist programmers with little formal software training. In addition, the community is split between different experiments that often diverge in timescales, size and resources.

Another peculiarity of HEP is that the experiment software is usually divided in two separate use cases, production (data acquisition, data reconstruction or simulation) and user analysis, whose requirements and life-cycles are completely different. The former is very carefully managed in a central and slow moving manner, following the schedule of the experiment itself. The latter is much more dynamic and strongly coupled with conferences or article publication timelines. Finding solutions which adapt well to both cases is not always obvious or even possible.

Principle areas of challenge are:

Effective use of developer effort

- The large fraction of short term students and collaborators found in our field requires a process for evaluating software contributions to common projects and for assuring not just their quality, but also their maintainability.
- For the same reason, we need to minimise the time required for people to begin to contribute effectively.

Knowledge sharing

- There is a strong need for knowledge sharing, including effective training. This is required by groups that are geographically separated, but also amongst different fields, with different skills, languages and cultures. E.g., some students might be able to track new trends better than older colleagues, but they might lack vision; software engineers might provide better implementations than postdocs, but may lack a complete understanding of the broader picture for the experiment needed to set priorities.
- There is an historical and stubborn compartmentalisation between different experiments, so propagating knowledge horizontally across experiments is particularly hard.

Reusing code effectively

- While striving towards common solutions, the group recognises that a single platform or set of tools will not fit all use cases, but we emphasise that generic best practices and recommendations can be made. A top-down approach, where a given tool or solution is mandated has not proven to be viable in the past. However, if we can identify success stories and make sure they can be extended (if needed) and advertised as possible general solutions, duplicate efforts or developments are more likely to be avoided.

Validation of complex output

- Efficient validation of the complex outputs of HEP code, involving inputs from highly specialised experts and unique sources, is hard to do, especially taking into account stochastic processes and long tails.

Data, code and knowledge preservation

- Long term maintainability of the code to handle data that was obtained decades before as required by the lifetime of a HEP experiment.

Code lifecycle and deprecation

- In a highly demanding software environment such as the HEP communities, there is great pressure to adopt updated versions of tools and libraries for performance or design benefits. However, there is little corresponding pressure to deprecate old components that may have been used for years, causing a bloat of the active software stack and provoking crises when abandoned upstream libraries start to fail to build. Hence there is a need to engage in effective, smooth and continuous lifecycle management of the codebase.

Hardware and software evolution

- Hardware trends are now towards increasing processing capacity through concurrency (many cores and vectorisation) rather than any increase in serial processing capacity. This is at odds with the traditional HEP software workflows, which have largely been serial. Memory latencies and a deep memory and storage hierarchy have become key drivers of performance. Increasingly specialised processors are also arriving in the marketplace, which are not naturally suited to HEP codes. Adapting to this new hardware environment and maintaining the efficiency of HEP code becomes increasingly hard.

- New innovations in software development usually come from outside of the HEP community. These can provide significant advantages in exploiting new hardware or aiding efficient distributed development and such technologies need to be tracked, investigated and deployed.

Software deployment

- As HEP software today runs in widely heterogeneous environments, from traditional grid computing sites to High Performance Computing sites, including the gamut of academic and commercial cloud services, there is a challenge to uniformly provide the appropriate software in all of these environments. End user analysis code also needs to be managed and distributed into these environments. CVMFS [2] has been hugely successful here, however it does not cover all cases and a viable common solution may emerge and be adopted more widely.

Recognition of software development

- Writing high quality software is a skilled activity that greatly contributes to the success of the field. Ensuring that software developers receive recognition for their contributions will help retain people in the field and help their career development.

3 Meeting the Challenges

The previous section introduced a brief summary of the main challenges this working group has identified. In the next paragraphs we both expand on these and identify viable existing solutions and areas where more investigation is required.

3.1 Effective use of developer effort

3.1.1 Design documentation and training

For developers to be able to contribute effectively to experiment software it is first of all necessary for them to have a clear idea of how to write code that will mesh effectively with the framework or the rest of the software stack. Thus it is essential that developers can access clear documentation, with good examples as to how to model their code. Effective contact with experts should be available so that good design choices are made from the outset.

Once a clear picture of the framework is available to new developers the first task of the contributor should be to make their intentions clear to others. A common technique is to use a request for comments document which outlines the design and allows other developers to provide feedback before substantial coding effort is expended. Such documents can be accompanied by demonstrator or prototype code to better illustrate the purpose of the of the changes. This approach allows documentation and testing to be incorporated into the development itself and not left as an afterthought. This model was used by the Concurrency Forum [3] in the past and was very successful in selecting the most promising approaches for the community and disseminating knowledge amongst different experiments.

The task for developers who might contribute a general purpose piece of code that is used across experiments is more challenging as active solicitation of input will need to be sought. However, if experiment documentation is open to the HEP community then different experimental boundary conditions will be more easily understood and translated into the design and interface of a software product.

In general, good software design principles should be followed and thus generic training in software design, but with a focus on the HEP problem space, is a valuable investment for the community. We note that several computing schools exist already, but that overall only a small fraction of HEP students attend them as they are considered quite specialist. Universities, in both their undergraduate and graduate programmes, play an important role too in core skills training (and in some institutes also in relevant advanced topics), but this can be uneven. Effort should be made to incorporate more generic training into the education programmes of the experiments; centering these activities around some of the larger labs will also allow sharing of the training effort across different experiments.

3.1.2 Standard development tools

To maximise the productivity of developers it is very beneficial to use development tools that are not HEP-specific. There are many open-source projects and tools that are of similar scale to large experiment software stacks and standard tools are usually well documented. Many simple questions can be answered using standard resources, such as Stack Overflow.

Insofar as an experiment requires customisation of tools, documentation and training are evidently important. However, the costs of such customisation can be easily outweighed by the cost of maintenance and training, as well as a possible loss of generic skills for users.

For source control in particular, the open-source world has moved strongly towards distributed version control as superior to centralised solutions. The advantages for the individual developer are numerous, including independence from central services and greater freedom to experiment. Finished code enhancements can be proposed using a pull request workflow so that high quality contributions are made with the central repository receiving pristine patches. We note that the community has generally chosen to move to git. This standardisation is very welcome as it also brings an alignment with many open-source projects and commercial organisations.

The HEP current community is widely using CMake for the builds of software packages. This is an open-source system dedicated to building, testing, and installing software that captures the specific build specifications for each particular package in a platform independent way. It is highly regarded because of its modular and scalable characteristics and is also very widely used outside HEP with a lot of support available. CMake's use of plugin modules allows scope for sharing between HEP experiments in the cases of building HEP specific code, though at the moment probably the best use is not yet made of this feature in our community. CMake can orchestrate the builds of large numbers of packages (e.g., the LCG releases of over 300 packages), but can become quite specific when doing so and thus more limited. The HSF Packaging group found Spack [4, 5] to be a promising more general solution for the task of building an HEP software stack, however, it currently has a relatively small user base, centered on HPC, and might just become a niche product with little traction in the wider development community. More generic tools, such as Homebrew or Conda are interesting but may not have all the features needed by HEP experiments. Thus this area still requires close attention to active developments in the open-source world.

For reporting problems, tracking bug fixes and planning improvements to the software issue trackers should be used. The best of these offer multi-level grouping of issues and provide direct support for useful aspects of agile development discussed below. Optimal choices will offer good integration with source code management (e.g., GitHub Issue Tracker, Jira, GitLab Issue Tracker) and the choice should usually be made in parallel with an source code management tool.

3.1.3 Development environment

It is important that developers can focus on the design and implementation of the code and do not have to spend a lot of time on technical issues. Clear procedures and policies must exist to perform administrative tasks in an easy and quick way. This starts with the setup of the development environment, for example by having a minimal set of requirements on the operating system and the installed packages. Supporting different platforms not only allows the developers to use their machine directly for the development, it also provides a check of portability basically for free.

Other typical workflows are the update of versions or the submission of code for review. It decreases the turnaround time and reduces frustration if code quality criteria and policies are checked as early as possible, ideally on commits to the local repository or even by the editor. Modern IDEs, which offer good integration with modern development tools, can be particularly valuable for novice coders. They provide support for developers in navigating the code base as well as catching elementary errors. It would be of great benefit for the community to ensure that standard project templates (e.g., HSF Project Template [6]) work with minimal configuration with standard IDEs, such as Eclipse, XCode, KDevelop, Qt Creator, etc. For large experiment code bases, the scaling of these IDEs to many millions of lines requires investigation.

Finally, support is important. A system that enables developers to get quick and competent advice from experts will improve their productivity.

3.1.4 Social coding sites

The advantages of social coding sites are that they allow developers to share and discuss code through very streamlined and highly functional web interfaces. Distributed version control systems are key enablers for these sites. There are commercial choices, such as GitHub or BitBucket, that can serve a community well; alternatively a privately hosted service, such as CERN's GitLab instance, may mesh more easily with other related services. We note that "bridging" code between different service platforms has been developed by a number of experiments and could be shared across the community. Smaller projects would probably benefit from the increased exposure and larger development community from being hosted on GitHub. For attribution and credit, GitHub also offers a more standard platform that can be helpful to a developer's career. However, the key requirement here is the ability to discuss and revise code changes in a recorded fashion as they become part of the code repository.

3.1.5 Continuous integration

Proper testing of changes to code should always be done in advance of a request being accepted. Continuous integration, where merge or pull requests are built and tested in advance is now standard practice in the open-source community and in industry. HEP software should not be different. Not only should continuous integration run unit and integration tests, it can also incorporate code quality checks and policy checks that will help improve the consistency and quality of code at low human cost.

For running continuous integration and build orchestration many options exist (Jenkins, Gitlab CI, Travis, Bamboo) and the particular choice of which one to use is a relatively pragmatic decision, with only a very limited impact on the ability to cooperate around software.

3.1.6 Code review

Incorporation of code into the code base should usually also involve sign off from at least one relevant expert who can check for architectural violations, anti-patterns or even just simple coding errors. Code review should be seen as a process of dialogue between the developer and the reviewer (community expert) and it should be firm, but friendly.

As well as a way to validate code, reviews can also be a way for newcomers to learn about the architecture of a project. As part of a mixed experience reviewing team, fresh eyes on a piece of software can produce original comments, but the discussions occurring as a side effect of the review effectively helps new developers understand the issues at stake.

3.1.7 Agile development

HEP is a community where the developer of a piece of software is also likely to be the 'customer' as well. However, despite this, many useful ideas can be taken from the various agile methodologies, in particular with regard to solving only the problem at hand and keeping development cycles as short as possible to find iterative and evolutionary solutions. Agile development methodologies for physicists, and how to select the most appropriate one, might be best taught by example rather than as formalism.

One aspect of agile methodology that would serve HEP rather well is the concept of a user story that describes the purpose of a system, rather than requirements capture that was used in the past. Such a method is more flexible in adapting to changing requirements, which can be quite a common situation in HEP, especially in the analysis domain.

HEP would benefit from adopting agile retrospectives. A retrospective is a formalised way for contributors to meet regularly to discuss ways to improve their software development process. Since a retrospective occurs regularly, there is a chance to catch issues affecting the development process as they arise. Issues can be tracked and mitigated over time rather than ballooning into daunting barriers. Additionally, the focus is on learning from failures quickly, without placing blame. This welcomes feedback, positive or negative, toward the goal of improving the software development process.

Retrospectives can be structured as needed to suit HEP, but the standard approach lends itself nicely to solving current problems since the last retrospective:

- Gather data. What went well? What didn't go well? What needs to be improved? Each person who has input should have a chance to succinctly state their observations.

- Discuss top issues in prioritised order. Based on the feedback of the group, discuss top issues to reach an understanding about the root causes.

- Assign action points. Based on the pain points discussed, assign action items that are small enough in scope that they can be resolved before the next retrospective.

This setting of information sharing and collaboration can yield clear productivity benefits. For example, it is possible that a developer experiences issues that slow down their productivity without being aware of it. Perhaps the developer became accustomed to the build time being very high and thinks of it is as given constraint. In a retrospective, a discussion about build times may arise along with known solutions for reducing the build times. This will elicit awareness about the issue, a solution, and a subsequent gain in productivity.

Agile development is very well supported by the modern development infrastructure outlined above.

3.2 Knowledge sharing

3.2.1 Documentation

As was mentioned above, proper training and documentation is key to efficacious use of developer effort. For documentation that has to be specific, favoured solutions would have a low barrier of entry for contributors, but also allow and encourage the review of material. Consequently it is very useful to host documentation sources in a repository with a similar workflow to code and to use an engine that translates the sources into modern web pages. An example would be using the Jekyll engine, as the main HSF website currently does, or using services such as Read The Docs.

Traditionally HEP has often used Doxygen for reference documentation, especially given its emphasis on C++. New documentation tools are also available that integrate Doxygen with better solutions in other languages, e.g., the python Sphinx documentation tool can use Breathe to integrate C++ and python documentation. Sites such as Read The Docs also take much of the pain out of producing an attractive documentation site.

3.2.2 Training

Code development, as a critical and transferable skill, is well recognised inside the HEP software community. Various schools exist that train students in good coding practice, but only a small minority of contributors to HEP code attend these. There is therefore scope for broader and more accessible training that experiments can play a role in encouraging collaborators to attend. Training events can start with generic material, shared between experiments, then move to separate experiment specific topics. This would be especially useful for experiments sharing a home laboratory and provides an additional benefit when different groups have managed to converge on common components.

Training and documentation are intimately linked and good training materials can be studied offline by students in their own time.

As much use as possible should be made of generic resources that already exist; there is a role here for the HSF to curate useful training materials (where their ongoing usefulness and validity needs to be managed) and encourage cooperation with other training initiatives, such as Software Carpentry [7].

3.2.3 Seminars and discussion forums

These are important to the community, in particular to discuss new technologies or tools at an early stage of development. A good example is the Software Technology Forum [8]. These forums also allow questions to be posed about problems that are encountered and identifying existing software that may provide a solution (thus avoiding re-inventing the wheel yet again).

In terms of knowledge sharing among developers, solutions such Stack Overflow are excellent for establishing communication between software developers and publishing answers on the web. In fact, this solution is used by many developers to find solutions to the daily problems they face. It seems that in general HEP software developers are consumers of these general help lists and we encourage the community to take more active role in contributing as well. Where a smaller community does not have the critical mass for their own Stack Exchange service other products, like Discourse, can be installed on-premises.

In addition, attempts have also been made to set up general software discussion mailing lists in the past. However, it seems that after some initial flurry of activity these are not really very successful. They may be too far away from most developers day-to-day concerns and there is probably some reluctance to pose questions to a wide list. Though being a fast and attractive solution for discussions about a particular issues they are not as viable for long term or broad knowledge sharing. There may be some use in trying alternatives, such as a Slack channel, at least to prototype with low investment.

3.2.4 Workshops and community reviews

Hosting workshops on specific topics is a particularly useful way to bring together experts from different experiments. These have an essential role in introducing new ideas to the community and providing an environment in which people can meet and interact. The HSF has also organised community meetings on aspects of future HEP software development that are of particular interest to the community in a strategic sense. Two such meetings have been organised so far: one on Geant V simulation [9], and the other on the analysis ecosystem [10]. These meetings can provide very valuable feedback to developers on the priorities of the experiments and the most critical features to develop and support. Organising further meetings on such topics provides important strategic feedback on development.

3.2.5 Conferences

HEP has a strong tradition of software and computing conferences (ACAT and CHEP are good examples). These continue to be a critical part of the lifecycle of software and of the community that supports it, offering recognition of work done as well as dissemination of knowledge about available solutions that can, hopefully, be adopted by others. Although they focus on completed pieces of work, they complement other activities well and provide an important space for social interaction.

It would be beneficial for the field as a whole to increase its participation in general conferences and software focused events. This would help generate relationships and collaborations outside the direct field with experts who may have interesting observations and suggestions.

3.2.6 Journal publication

Journals disseminate information to the wider community in a permanent way and so form an important part of the collective memory of the community. Journals also have another significant role to play in recognition of software work, which is discussed at greater length in Section 3.9.

3.3 Reusing code effectively

Effective reuse of code requires good design, documentation and support. Good design starts from a good understanding of the problem to be solved, with an appreciation of the important external interface to provide to clients. APIs should be stable, with scope to change the internal details of an implementation as needed. Training software developers in good design principles will certainly help in this regard; however, often the reuse potential of code is only discovered post-facto and then some advice and expertise in refactoring will be useful for the longevity of the package. Here Agile methodologies can help to focus on the key areas of responsibility and avoid over designing interfaces for imagined situations.

There is scope to improve the training in these areas within the HEP community as discussed above.

In all cases good documentation for code will greatly help adoption (the same solutions apply here as were discussed above) and this provides a key aspect of user support. Utilising popular standard development tools encourages collaboration and provides issue tracking capabilities.

3.3.1 Software Licenses

All code should have a clear copyright holder, which gives the legal ownership of the software. Applying a license specifies how the software can be used by others. Open-source licenses are now widely accepted by the HEP experiments, which we believe is the correct approach. Open source licenses fall into various categories

- Copyleft licenses mandate that any public releases with changes to the code must be licensed under the same terms and, in addition, that any software which uses the copyleft code must also itself be distributed under a copyleft license (which is why these licenses are sometimes referred to as ‘viral’). The General Public License, GPL, is the best known of these.

- Weak copyleft licenses (such as the Lesser General Public License, LGPL or the Mozilla Public License, MPL) remove the latter copyleft via use requirement, but still mandate that direct modifications to the package itself be redistributed under the same terms.

- Permissive licenses (Apache, MIT, BSD) generally allow for public modifications to be made without requiring them to be released under the same terms as the original code.

There is a modern report from the HSF on licensing topics [11] and we do not repeat the discussion here. Instead we encourage code authors to ensure that copyright and license for code is well established at the beginning of the project, including the status of contributions to the code. The implications of the chosen license should be properly understood, especially in so far as it affects contributors to the code base and users of the code who may incorporate it into a larger software stack, together with their own code (the GPL has a fairly profound effect in this regard).

3.4 Validation of complex outputs

The outputs of HEP software packages can be extremely complex and thus difficult to validate. This is especially true of the simulation of modern high energy physics detectors, which are incredibly complex machines and need to be accurately modeled to understand their performance for rare decays and weak signals. Up to now most experiments have developed their own infrastructure for comparing results. Comparison of distributions is a relatively well understood topic in statistics, so having standard tools that help compare outputs from different versions of software would help save effort between experiments and offers scope for improving the quality of our validation.

3.5 Data and code preservation

The longevity of code in HEP is becoming increasingly important. Large experiments have multi-decade active lifetimes, with "data preservation" now considered an important topic after an experiment has finished taking data. Data taken in the early years of the experiment may need to be reanalysed years afterwards with older software that has not been built for a long time. Software virtual machines or containers can help a great deal in preserving the working environment, including the source code itself. Should changes need to be made to software to correct for a long dormant bug or add a necessary new feature, having a virtual machine or container with the source code and build environment, in addition to any binary products, is important. Here the use of standard tools, as encouraged above, can help, with the state of the code and externals being encapsulated in a source repository tag. This is becoming a prerequisite to publication in some journals, so being able to trace the software used to produce some results, all the way through to an analysis, is crucial. Experiments need to strongly encourage their members to work in a preservable way.

In the design of code, relying on standard language features is more sustainable than utilising external libraries that may become deprecated. Of course, libraries that do tasks well are preferable to inferior home grown implementations and achieving some uniformity in the community will help for longer term support issues when they arise.

For further details on this topic we refer to the Data Preservation Community White Paper group [12].

3.6 Code deprecation

The complexity of HEP software and the generic nature of many of the sub-tasks that need to be performed mean that many external libraries are essential to our workflows. It would be completely unfeasible and a waste of effort to reproduce such code internally. However, there are often many solutions to the same problem and picking the one that has the best long term prospects or becomes the most widely adopted is not possible a priori. Sometimes externals will simply be eclipsed by alternatives and sometimes they will change their APIs in backward-incompatible ways. The problem is often exacerbated by the fact that the HEP-specific client may itself be only in maintenance mode and the original author may not even work in the field anymore.

In these cases evolving away from deprecated code is required. This can be a labor intensive operation, but often many aspects of it are automatable. There is a good example in the refactoring of C++, which is a hard problem, but with the development of Clang and full knowledge of the abstract syntax tree (AST) of the code, there are significant possibilities for using this knowledge to tackle much of the drudge work of refactoring. There have been successful examples of using Clang in this way [13] and we believe this is an area where investment could be very profitable, both specifically for HEP and as a contribution to the wider open-source community. Tools to further help validate the updated code can be shared between experiments, e.g., support for any migration to new versions of ROOT [14] or Geant4 [15].

Changing software versions and evolving platforms is a natural part of the lifecycle of production environments and can be helped by migration to more self-contained deployment models, e.g., by using containers instead of a site provided environment.

3.7 Hardware and software evolution

The evolution of processors in recent years have given rise to highly parallel architectures (from many core CPUs to GPUs); in addition, thanks to the push coming from the mobile market, viable low-power solutions are also now common (e.g., ARM architectures).

3.7.1 Effective exploitation of parallel hardware

Implementation and optimisation of software on parallel architectures requires different skills, tools and training (generally more advanced) than the ones required for the serial world. In order to allow physicists to effectively exploit parallel architecture, means are required to insulate end user programmers from many of the low-level difficult details of parallel programming.

Many specific details of parallel architectures can be masked by the adoption of appropriate libraries. Generally HEP problems fit better into a task based scheduling pattern, rather than to an optimiser of kernels run in tight loops. The community has utilised Intel's Threaded Building Blocks (TBB) [16, 17] successfully in many areas. Should TBB continue to develop and be a good fit for our problems this common solution also helps solve the problem of resource balancing between different parts of the code. Should the solutions adopted become fragmented then overall resource balancing becomes much harder and may become difficult to solve. Evolution of the C++ standard will most likely bring more concurrency primitives into the language, however, so some evolution here is to be expected and should be planned for. This would mean appropriate zero cost abstractions when possible.

3.7.2 Achieving performance portability

The fact that different parallel architectures (e.g., CPUs and GPUs) have different sweet-spots for performance makes compile time performance portability extremely difficult to obtain. This is true across architectures, but also between different generations of the same architecture. Past abstraction techniques might not work and development needs to target specific hardware for best performance. However, it is strongly advisable that the design of the code separates physics logic from performance optimisation. This helps to avoid premature optimisation and a harmful reduction in code maintainability. Options for runtime optimisation would also be possible (e.g., fat libraries with code for various vector architectures) and may help to avoid an explosion in build target architectures. Such techniques are an area where common community investigation would be worthwhile, especially when common tools are used in multiple projects.

When aiming for cross-architecture performance portability, one important concern is data layout, as different architectures have different preferences in this respect. For example, GPUs perform best when memory accesses from different threads are coalesced (as it optimises memory bus utilisation), whereas CPUs perform best when writes from different threads are relatively far apart in RAM (to avoid the cache trashing effect known as "false sharing"). These differences can be abstracted away through the use of data structure generation mechanisms, which are still in their early days but are begining to be offered by some programming environments such as Kokkos [18], and some domain specific languages, such as those used in the context of the H.E.S.S. Observatory [19] and in the Cherenkov Telescope Array reconstructions [20].

3.7.3 Tracking of new software technologies and tools

Compared to when HEP started as a field, the importance and ubiquity of software development has increased hugely. If in the late 80s and 90s many of the tools and practices were actually started inside our field itself, or at least within academia, it is now true that a large amount of development happens outside the traditional HEP field. Starting from the contributions of "bedroom coders", to the scale of large corporations like Google, Apple, or Facebook, a large number of high quality tools and libraries are now available as open-source projects for everyone to use. While this affords the field great opportunities, the rate at which these tools and libraries change is something that necessitates a continuous attention and an in-depth scrutiny of their potential, as well as managing inevitable deprecations. As was pointed out above, pooling community knowledge here will make optimal choices in new technology more likely.

3.7.4 Dealing with hardware diversity

The increasing number of different architectures, operating systems and compilers with different versions give rise to a large number of possible platforms that combine these parameters. Experiment software should be tested on a large range of platforms to ensure a competitive and effective use of these new technologies, which requires good test cases and striving to minimise the operational and human costs of multiple platforms. Use of open-source orchestration toolkits for managing these stacks can help a lot. Jenkins has received much attention, but alternatives, such as Travis, exist and there may be scope for a community evaluation. Aspects such as application independence, adaptation and modularity (a plugin-based structure) are important. Basic platform types can share a lot of common infrastructure (e.g., x86_64, AArch64 and PowerPC) that minimise the cost of adding new flavors if common components are used.

There is an important link here when deciding what level of validation is considered acceptable on each platform, especially if platforms do not produce binary identical results. In order to evaluate and prepare for the incorporation of such new platforms having early access is extremely important. CERN's TechLab and OpenLab projects help provide that, but there is a need to ensure that the whole community can benefit and more sites could be involved in this activity.

3.8 Software deployment

Deployment of HEP software has been revolutionised by the widespread adoption of CERN Virtual Machine File System (CVMFS) [2] for flexible and ubiquitous access to a common filesystem namespace with efficient distribution of content that can be strongly cached at multiple levels. We expect that CVMFS will remain the mainstay of software distribution to most computing sites in the foreseeable future.

However, CVMFS cannot cover all possible use cases. Sites that have no outbound network access (common in the HPC world) or are mobile and perhaps temporarily disconnected (e.g., developer laptops) require additional distribution mechanisms. Here, containerisation offers a great deal of promise as a way to isolate the software environment from the underlying hardware and to conveniently provide all the needed runtime components. This is particularly useful when other constraints drive the base operating system away from the standard one adopted and validated by the experiment. At the moment Docker is favored as being exceptionally convenient for development, with automated conversion to other container implementations (e.g., Shifter or Singularity) being possible. There should be no reason to deeply bind anything in the install process into any particular container implementation.

Containers also play a role in data and code preservation as already noted. While containers are architecture specific, there is currently no serious risk that, e.g., x86_64 platforms will be unavailable in the foreseeable future.

3.9 Recognition of software development

Proper recognition of the contribution that software makes to the success of High Energy Physics is a key element of sustaining that effort and establishing software as a 'first class citizen' in the field. As an academic discipline, HEP primarily recognises publications in refereed academic journals and the citations of those publications as indicators of merit. Therefore we strongly encourage authors of software to submit publications of that software to such journals, of which there are now many [21]. It is also equally important that publications from the field appropriately cite the software that they have used.

The correct level of granularity of software versions for publication will need to be judged by authors themselves, as well as reviewers. Significant improvements in algorithms, in either machine resource consumption or in physics performance, would certainly merit a new publication, as might a major release of software with significant new features. There is also a strong case for having an overall publication that encompasses a major piece of combined software used by an experiment. One example is an article on an experiment's offline software stack (that itself includes citations of the other software used within the combined software). Such publications would then be highly citable in physics papers, analogous to the common citations of the detector design papers.

Currently, if HEP software has an article written about it, it will tend to be in the conference proceedings of, e.g., CHEP or ACAT. Although these are refereed, in general the barrier for entry is low, and as such they are not considered as prestigious as refereed journals as the quality is mixed. Without some reorganisation of the community, and a more strict refereeing process, it is unlikely that conference proceedings will become the journals of choice for recognition in our field. However, conference journals (e.g., Journal of Physics: Conference Series) usually do not allow resubmission of articles to other journals without extended content. Software authors should be aware of these issues when deciding where best to publish.

There are also now interesting projects to directly publish software itself, for example to Zenodo [22] or figshare[23], as has been recommended by the FORCE11 Software Citation Working Group [24]. We are very encouraging of such efforts, and believe it would be useful for HEP software authors to participate, but at the moment the actual recognition accrued from such a publication is unclear. Through its work in reviewing papers, the HEP community could choose to suggest to authors that they cite the software they use, whether directly or via software papers. Over time, this small effort on the part of reviewers could be sufficient to change community practice regarding software credit.

For further discussion on this topic see also the Careers and Training Community White Paper [25].

4 Roadmap for the next 10 years

In the areas covered by this white paper HEP must endeavor to be as responsive as possible to developments outside of our field. In terms of hardware and software tools there remains great uncertainty as to which platforms will offer the best value for money in a decade. It therefore behooves us to be as generic as possible in our technology choices, retaining the necessary agility to adapt to this uncertain future.

Our vision is characterised by HEP being current with technologies and paradigms that are dominant in the wider software development world, especially for open-source software, which we believe to be the right model for our community. In order to achieve that aim we propose that the community establishes a development forum that allows for technology tracking and discussion of new opportunities. The HSF can play a key role in marshalling this group and in ensuring its findings are widely disseminated. In addition, having wider and more accessible training for developers in the field, that will teach the core skills needed for effective software development, would be of great benefit.

Given our agile focus, it is better to propose here projects and objectives to be investigated in the short to medium term, alongside establishing the means to continually review and refocus the community on the most promising areas. The main idea is to investigate new tools as demonstrator projects where clear metrics for success in reasonable time should be established to avoid wasting community effort on initially promising products that fail to live up to expectations.

4.1 Short term projects (1-2 years and ongoing activities)

- Establish a common forum for the discussion of HEP software problems. This should be modeled along the lines of the Concurrency Forum [3], which was very successful in establishing demonstrators and prototypes that were used as experiments started to develop multi-threading frameworks.

- Continue the HSF working group on packaging, with more prototype implementations based on the stronger candidates identified so far.
- Provide practical advice on how to best set up new software packages, developing on the current project template work and working to advertise this within the community.
- Work with HEP experiments and other training projects to provide accessible core skills training to the community. This training should be experiment neutral, but could be usefully combined with the current experiment specific training. Specifically this work can build on and collaborate with recent highly successful initiatives like the LHCb StarterKit [26] and ALICE Juniors [27] and with established generic training initiatives such as Software Carpentry [7].
- Strengthen links with software communities and conferences outside of the HEP domain, presenting papers on the HEP experience and problem domain. SciPy, SC (informally known as Supercomputing), RSE Conference, and Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE) would all be useful conferences to consider.
- Write a paper that looks at case studies of successful and unsuccessful HEP software developments and draws specific conclusions and advice for future projects.

4.2 Medium term projects (3-5 years)

- Prototype C++ refactoring tools, with specific use cases in migrating HEP code.
- Prototyping of portable solutions for exploiting modern vector hardware on heterogenous platforms.
- Develop tooling and instrumentation to measure software performance, especially in the domain of concurrency. This should primarily aim to further the developments of existing tools, e.g., igprof [28], rather than developing new ones.
- Develop a common infrastructure to gather and analyse data about experiments' software, including profiling information and code metrics, to ease sharing of this information across experiments.

- Develop tool(s) that allow developers to understand the usage of their software and to be credited for this usage, possibly via using these metrics associated with software citation.
- Undertake a feasibility study of a common toolkit for statistical analysis that would be of use in regression testing for experiment's simulation and reconstruction software.

It would be highly beneficial for the group to continue to function, through the means of the forum proposed above, and to have at least one meeting a year devoted to reviewing our activities and updating our knowledge of best tools and practices.

References

[1] The HEP Software Foundation. *A Roadmap for HEP Software and Computing R&D in the 2020s*. Tech. rep. HSF-CWP-2017-01. HEP Software Foundation, 2017. arXiv: 1712.06982 [physics.comp-ph].

[2] J. Blomer et al. "The Evolution of Global Scale Filesystems for Scientific Software Distribution". In: *Computing in Science Engineering* 17.6 (Nov. 2015), pp. 61–71. ISSN: 1521-9615. DOI: 10.1109/MCSE.2015.111.

[3] *Concurrency Forum*. URL: http://concurrency.web.cern.ch/.

[4] Elizabeth Sexton-Kennedy, Benedikt Hegner, and Brett Viren. *HSF Packaging Working Group Report*. Tech. rep. HSF-TN-2016-03. HEP Software Foundation, 2016. URL: http://hepsoftwarefoundation.org/notes/HSF-TN-2016-03.pdf.

[5] Todd Gamblin et al. "The Spack Package Manager: Bringing Order to HPC Software Chaos". In: *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. SC '15. Austin, Texas: ACM, 2015, 40:1–40:12. ISBN: 978-1-4503-3723-6. DOI: 10.1145/2807591.2807623. URL: http://doi.acm.org/10.1145/2807591.2807623.

[6] *Common HSF Tools Repository*. URL: https://github.com/HEP-SF/tools.

[7] *Software Carpentry*. URL: https://software-carpentry.org.

[8] *Software Technology Forum*. URL: https://indico.cern.ch/category/7857/.

[9] Gloria Corti et al. *HEP software community meeting on GeantV R&D Panel Report*. Tech. rep. HSF-GeantV-2016. HEP Software Foundation, 2016. URL: http://hepsoftwarefoundation.org/assets/GeantVPanelReport20161107.pdf.

[10] HEP Software Foundation. *HEP Analysis Ecosystem Workshop Report*. Tech. rep. HSF-Analysis-Ecosystem-2017. HEP Software Foundation, 2017. URL: hthttp://hepsoftwarefoundation.org/assets/AnalysisEcosystemReport20170804.pdf.

[11] Michel Jouvin et al. *Software Licence Agreements HSF Policy Guidelines*. Tech. rep. HSF-TN-2016-01. HEP Software Foundation, 2016. URL: http://hepsoftwarefoundation.org/notes/HSF-TN-2016-01.pdf.

[12] The HEP Software Foundation. *HEP Software Foundation Community White Paper Working Group – Data and Software Preservation*. Tech. rep. HSF-CWP-2017-06. HEP Software Foundation, 2017.

[13] Hyrum Wright et al. "Large-Scale Automated Refactoring Using ClangMR". In: *Proceedings of the 29th International Conference on Software Maintenance*. 2013. URL: https://research.google.com/pubs/pub41342.html.

[14] R. Brun and F. Rademakers. "ROOT: An object oriented data analysis framework". In: *Nucl. Instrum. Meth.* A389 (1997), pp. 81–86. DOI: 10.1016/S0168-9002(97)00048-X.

[15] S. Agostinelli et al. "GEANT4: a simulation toolkit". In: *Nucl. Instrum. Meth.* A506 (2003), pp. 250–303. DOI: 10.1016/S0168-9002(03)01368-8.

[16] Chuck Pheatt. "Intel®; Threading Building Blocks". In: *J. Comput. Sci. Coll.* 23.4 (Apr. 2008), pp. 298–298. ISSN: 1937-4771. URL: http://dl.acm.org/citation.cfm?id=1352079.1352134.

[17] *Intel Threading Building Blocks*. URL: https://www.threadingbuildingblocks.org/.

[18] H. Carter Edwards, Christian R. Trott, and Daniel Sunderland. "Kokkos: Enabling manycore performance portability through polymorphic memory access patterns". In: *Journal of Parallel and Distributed Computing* 74.12 (2014). Domain-Specific Languages and High-Level Frameworks for High-Performance Computing, pp. 3202–3216. ISSN: 0743-7315. DOI: https://doi.org/10.1016/j.jpdc.2014.07.003. URL: http://www.sciencedirect.com/science/article/pii/S0743731514001257.

[19] *High Energy Stereoscopic System Observatory*. URL: https://www.mpi-hd.mpg.de/hfm/HESS/.

[20] *The Cherenkov Telescope Array observatory*. URL: https://www.cta-observatory.org/.

[21] *Sustainable Software Institute: In which journals should I publish my software?* URL: https://www.software.ac.uk/which-journals-should-i-publish-my-software.

[22] *Zenodo*. URL: https://zenodo.org.

[23] *figshare*. URL: https://figshare.com.

[24] Arfon M. Smith, Daniel S. Katz, and Kyle E. and Niemeyer. "Software citation principles". In: *PeerJ Computer Science* 2 (Sept. 2016), e86. ISSN: 2376-5992. DOI: 10.7717/peerj-cs.86. URL: https://doi.org/10.7717/peerj-cs.86.

[25] The HEP Software Foundation. *HEP Software Foundation Community White Paper Working Group – Careers & Training*. Tech. rep. HSF-CWP-2017-02. HEP Software Foundation, 2017.

[26] Albert Puig and LHCb Starterkit Team. "The LHCb Starterkit". In: *Journal of Physics: Conference Series* 898.8 (2017), p. 082054. URL: http://stacks.iop.org/1742-6596/898/i=8/a=082054.

[27] H. Beck. *The Junior Community in ALICE*. Presented at EPS conference. July 2017. URL: https://indico.cern.ch/event/466934/contributions/2589553/attachments/1489205/2

[28] G. Eulisse and Lassi A. Tuura. "IgProf profiling tool". In: *Computing in high energy physics and nuclear physics. Proceedings, Conference, CHEP'04, Interlaken, Switzerland, September 27-October 1, 2004*. 2005, pp. 655–658. URL: http://doc.cern.ch/yellowrep/2005/2005-002/p655.pdf.