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ISSUES IN RESEARCH SOFTWARE

Summary of the First Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE1)

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Challenges related to development, deployment, and maintenance of reusable software for science are becoming a growing concern. Many scientists' research increasingly depends on the quality and availability of software upon which their works are built. To highlight some of these issues and share experiences, the First Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE1) was held in November 2013 in conjunction with the SC13 Conference. The workshop featured keynote presentations and a large number (54) of solicited extended abstracts that were grouped into three themes and presented via panels. A set of collaborative notes of the presentations and discussion was taken during the workshop.

Unique perspectives were captured about issues such as comprehensive documentation, development and deployment practices, software licenses and career paths for developers. Attribution systems that account for evidence of software contribution and impact were also discussed. These include mechanisms such as Digital Object Identifiers, publication of "software papers", and the use of online systems, for example source code repositories like GitHub. This paper summarizes the issues and shared experiences that were discussed, including cross-cutting issues and use cases. It joins a nascent literature seeking to understand what drives software work in science, and how it is impacted by the reward systems of science. These incentives can determine the extent to which developers are motivated to build software for the long-term, for the use of others, and whether to work collaboratively or separately. It also explores community building, leadership, and dynamics in relation to successful scientific software.

Keywords: sustainability; software development; policy; career paths

1 Introduction

The First Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE1, http://wssspe.researchcomputing.org.uk/WSSSPE1) was held on Sunday, 17 November 2013, in conjunction with the 2013 International Conference for High Performance Computing, Networking, Storage and Analysis (SC13, http://sc13.supercomputing.org).

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Because progress in scientific research is dependent on the quality of and accessibility to software at all levels, it is now critical to address many challenges related to the development, deployment, and maintenance of reusable software. In addition, it is essential that scientists, researchers, and students are able to learn and adopt software-related skills and methodologies. Established researchers are already acquiring some of these skills, and in particular a specialized class of software developers is emerging in academic environments as an integral part of successful research teams. This first WSSSPE workshop provided a forum for discussion of the challenges around sustaining scientific software, including contributed short papers in the form of both positions and experience reports. These short papers, as well as notes from the debates around them, have been archived to provide a basis for continued discussion, and have fed into the collaborative writing of this report. Some of the workshop submissions have been extended to full papers, which form part of the same special journal edition in which this report appears. The workshop generated a high level of interest; an estimated 90 to 150 participants were in attendance at different times of the day. The interest and discussions have already led to follow-up activities: A smaller Python-specific workshop is planned to be held at the 2014 SciPy conference, and a follow-on WSSSPE2 workshop has been accepted for the SC14 conference. In addition, funds to support the workshops have been obtained from the US National Science Foundation (NSF) and the Gordon and Betty Moore Foundation, and the original workshop website has been turned into a community website to engender further discussion and progress. Additionally, a minisymposium at the 2014 Society for Industrial and Applied Mathematics (SIAM) Annual Meeting on "Reliable Computational Science" (SIAM AN14, http://meetings.siam.org) is being co-organized by a WSSSPE1 participant to further explore some of the key issues raised at the workshop.

This report attempts to summarize the various aspects of the workshop. The remainder of this paper first gives an overview of the process with which the workshop was organized (§2), then proceeds with summaries of the two keynote presentations (§3), followed by summaries of the workshop papers grouped by the three thematic workshop panels to which they were assigned (§4–6). Three broader cross-cutting issues surfaced repeatedly, and are discussed separately (§7), as are use cases for sustainable software (§8). The summaries are based not only on the papers and panel presentations, but also on the many comments raised in both the onsite and online discussions that accompanied the workshop elements, as documented by collaborative note taking during the workshop [1]. We conclude with issues and lessons learned, as well as plans for future activities (§9). The original call for papers is included in Appendix A. The short papers accepted to the workshop are listed in Appendix B, and a partial list of workshop attendees can be found in Appendix C (see supporting information).

2 Workshop Process and Agenda

WSSSPE1 was organized by a relatively small group of five organizers and a larger program committee of 36 members. The program committee peer-reviewed submissions, but also had early influence in the workshop's organization, such as articulating the Call for Papers (see Appendix A).

Aside from setting the stage for the relevance of software sustainability and corresponding training and workforce issues to science, the call for papers enumerated the topics it was interested in as challenges to the ecosystem of which scientific software is a part, and in which software developers, users, and funders hold roles. These challenges roughly followed NSF's Vision and Strategy for Software [2], and specifically included the development and research process that leads to new (or new versions of existing) software; the support, community infrastructure, and engineering for maintenance of existing software; the role of open source communities and industry; aspects of the use of software, such as reproducibility, that may be unique to science; policy issues related to software sustainability such as measuring impact, giving credit, and incentivizing best practices; and education and training.

The workshop's goal was to encourage a wide range of submissions from those involved in software practice, ranging from initial thoughts and partial studies to mature deployments. Consequently, the organizers aimed to make submission as easy as possible. Rather than requiring adherence to a formal submission system and a full research paper-style template, submissions were intentionally limited to short 4-page papers, articulating either a position on one or more of the topics, or reporting experiences related to them. Furthermore, for submission authors were asked to self-archive (and thus self-publish) their papers with a third-party service that issues persistent identifiers, such as Digital Object Identifiers (DOIs), and to then submit the URL to the archived paper by email. This had the side effect that every submitter would also have a publicly available and citable version of their workshop contribution.

This process resulted in a total of 58 submissions. Almost all submitters used either arXiv [3] or Figshare [4] to archive their papers. The submissions were then subjected to peer review by the program committee, resulting in 181 reviews, an average of 3.12 reviews per paper. Reviews were completed using a Google form, which allowed reviewers to choose papers they wanted to review, and to provide general comments as well as relevance scores to the organizers and to the authors. Based on the review reports, the organizers decided to list 54 of the papers (see Appendix B for a full list) as significant contributions to the workshop. The high acceptance rate may come as a surprise, but it is nonetheless consistent with the goal of fostering broad participation, and as a corollary of the chosen submission process paper acceptance was no longer a means to filter the papers' public availability.

Roughly following the call for papers topics, the accepted submissions were grouped into three main categories, namely *Developing and Supporting Software*, *Policy*, and *Communities*. Each category was assigned to a panel, with three to four panelists drawn from authors of the associated submissions, who were each assigned to read and summarily present a subset of the papers associated with the panel. The process from organizing and advertising the workshop, to collecting and reviewing the papers, and putting together the agenda was documented by the organizers in a report [5], which they self-archived in the same way as contributed papers.

The workshop received submissions from eight North American and European countries. In some instances authors collaborated across multiple countries towards jointly authored papers. A majority of contributions came from the US with 42 papers where at least one author was affiliated with a US institution. A total of 10 submissions were from Europe and 4 were from Canada. This is not surprising for a workshop being held in the US. We believe future versions of the workshop will have contributions from more countries and more continents.

In terms of subject of the papers, the submissions were dominated by the domain of practice of sustainable software engineering and management with about 32 papers based on these themes. These papers were further based on a variety of disciplines including infrastructure and architecture, user engagement, and governance. Additionally, 18 papers were based on the sciences and applied mathematics domains with disciplines including High Energy Physics, Bioinformatics, Nanotechnology, Chemistry, and material sciences. Others were included topics such as science gateways and visualization. Again, given that this workshop was held with a computer and computational science conference, these numbers are not surprising.

The workshop also included two keynote presentations. Remote participation was facilitated by a live-cast of keynotes and panels via Ustream.tv (http://ustream.tv). In each panel, the paper summary presentations were followed by active discussion involving panelists, onsite attendees, and often online participants. The latter was facilitated by having a shared Google Doc [1] for collaborative note taking. Some of the online discussion also took place on Twitter (hashtag #wssspe).

3 Keynotes

The WSSSPE1 workshop began with two keynote presentations, which resonated with the audience and spurred a number of topics discussed throughout the meeting.

3.1 A Recipe for Sustainable Software, Philip E. Bourne

The first keynote [6] was delivered by Philip E. Bourne of University of California, San Diego. Bourne is a biomedical scientist who has also formed four software companies. He co-founded PLOS Computational Biology [7] and helped develop the RCSB Protein Data Bank [8]. He is working on automating three-dimensional visualizations of cell contents and molecular structures, a problem that has not been solved and when done, would serve as a key function of software in biomedical sciences.

Bourne's presentation was based on his own software experiences. He emphasized that sustainability for software "does not just mean more money from Government" (see also Section 7.1). Other factors to consider, he mentioned, encompass costs of production, ease of maintenance, community involvement, and distribution channels.

In places, Bourne said, development in science has improved thanks to open source and hosting services like GitHub [9], but for the most part it remains arcane. He argued that we can learn much from the App Store model about interfaces, ratings, and so on. He also mentioned BioJava [10] and Open Science Data Cloud [11] as distribution channels. On a related note, Bourne observed a common evolutionary pathway for computational biology projects, from data archive to analytics platform to educational use, and suggested that use of scientific software for outreach might be the final step.

Bourne shared with the audience a few real challenges he encountered. His first anecdote was that he has looked into reproducibility in computational biology, but has concluded that "I have proved I cannot reproduce research from my own lab" [12].

Another problem Bourne experienced was staff retention from private organizations which reward those combining research and software expertise (the "Google Bus"). However, he is a strong supporter of software sustainability through public-private partnerships. He noted that making a successful business from scientific software alone is rare: founders overvalue while customers undervalue. He noted that to last, an open source project needs a minimal funding requirement even with a vibrant community — goodwill only goes so far if one is being paid to do something else. He talked about grant schemes of relevance in the U.S., particularly with regard to technology transfer [13, 14].

Bourne also had problems with selling research software: the university technology transfer office wanted huge and unrealistic intellectual property reach through, whereby they would get a share of profits from drugs developed by pharmaceutical companies who use the software. He advocated for a one-click approach for customers to purchase university-written software.

He then presented arguments on directly valuing software as a research output alongside papers, a common discussion within this field. He mentioned an exploration of involving software engineers in the review process of scientific code [15], and discussed how publishing software reviews could change attitudes.

On the notion of *digital enterprise*, where information technology (IT) underpins the whole of organizational activities, he contended that universities are way behind the curve. In particular, he highlighted the separation of research, teaching, and administration into silos without a common IT framework as a blocker to many useful organizational innovations: "University 2.0 is yet to happen." He argued that funders such as NSF and NIH can help train institutions, not just individuals, in this regard.

Bourne concluded by discussing his 2011 paper "Ten Simple Rules for Getting Ahead as a Computational Biologist in Academia" [16] and argued that computational scientists "have a responsibility to convince their institutions, reviewers, and communities that software is scholarship, frequently more valuable than a research article".

3.2 Scientific Software and the Open Collaborative Web, Arfon Smith

The second keynote [17] was delivered by Arfon Smith of GitHub. Smith started with an example from his past in data reduction in Astronomy, where he needed to remove interfering effects from the experimental apparatuses. He built a "bad pixel mask," and realized that while it was persistent, there was no way or practice of sharing these data among scientists. Consequently many researchers repeated the same calculations. Smith estimated that plausibly 13 person-years were wasted by this repetition.

"Why didn't we do better?" Smith asked of this practice. He argued this was because we were taught to focus on immediate research outcomes and not on continuously improving and building on tools for research. He then asked, when we do know better, why we do not act any different. He argued that it was due to the lack of incentives: only the immediate products of research, not the software, are valued. He referenced Victoria Stodden's talk at OKCon [18] which he said argued these points well.

C. Titus Brown [19], a WSSSPE1 contributor, argued that with regard to reusable software, "we should just start doing it." Smith replied that documentation should be "treated as a first class entity." He noted that the open source community has excellent cultures of code reuse, for example, RubyGems [20], PyPI [21], and CPAN [22], where there is effectively low-friction collaboration through the use of repositories. This has not happened in highly numerical, compiled language scientific software. An exception he cited as a good example of scientific projects using GitHub is the EMCEE Markov Chain Monte Carlo project [23] developed by Dan Foreman-Mackey and contributors.

He argued that GitHub's *Pull Request* code review mechanism facilitates such collaboration, by allowing one to code first, and seek review and merge back into the trunk later.

"Open source is …reproducible by necessity," Smith quoted Fernando Perez [24], explaining that reproducibility is a prerequisite for remote collaboration. He pointed out that GitHub could propel the next stage of web development, i.e., "the collaborative web," following on from the social web of Facebook.

In conclusion Smith reiterated the importance of establishing effective incentive models for open contributions and tool builders, for example, meaningful metrics and research grants such as [2]. He urged computational scientists to collaborate and share often their research reports, teaching materials, code, as well as data by attaching proper licenses.

4 Developing and Supporting Software

The panel on Developing and Supporting Software examined the challenges around scientific software development and support, mainly focused on research groups that in addition to pursuing research also produce code in various forms. There was widespread agreement that developing and maintaining software is hard, but best practices can help. Several participants added that documentation is not just for users, and writing application programming interface (API) documentation, tutorials for building and deploying software, together with documented development practices can be very helpful in bringing new developers into a project.

Two subjects that prominently surfaced in this panel also came up throughout other parts of the workshop, and are therefore deferred to the section on Cross-cutting Issues (§7). These are the lack of long-term career paths for specialists in the various software development and support areas (see §7.2), and the question of what "sustainable" should mean in the context of software (see §7.1).

4.1 Research or Reuse?

Software is developed for many different purposes, and the requirements can vary significantly depending on the intended audience. Most end-users make use of either a graphical user interface of some kind, or a command line that may offer input and output formats for running the code and analyzing its output(s). When discussing backward compatibility it is these various interfaces that are discussed. For software that builds on other software frameworks it is the APIs that are most important, and this can encompass issues such as the source and binary interfaces to the software libraries developed—with each potentially having a high maintenance cost if they are to remain compatible over many years. When using command-line programs it is generally the command-line switches as well as the input/output formats that could incur significant costs if they are changed.

There was discussion that backward compatibility is not always desirable, and it can be very costly. This must be balanced with the aims of a given project, and how many other projects depend on and use the code when backwards incompatible changes are to be made. There are many examples in the wider open source software world of strategies for dealing with this, and again best practices can go a long way to mitigating issues around backwards compatibility. Many projects live with sub-optimal code for a while, and may allow backwards compatibility to be broken at agreed-upon development points, such as a major release for a software library.

There were 13 articles about different experiences in this area, but little about GUI testing, performance, scalability, or agile development practices. There were several unique perspectives about issues such as managing API changes, using the same best practices for software as data, and going beyond simply "slapping an OSI-approved license on code."

It should be noted that several articles that discussed long-term projects, that could be said to have reached a sustainable period. The Visualization Toolkit (VTK) was described [25] as being one of the oldest projects serving as a basis for several other tools such as ParaView [25], VisIt [26], and VisTrails [27]. Other examples of long-term, sustainable projects included MVAPICH [28] and R/qtl [29], which both began development in 2000, and DUNE [30], which is also over a decade old. In addition to how long a project has been active, other metrics are important, such as number of developers, number of institutions, and whether there are active developers acting as advocates for the continued viability of a project beyond individual projects and/or institutions.

4.2 The Importance of Communities

Communities are extremely important in software projects, and both their building and continued engagement need attention during the project life cycle. Several of the submitted papers discussed how communities have been built around projects, and what is needed to enable a project to grow [31, 25, 32, 33, 34]. The latter includes public source-code hosting, mailing lists, documentation, wikis, bug trackers, software downloads, continuous integration, software quality dashboards, and of course, a general web presence to tie a project's channels and artifacts together.

There was extended discussion about the challenge of fostering communities in which users help each other, rather than always deferring to the developers of project to answer user queries. Participants offered examples that this is indeed possible, such as mailing lists in which developers do not participate much because users actively respond to questions from other users, but also asked whether by doing too much the "core team" could end up setting unrealistic expectations. Team Geek [35] and Turk's paper on scaling code in the human dimension [36] discuss how development lists tend to have many more people contributing when they are welcoming to people.

4.3 Software Process, Code Review, Automation, Reproducibility

The papers submitted to this panel included many general recommendations for processes, practices, tools, etc. One of the papers [37] suggested that a "Software Sustainability Institute" should be vested with the authority to develop standardized quality processes, a common repository, central resources for services and consulting, a think tank of sorts, and a software orphanage center (i.e., a place to 'take care' of software when the original developers have stopped doing so). The idea of one common repository received some resistance, with so many compelling alternatives available, e.g., Bitbucket or GitHub. The centralized communication or point of contact was seen as reasonable, with the statement that "vested with authority" is perhaps too strong. However, "providing tools if needed" might be more appropriate.

What about actual software engineering principles, such as modularity and extensibility? This is how industry maintains software, and ensures it continues to be useful. Often, rewriting software is considered to be too costly, but with a modular design it can be kept up to date. Extensibility is expected to keep it relevant, if built into the project. One counterpoint raised by Jason Riedy was that trying to take advantage of the latest and greatest hardware often makes this painful, hence the lack of papers mentioning "GPUs and exotic hardware."

The question of whether funders, such as the NSF, can mandate software plans in much the same way as they do data management plans, was raised. Daniel Katz responded that software is supposed to be described as part of the NSF data management plan, and that in NSF's definition, data includes software. A comment from Twitter (@biomickwatson) raised the issue that this requires reviewers and funders who understand the answers that are given in these plans. Daniel Katz responded that in programs focused on software or data this can be done effectively, but agreed that in more general programs this is indeed a problem.

4.4 Training Scientists to Develop and Support Software

Part of the panel discussion focused around community structures and how academic communities are not taught how to evaluate cross-disciplinary work. One question raised was whether software developers can be effective if they are not part of the appropriate domain community, with responses that this depends on the specific problem and situation, and that "T-shaped" people who have both disciplinary depth as well as interdisciplinary and collaboration skills are important [38, 39, 40]. The discussion focused on whether we could teach software developers and domain scientists to collaborate together more effectively rather than trying to teach software developers about domain science and domain scientists about software development practices. The end goal of this would be to have a single community with a spectrum of expertise across domain science and software development, rather than two separate communities [41].

The role of the growing field of team science with software development was discussed. Team science deals with understanding and improving collaborative and team-based scientific research, and issues such as virtual organizations, and tool development across software development communities [32, 33]. Further, how should these skills and best practices then be introduced to students?

4.5 Funding, Sustainability Beyond the First Grant/Institution

Are there significant differences in projects that have been running for 1, 3, 5, or 10+ years? Are there shared experiences for projects of a similar stage of maturity? It was noted that computing and communication have changed significantly over the past decade, and many of the experiences are tied to the history of computing and communication. See the history of GCC, Emacs, or the Visualization Toolkit for examples. Others felt that computing has changed less, but communication and the widespread availability of tools has. It was noted that email lists, websites, chat rooms, version control, virtual and physical meetings are all over 20 years old.

It appears that while some of the basics of computing may be similar, the tools commonly used for computing have changed quite significantly. Reference was made to Perl, which was commonly used, giving way to whole new languages, such as Python, for gluing things together and how this induces many students into entirely rewriting the scaffolding, leaving the old to rot and the experiments to become non-reproducible as the tools change. There was discussion of this tendency along with the

Paper/Authors	Software	Sustainability	Approach to Understand or Evaluate Sustainability
Calero, et al. [43]	General notion of software. Not explicitly defined.	Sustainability is linked to quality.	Add to ISO
Venters, et al. [44]	Software as science software; increasingly complex; service-oriented computing	Extensibility, interoperability, maintainability, portability, reusability, scalability, efficiency	Use various architecture evaluation approaches to assess sustainability
Pierce, et al. [45]	Cyberinfrastructure software	Sustainable to the extent to which there is a community to support it	Open community governance
Katz, et al. [46]	E-research infrastructures (i.e. cyberinfrastructure)	Persisting over time, meeting original needs and projected needs	Equates models for the creation of software with sustaining software
Lenhardt, et al. [47]	Broadly defined as software supporting science	Re-use; reproducible science	Comparing data management life cycle to software development life cycle
Weber, et al. [48]	Software broadly defined; a software ecosystem	Software niches	Ecological analysis and ecosystem

Table 1: Summary of Modeling Sustainability papers from Policy Panel. Adapted from [42].

enormous differences in the speed and ease of sharing—having to ship tapes around in the early days of software development (which shaped development of GCC and Emacs in their formative years) as opposed to the immediate sharing of the latest development online, using revision control systems like CVS, Subversion, Git, Mercurial, Bazaar, etc.

The question was also posed as to whether the distinction between researcher and developer is sensible, with James Hetherington commenting that in the UK a more nuanced view of research software engineers and researcher developers is examined. Should this be less of a contract relationship, and more of a collaborative relationship? This is also at the core of the business model that Kitware presented in its submission to the workshop. Are other ingredients missing such as applied mathematicians? Should this be defined more in terms of skill sets rather than roles and/or identities? This builds on the comments from Vaidy Sunderam that scientists are generally good writers, and have mathematical skills, so why can't they learn software engineering principles?

Miller commented that all of the infrastructure that sits around a new algorithm that we need to make it useful and sustainable requires different skill sets than the algorithm developer. Friere commented that there are no good career paths for people with broad skills, no incentives for them to continue in these roles. There was debate around people doing what interests them, and learning computing leaves people cold, but is it that it leaves the people who find career paths in academia cold versus the full spectrum of people involved in research? Is this also caused by poor teaching, or because the benefits for doing this are perceived as too small? It could also be attributed to their focus being on science, not software engineering, or do people with the passion for software engineering in science simply have no viable career path and either adapt or seek out alternate career paths?

5 Policy

The panel on policy discussed workshop contributions dealing with the wide range of software sustainability aspects that relate to establishing, promoting, and implementing policies. Six papers presented frameworks for defining, modeling, and evaluating software sustainability, the basis of establishing policies. Four papers advocated mechanisms for more properly assessing the impact of scientific software, and for crediting and recognizing work that promotes software sustainability, all of which are instrumental in effectively promoting policies that aim to change current practices. Four papers discuss facets of implementing software sustainability, and models of implementation across different facets.

5.1 Modeling Sustainability

The workshop submissions grouped under this section provide frameworks for thinking about, researching, and understanding which elements of sustainability are important and how they are related to each other. Although there is substantial overlap between the frameworks, they have different emphases and extents. Each paper in this group included a definition of sustainability, with many overlaps between them (see **Table 1**). Perhaps unsurprisingly, the issue of how to define sustainability came to the fore multiple times during the workshop, and it is thus summarized in depth separately in §7.1.

Table 1 is based on a summary by Lenhardt [42], which shows for each contribution to the Modeling Sustainability panel what it meant when referring to software, how it defined software sustainability, and which approach it suggested to understand or evaluate sustainability.

One area in which there was not complete overlap was whether the word (and thus the effort called for by the WSSSPE workshop) involved environmental sustainability. Of course the word sustainability has strong connotations from consideration of environmental issues, evoking some mention of the areas in which software interacts with overall environmental resource usage, particularly energy efficiency. The two papers in this area which mentioned this [44, 43] did so without integrating that analysis into the question of software being around long-term, suggesting that questions of environmental impact of scientific software is a conceptually distinct area of inquiry.

One group of papers presented frameworks that were primarily about characteristics of software artifacts, connecting with the long discourse on software quality. This approach is realized in adjectives that can be applied to pieces of software but might also extend to describe software projects. Thus Calero et al. [43] propose adding elements to the ISO standards for measuring software quality. Specifically, they propose an additional dimension of quality they call "perdurability" with three defining characteristics: reliability, maintainability, and adaptability. This overlaps with the framework by Venters et al. [44] who employ the features "extensibility, interoperability, maintainability, portability, reusability and scalability," anticipating the sorts of work that people would need to do with a software artifact in the future, "as stakeholders requirements, technology and environments evolve and change." Venters et al. argue that these choices need to be made early because they are related to the architecture of the software and involve trade offs that ought to be analyzed alongside each other. Lenhardt et al. [47] compare the software lifecycle to the data lifecycle to argue for the inclusion of metadata throughout a piece of software's life (discussing, for example, how it has been built and tested and what "data in" and "data out" has been considered). In addition, their analogy suggests that the software lifecycle might add a phase of "preservation" and draw on the understanding of what that involves from studies of data. In sum, then, these frameworks focused on what needs to be accomplished to have more sustainable software.

A second theme in these papers was the continued availability of resources to accomplish the goals of sustainability. The elements of these frameworks focused far more on the organization of a software project than they did on characteristics of the artifact itself (although it is certainly true that the adjectives discussed above could be applied to a software project). For example Pierce et al. [45] focus on the way that the project is run, particularly in terms of how those involved communicate and jointly set priorities, a process they call governance. In particular they argue that because sustainability is related to having ongoing resources, governance must be open to receive diverse input (by occurring online, asynchronously, or publicly) and thus have the potential to "transform passive users into active contributors." They argue that the Apache Software Foundation's incubation process teaches this and could be learned from by projects throughout scientific software. Katz and Proctor [46] also discuss governance, describing two modes: "top-down" and "bottom-up" governance. They place governance alongside technical questions about the software, political questions about who is funding the work surrounding the software, and the manner in which resources come to the project both initially (commercial, open source, closed partnerships, grant funded) and long-term (all four plus paid support).

Frameworks also concerned themselves with the context in which software projects exist, moving in abstraction from the software artifact itself to the organization of its production and the shape of the space in which an artifact or project exists. These frameworks take the form of contingency theories in that they outline a different set of challenges and argue that different project organizations (and presumably artifact attributes) are necessary to persist long term in spaces with particular characteristics. Katz and Proctor [46] propose thinking of this idea of space in terms of three axes: temporal (long or short term needs), spatial (local or global use) and purpose (specific to general). They propose that different project organizations will be needed in different locations and argue that we should concentrate research to understand those connections. Weber et al. [48] describe their spaces by analogy with natural ecosystems as "niches" which sustain particular pieces of software. They define "a software niche as the set of technical requirements, organizational conditions and cultural mores that support its maintenance and use over time." They call for better understanding and modeling of niches (as well as further exploration of the usefulness of ecosystem metaphors).

5.2 Credit, Citation, and Impact

How work on scientific software is recognized and rewarded strongly influences the motivation for particular kinds of work on scientific software. A recurring theme of the panel discussion was that software work in science is inadequately visible within the reputation system underlying science; in other words it often doesn't "count". In his paper for this workshop, Katz placed software work along with other "activities that facilitate science but are not currently rewarded or recognized" [49]. Priem and Piwowar argued for the need to "support all researchers in presenting meaningful impact evidence in tenure, promotion, and funding applications." [50]. Knepley et al. argued that the lack of visibility of software that supported a piece of science "can have detrimental effects on funding, future library development, and even scientific careers." [51].

These papers, and the discussion at the workshop, join a nascent literature seeking to understand what drives software work in science and how the reward systems of science thereby shape the type of software work undertaken. This study includes the extent to which developers are motivated to build software for the long-term, for the use of others, and whether to work collaboratively or separately [52, 53, 54]. Software work is not only motivated by direct citations, but the visibility of software work in the literature is important to those who write software used in science.

Papers and discussion concentrated on three overarching questions: How ought software work be visible, what are the barriers to its visibility, and what can be done to make it more visible?

Most of the papers in this area focused on visibility of software in scientific papers, since scientific papers are the most widely accepted documentation of achievement in science. It was noted that there appear to be no widely accepted standards on how the use of software towards a paper ought to be mentioned, and that journals, citation style guides and other guides to scientific conduct are vague about how to describe software. To address this, papers advocated the need for a fixed identifier for software, either directly through a mechanism such as a Digital Object Identifier [49, 51] or via a published paper written to document the software (and perhaps its creation), a "software paper" [55]. However, as was pointed out during the panel discussion, one of the problems with papers as the cited product is that their author list is fixed in time, which discourages potential contributors who are not on the original author list from designing incremental improvements as integration work rather than separate (and hence possibly rewritten) software products [52].

Another approach is to reduce the difficulty of citing all software underlying a research paper. For example, scientists often work with software that itself wraps other software, leading to attribution stacking that can make it non-obvious or even difficult to determine what attributions would be appropriate. Knepley et al. [51] approach this by proposing a mechanism by which the software itself, after it has run, provides the user with a set of citations, according to the pieces of code actually executed. They describe a prototype implementation whereby the citations are embedded in libraries and reported along with the results, via a command-line interface [51]. Discussion highlighted the difficulty that attempting to acknowledge the contributions of all pieces of dependent code within a paper faces the difficulty of creating very long citation lists, straining the analogy of code used to papers cited. Katz approaches this issue by proposing a system of "transitive credit," recording dependencies and relative contributions outside particular papers, relieving authors from the responsibility of acknowledging each and every dependency. Instead authors would acknowledge the percentage contribution of the software they used directly and an external system would then be able to recursively allocate that credit to those who had provided dependencies [49]. Finally Priem and Piwowar argued that machine learning techniques could examine the body of published literature and extract mentions of software, coping with the multitude of informal ways in which authors mention software they used [50]. A point raised in the panel discussion was that instead of asking users to improve their software citation practices, one can also ask how software projects can better monitor the literature to improve their ability to show impact. For example, the nanoHUB project scans the literature using keywords and names of known users to discover papers that are likely to have used their software and platform, and assigns graduate students to read each paper, highlighting mentions of software use and sometimes following up with the authors to identify stories for demonstrating impact. A process for tracking software-using publications with the goal of increasing impact visibility is now described at http://publications.wikia.com.

Potential visibility, and thus acknowledgement of scientific software products is not restricted to publications. Another key location for visibility is in the grant funding process, and as emphasized by NSF representatives at the meeting, recent changes to grant proposal and reporting formats now allow both applicants and awardees to report and highlight software products as much as publications. Nonetheless, whether peer review panels would value these contributions in the same way as publications remains to be seen.

Priem and Piwowar argued that assessing the impact of software work requires looking beyond publications, including evidence of contribution and impact recorded in social coding-oriented resources such as GitHub, and conversations about software in issue trackers, mailing lists, twitter and beyond [50]. In keeping with a principle of the "altmetrics" approach, they advocate that scholars should have resources that empower them to tell their own stories in the manner most appropriate for them and their audiences.

5.3 Implementing Policy

The workshop contributions in this group were concerned with the aspect of how implementation of best practices and other recommendations for improving scientific software sustainability could be promoted. Specifically, if scientific software is to become more sustainable, corresponding policies and guidelines need to be such that the scientific community can follow and implement them. This is considerably more challenging that it might seem at first, because in the reality of science today resources, both financial and personnel, that could be devoted to implementation are very limited, and the reward system does not encourage scientists to do so. Furthermore, implementing sustainability-targeting policies and guidelines often takes a variety of specialized software engineering expertises, which are not necessarily found in a single engineer, and much less so in a domain scientist cross-trained in programming. Adding to the policy implementation challenges, applicable sustainability-promoting practices and guidelines will change through a software project's lifecycle, in particular as it gains maturity.

Two of the papers in this group focus on specific facets of software design that are important factors in a project's sustainability but are often addressed only late in the scientific software development cycle, if at all: Krintz et al. [56] look at API governance, and Heiland et al. [57] discuss maturity models for software security. The other two papers discuss implementation strategies for science from the perspective of facilitating many or all facets of sustainability-oriented software design: Blanton and Lenhardt [58] contrast large projects that have software infrastructure development built-in, with cross-training domain scientist PIs in software engineering best practices. Huang and Lapp [59] discuss how various specialized software engineering skills could be turned into shared instrumentation with low barriers to access.

Krintz et al. [56] describe how in an era in which computing frequently takes place in a distributed cloud, the control over digital resources is increasingly shifting from physical infrastructure to APIs, in particular web-service APIs. Yet, as Krintz et al. observe, unlike for physical IT infrastructure in data centers, science communities have developed very little in the way of practices and technology for API governance, referred to by Krintz et al. as the "combined policy, implementation, and deployment control". Web APIs can and do change, sometimes quite frequently, raising the need to port dependent applications. The effort required for porting is notoriously difficult to estimate, making it nearly impossible for IT organizations to assess and thus properly manage the impact of API changes. To address this, Krintz et al. propose a mechanism that evaluates the porting effort between two versions of a web-service API in a formal and automated way. To analyze the porting effort, they divide API changes into *syntactic similarity*, the changes in inputs and outputs, and into *semantic similarity*, the changes in the API's behavior. In initial tests, their method showed good congruence with human developers in scoring porting effort, offering the possibility that API governance can become as solid a part of scientific IT management as data center infrastructure management is today.

Many facets of engineering for software sustainability strongly depend on the maturity level of the software. However, the maturity level of a software project meant to be sustained changes tremendously over its development life cycle, and the eventual maturity level is often difficult to predict during initial development. Using software security as their case study, Heiland et al. [57] discuss how Maturity Models can be used to formalize best practices appropriate for the different levels of maturity that a software project may go through over its lifecycle. Cybersecurity is also an example of a sustainability-relevant aspect in software design that is rarely given due diligence in science. In particular in industry, cybersecurity best practices for different stages of life cycle and maturity have been formalized as Software Security Maturity Models, and are widely used, yet awareness of these among scientific software development communities remains low. In providing a path to tightening security practices as software matures, such models align with the objective of providing implementation approaches that the scientific community can actually follow.

API governance and cybersecurity measures appropriate for a project's maturity are all but two facets of sustainability-oriented software development. Others include user-centered interface design, test engineering, dependency management, and deployment operations. Each of these facets requires specialized skills and training in software engineering. How can the implementation of best practices and guidelines along many or all of these different facets be facilitated in scientific software development? Blanton and Lenhardt [58] contrast two models. In one, the time and personnel devoted to software engineering is "co-funded" with the driving science project. This typically implies large multi-year collaborative projects that to succeed require significant software infrastructure to be built, and which thus have the funding to support one or several software engineers. The sustainability of such projects then depends on sustaining the funding. In the other model, domain scientists also take the role of software developers, whether by necessity such as funding limitations, or due to cross-disciplinary professional interests. For this to result in sustainable software products, the domain scientists need to be (or become) cross-trained in software engineering standards and best practices.

In practice, there are example for both extremes of the spectrum. For example, in the life sciences the iPlant Collaborative [60], the Galaxy Project [61], and Qiime [62] are large multi-year projects with significant software infrastructure funding and deliverables. Typically though these are the exception rather than the rule, and particularly in the long tail of science the scientist-developer predominates, even for software that is widely used or crosses domain boundaries such as rOpenSci [63]. For better training domain scientists at least in basic software engineering best practices, initiatives such as Software Carpentry [64] have demonstrated how this could be achieved at scale.

However, there may also be a middle ground between the two extremes. Huang and Lapp [59] propose a Center of Excellence model that leverages economies of scale to make software engineering experts and their skills accessible to the long tail of science. As Huang and Lapp discuss, this model could effectively turn the utilization of software engineering expertise from a complex human resource recruitment and management challenge, to buying time, when and to the extent needed, on shared instrumentation. There is precedence to using such a model to lower access barriers for long tail science, in particular for new experimental technologies. For example, although the acquisition and operation of next-generation high-throughput DNA sequencers requires substantial investments of money, time, and expertise, the establishment of "core facilities" on many university campuses has made these technologies accessible to a wide swath of scientists, with transformative results for science.

One of the important conclusions from this group of papers is that creating sustainable software requires paying attention not to one or two, but to several different facets of software engineering, each with corresponding best practices and standards of excellence. Even if a science project requires and has funding for a full software engineering FTE, what the project really needs could be fractions of different engineers with different specialty training. The vast majority of long tail science projects lacks the funding for even one full software engineer, let alone one who combines expertise in all of the applicable facets of engineering. Some scientists in the long tail will have the professional interests to cross-train enough in software engineering to be successful with creating sustainable software, but it is unrealistic to expect this expertise and interest of all or even the majority. This is where a software engineering center of excellence could provide a critical resource by enabling scientists in the long tail to complement their resources and expertise with facets that are missing, but which, if applied at the right time, would improve the chances of a software product to become sustainable. Such complementary expertise also need not be restricted to software engineering in the strict sense; for example, it could consist of community building, leadership, and support for some period of transition to sustainability.

In summary, implementing software sustainability practices on a broader basis requires on the one hand the development of guidelines and practices that are suitable for the exploratory research context in which most scientific software is created, and on the other hand a skilled workforce trained in a variety of software engineering facets and community building. The capabilities afforded by such a workforce need to be accessible not only to large projects with sufficient funding to provide competitive employment, but also to the many smaller projects in the long tail of science. Sufficiently cross-training domain scientists could be one way to achieve this; another, complementary approach is to instrument the necessary capabilities so they can be shared.

6 Communities

Across all talks and papers submitted, authors implicitly and explicitly recognized the concept of "communities" as a driving and unifying force within software projects. Despite that, the actual nature of the communities, the incentive structures that bind them together, the infrastructure they utilize for communication and even the types of individuals that make up those communities were different. Some of these communities were primarily composed of members of industry, some were funded and driven by individuals focused on developing software as opposed to utilizing it, and others were primarily composed of scientist practitioners, and were true communities of practice.

These varying structures and compositions result in differing modes of interaction within communities, styles of development, and the structure of planning for future development of software. In this section, we summarize the different types of communities in scientific software as well as the resultant impact on sustainability and development of functionality.

6.1 Communities

Drawing on experiences from high-energy physics, Vay et al. [65] proposed developing teams of technical specialists to overcome a lack of coordination between projects. Maximizing scientific output requires maximizing the usability of the scientific code while minimizing the cost of developing and supporting those code. This included targeting different architectures for their software to be deployed, as well as coordination between technically-focused individuals and usage of a common scripting language between projects. Instead of fragmenting the development of simulation codes across institutions, the paper suggests that a cohesive strategy reducing duplication and increasing coordination will broadly increase the efficiency across institutions. The approach proposed is of de-fragmenting the existing ecosystem in a non-disruptive way.

Maheshwari et al. [66] focuses on "technology catalysts" and their role in the modern scientific research process. A technology catalyst is an individual with knowledge of technological advancements, tasked with user engagement to create scientific or engineering applications, using suitable tools and techniques to take advantage of current technological capabilities. One of the tasks of technology catalysts is to seek community collaborations for new applications and engage users, thus benefiting both science, by effective running of scientific codes on computational infrastructure, and technology, by conducting research and seeking findings for technology improvement. The particular engagements described in the paper came up from the lead author's work as a postdoctoral researcher at Cornell and Argonne, where interaction with the scientific communities in both institutions resulted in these collaborations.

At NESCent, a combination of in-house informatics individuals and domain scientists collaborate to develop software to study evolutionary science. The report [33] studied the success of a "hackathon" model for development, where short-form, hands-on events combining users, researcher-developers and software engineers targeted specific code improvements. From this experiment, the authors identified several key outcomes as well as lessons-learned: specifically, the co-localization of developers was seen as having a strong impact, enabling casual conversation that led to discrete outcomes. The formation of the discussion mailing list, specifically in response to the social capital built at the hackathon, was seen as spurring on longer-term benefits to the community and fostering sustainability.

Hart et al. [67] addresses the success of the rOpenSci project in developing collaboration supporting tools for Open Science. This software collective, organized around the statistical programming environment R, develops access mechanisms for data repositories and attempts to reduce the barrier to entry for individuals wanting to access data repositories and study the data contained therein. The collective fosters direct collaboration between individuals and data providers, designed to "train academics in reproducible science workflows focused around R." Two central challenges are engagement of existing users within ecology and evolutionary biology (EEB), and how the community can make inroads and traction in other disciplines. Currently, the collective is exploring addressing these challenges through the use of social media, holding workshops and hackathons. This helps to both raise the profile of the collective within EEB and in other domains. However, the overarching challenge identified in the paper was that of incentivizing maintenance of software, which is difficult in academia.

Christopherson et al. [32] outlines the degree to which research relies on high quality software. There are often barriers and a lack of suitable incentives for researchers to embrace software engineering principles. The Water Science Software Institute is working to lower some of these barriers through an Open Community Engagement Process. This is a four-step iterative development process that incorporates Agile development principles.

Step 1: Design - thorough discussion of research questions
Step 2: Develop working code
Step 3: Refine based on new requirements
Step 4: Publish open source

Christopherson reports on the application of Steps 1–3 to a computational modeling framework developed in the

1990s. Step 1 was a 2-day, in-person specifications meeting and code walk-through. Step 2 was a 5-day hackathon to develop working code, and Step 3 was a 3-day hackathon to refine the code based on new requirements. The team worked on small, low-risk units of code. It was challenging, revealed unanticipated obstacles, programmers had to work together, and experimentation was encouraged. The paper recommended: start small and gradually building toward more complex objectives, consistent with Agile development; develop consensus before coding, by repeating step 1 before all hackathons; ensure newcomers receive orientation prior to the hackathon, such as a code walk-through or system documentation; and co-locate collaborators whenever feasible.

Pierce et al. [68] describes how science gateways can provide a user-friendly entry to complex cyberinfrastructure. For example, more than 7,000 biologists have run phylogenetic codes on supercomputers using the CIPRES Science Gateway in 3½ years. Over 120 scientists from 50 institutions used the UltraScan Science Gateway in one year, increasing the sophistication of analytical ultracentrifugation experiments worldwide. The new Neuroscience Gateway (NSG) registered more than 100 users who used 250,000 CPU hours in only a few months.

Gateways, however, need to keep operational costs low and can often make use of common components, such as authentication, application installation and reliable execution and help desk support. Science Gateway Platform as a Service (SciGaP) delivers middleware as a hosted, scalable third-party service while domain developers focus on user interfaces and domain-specific data in the gateway. While SciGaP is based on the Apache Airavata project and the CIPRES Workbench Framework, community contributions are encouraged by its open source, open governance and open operations policies. The goal is robust, sustainable infrastructure with a cycle of development that improves reliability and prioritizes stakeholder requirements. The project is leveraging Internet2's Net+ mechanisms for converting SciGaP and its gateways into commodity services.

Zentner et al. [69] describes experiences and challenges with the large nanoHUB.org community, where community is defined as a "body of persons of common and especially professional interests scattered through a larger society." Support is challenging because of the diversity of viewpoints and needs. The group constantly examines its policies to determine whether they are indirectly alienating part of the community or encouraging particular types of use. nanoHUB's 10-year history with over 260,000 users annually provides a lot of data to analyze: 4000 resources contributed by 1000 authors. nanoHUB serves both the research and education community and the contribution model allows researchers to get their codes out into the community and in use in education very rapidly. The primary software challenges are twofold — support for the HUBzero framework and challenges related to the software contributed by the community.

The group has learned that community contributions are maximized with a tolerant licensing approach. HUBzero uses an LGPLv3 license so contributors can create unique components and license as they choose. If they make changes to source code, the original license must be maintained for redistribution. As far as contributed resources, these must be open access, but not necessarily open source. This allows contributors to meet the requirements of their institutions and funding agencies. Quality is maintained via user ratings. Documentation is encouraged and nanoHUB supplies regression test capabilities, but the user community provides ratings, poses questions and contributes to wishlists and citation counts, all of which incentivize code authors.

Terrel [34] describes support for the Python scientific community through two major efforts: the SciPy conference and the NumFOCUS foundation. Since software sustainability relies on contributions from all sectors of the user community, these efforts support these sectors, and help develop and mature Python. The reliance on software in science has driven a huge demand for development, but this development is typically done as a side effort and often in a rush to publish without documentation and testing. While the software is often created by academics, software support can fall to industrial institutions. SciPy brings together industry, government, and academics to share their code and experience in an open environment. NumFOCUS in a non-profit that promotes open, usable scientific software while sustaining the community through educational programs; collaborative research tools and documentation; and promotion of high-level languages, reproducible scientific research, and open-code development. Governance is a loose grantor-grantee relationship with projects, allowing funds to be placed in the groups' accounts. This has raised money to hire developers for open code development, maintain testing machines, organize the PyData conference series, and sponsor community members to attend conferences.

Löffler et al. [70] describes the Cactus project, which was started in 1996 by participants in the USA Binary Black Hole Alliance Challenge. Cactus has a flesh (core) and thorns (modules) model, a community-oriented framework that allows researchers to easily work together with reusable and extendable software elements. Modules are compiled into an executable and can remain dormant, becoming active only when parameters and simulation data dictate. Users can use modules written by others or can write their own modules without changing other code. The community has grown and diversified beyond the original science areas.

The paper points out four keys to sustaining the community: modular design, growing a collaborative community, career paths, and credit. In modular design, the Cactus project went far beyond standard practices of APIs. Domain specific languages (DSLs) allow decoupling of components — for example I/O, mesh refinement, PAPI counters, and boundary conditions abstracted from science code. In academia, publications are the main currency of credit. Because the project connects code developments to science, the work is publishable and modules are citable. Because of the open source, modular approach, programmers can see the impact of their contributions and often continue work after graduation. Career paths remain a challenge, however. Tasks that are essential from a software engineering perspective are often not rewarded in academia. The best programmers in a science environment often have multidisciplinary expertise. This also is not rewarded in academia.

Wilkins-Diehr et al. [71] describes an NSF software institute effort to build a community of those creating science gateways for science. These gateways, as described in some of the other papers in this section, can be quite capable and can have strong scientific impact. Challenges are similar to those highlighted by other papers in this section: the conflict between funding for research vs infrastructure and the challenges around getting academic credit for infrastructure. The authors observe that development is often done in an isolated hobbyist environment. Developers are unable to take advantage of similar work done by others, finding themselves in isolation even when their projects have common goals. But often projects struggle for sustainable funding because they provide infrastructure to conduct research and many times only the research is funded. Gateways also may start as a small group research project, taking off in popularity once they go live, without any long term plans for sustainability. Subsequent disruptions in service can limit effectiveness and test the limits of the research community's trust.

Recommendations from an early study of successful gateways include: 1) Leadership and management teams should design governance to represent multiple strengths and perspectives, plan for change and turnover in the future, recruit a development team that understands both the technical and domain-related issues, consider sustainability and measure success early and often. 2) Projects should hire a team of professionals, demonstrate credibility through stability and clarity of purpose, leverage the work of others, and plan for flexibility. 3) Projects should identify one or more existing communities and understand the communities' needs before beginning, then adapt as the communities' needs evolve. 4) Funders should consider the technology project lifecycle, and design solicitations to reward effective planning, recognize the benefits and limitations of both technology innovation and reuse, expect adjustments during the production process, copy effective models from other industries and sectors, and encourage partnerships that support gateway sustainability.

6.1.1 What are communities?

The workshop did not directly answer the question "What are communities?" but instead a number of different answers were indirectly presented, through the depiction of individuals and stakeholders in different aspects of the scientific software lifecycle. In broad strokes, however, scientific software communities were generally accepted as consisting of individuals, often but not always composed of scientist practitioners, that were working with some degree of coordination toward a common goal enabled by software.

The discussion of development-focused communities centered around describing methods of interaction between individuals and the scientific software. The first type of interaction was the development of a specific piece of software, the second was a particular domain or discipline, and the final primary type of interaction was around the development of applications built on a particular piece of software that was perhaps developed by another group. As an example, in [25], the community described is comprised of both the for-profit company Kitware and the users and contributors to their software packages such as VTK. This structure, of the centralized development of core infrastructure around which communities of individuals applying that infrastructure and developing applications utilizing it, was similarly reflected in [34], where the core scientific python ecosystem is supported by a non-profit entity that fosters community investment in that ecosystem. In many ways, these two organizations (Kitware and NumFOCUS) attempt to cross domain boundaries and provide support for both the infrastructure and application sides of community building.

6.1.2 Measuring community

How might a project know when it has built a sustainable community? How might an outsider be able to assess the activity and sustainability of that community? These questions have been partially addressed in the literature. For example, a key metric in online communities in general is the cross-over point where there are more external contributors than internal ones. Richard Millington's book "Buzzing Communities" does an excellent job of outlining these measures, drawing on communities research in an accessible manner [72]. Some participants in the workshop have since prepared materials outlining current and future practices in measurement of scientific software and its ecosystem [73].

6.1.3 Additional Resources for learning about software communities

Scientific software communities were viewed as a subset of software communities as whole. As such, resources applicable to generic software communities – such as open source and proprietary technology companies – can be used as input and as guiding understanding of how to steward and develop scientific software communities. Because incentive structures are different in industry and volunteer-based open source communities, these can provide rough guidelines but not necessarily identically applicable. The analogy between corporations and scientific investigators (particularly in terms of competition, cooperation and competitive advantage) has been explored in the literature below, but because of the different incentive structure the analogy is not universally true.

The literature below, suggested by attendees, addresses both non-scientific software projects, as well as scientific projects. The selections address both descriptive and prescriptive approaches to communities.

Both [53] and [52] study how scientific software collectives self-organize and address issues of incentive, long-term support, and development of infrastructure as well as new features. As noted elsewhere in this summary, [36] shared prescriptions from two software communities in astrophysics.

From the perspective of developing prescriptions for successful scientific software development, both [74] and [75] share experiences and suggestions for developing sustainable practices. [74] proposes "ten simple rules" for developing open source scientific software, focusing on both the choices made during development and the sustainability of practices in the long term. [75] describes the development and long-term growth of the deal.II library, and how its place in its ecosystem of libraries, applications and domains has shaped its development and community trajectory.

From more traditional open source development, resources were shared that developed communities explicitly, such as [76] and [77], focusing on large-scale projects such as the Ubuntu Linux distribution and smaller-scale volunteer-developed projects like such as ThinkUp, respectively. The process of open source development, while less explicitly focused on community building, sketched in [78] was seen as a valuable resource, particularly when combined with the management and personal interaction techniques outlined in [35]. Growing diversity in communities was directly addressed in [79], where experiences growing the diversity of technical conferences in open source were described.

6.2 Industry & Economic Models

Several papers presented discussed the connection between industry and scientific software, from the perspective of both integrating efforts between the two and sustaining long-term development.

Hanwell et al. [25] reflect on the 15-year history of open source software development at Kitware. In particular, they focus on their success at growing their community of users through enabling multiple channels of communication, directly reaching out to individuals, and lowering the barrier to entry for contributions. This involves providing clear, test-oriented and review-based mechanisms for evaluating contributions, permissive licenses, and a service-based model for sustaining development. This model enables Kitware to receive both public funding, as well as private funding to support improvements and targeted developments of the software.

Foster et al. [80] discussed the approach of developing sustainability models around Software-as-a-Service (SaaS) platforms, with the target example being that of GlobusOnline. The authors build a case that both grant-based and volunteer-based development fall short in sustaining software, resulting in software that is disproportionately difficult to use compared to its functionality, which they note directly impacts the overall scientific productivity of its users. In contrast, by charging a subscription fee for hosted, centrally-managed software (similar to offerings by Dropbox, EverNote, GMail), the authors propose to manage the funding cycle and enable a greater focus on the aspects of software that directly impact individuals, rather than funders. Globus has deployed such a service, for which they have attempted to develop a sustainable economic model that reduces institutional obstacles to funding and subscription. However, they do identify that cultural obstacles do still remain, and they note a particular difference in culture between NSF- and NIH-funded researchers.

6.3 Education & Training

The papers describing education and training were focused primarily on how these aspects of community development impact on the long-term sustainability of software projects. [40] described the impact of the mandate within the International Centre for Theoretical Physics (ICTP) to foster resources and competences in software development and HPC, resulting in the development of educational curricula directed in this area. The paper itself described the changes made in these curricula as a result of the current changes in the HPC and scientific software landscape due to the advent of scripting languages, new programming paradigms and new types of hardware such as accelerator technologies. The development of a workshop, with carefully selected participants and an immersive approach to learning, was identified as a major success for educating and developing new scientific software developers from targeted domains.

Elster [81] also points out how the prevalence and rapid growth of multi and many-core systems forces awareness of data locality and synchronization issues if one want to teach people how to develop high-performing scientific codes.

[37] addressed education and training within computational chemistry frameworks, particularly as these frameworks attempt to address next-generation computer hardware and software and as chemistry courses emphasize lab work over computational education. The authors identify this lack of computational awareness and training as the primary challenge to future advances in computational chemistry. The authors propose a new institute for computational chemistry, emphasizing collaboration (and a licensing structure, such as LGPL or more permissive) and education of future generations of chemistry researchers.

7 Cross-cutting Issues

Three issues, how to define software sustainability, how career paths (or their lack) interact with achieving it, and the impact of software licenses, were raised across the workshop's panels. This section aims to synthesize these discussions from different perspectives.

7.1 Defining Sustainability

What is, or should be meant by "sustainability" in the context of software came up in many different parts of the workshop, specifically in the first keynote (§3.1), the Developing and Maintaining Software panel (§4), and the Policy panel (§5). It quickly became clear that at present there is no consensus among the community, whether within or across disciplines, on what this definition should be, and that a variety of different definitions were being assumed, used, or sometime expressly articulated by contributors and attendees. However, some concepts, particularly relating sustainability to change over time, were also evidently held in common. This common notion is, for example, captured in the definition used by the UK's

Scientific Software Sustainability Institute, quoted in [44]: "software you use today will be available—and continue to be improved and supported—in the future". Pierce et al [45] express this idea as software that continues to serve its users.

Philip Bourne, too, used the relation to change over time when he suggested in his opening keynote that sustainability can perhaps be defined as the effort needed to make the essential things continue. This leads to having to decide what it is that we want to sustain, whether what we want to sustain is valuable, and finally, who would care and how much if it went away. As was pointed out during a discussion session, OSS Watch, an advisory service for issues relating to free and open source software in the UK, proposes a Software Sustainability Maturity Model to address the issue of what level of sustainability a particular element of software needs to have, and where this is important. It, too, expresses sustainability in relation to change over time:

> "When choosing software for procurement or development reuse — regardless of the license and development model you will use — you need to consider the future. While a software product may satisfy today's needs, will it satisfy tomorrow's needs? Will the supplier still be around in five years' time? Will the supplier still care for all its customers in five years' time? Will the supplier be responsive to bug reports and feature requests? In other words, is the software sustainable?" [82]

Attendees suggested that having a definition of sustainability on which the community can agree is key. A related question that was raised is what the goal of sustainability should be, with a wide range of possible answers, including more reproducible science, software persistence, and quality. And given a goal of sustainability, how would success in achieving it be measured? How would one know that a piece of software has reached sustainability? Participants pointed out that for truly sustainable software there should be no endpoint at which sustainability can be claimed, because the software products would continue to be used and useful beyond the single institution, grant, and developer or development team that created them. This may mean that sustainability needs to be addressed throughout the full software life cycle. It was also pointed out that software sustainability is not isolated from other attributes of scientific software and its use, such as usability, and provenance. Similarly, the question was considered, albeit only briefly, whether proprietary versus open-source license plays a role in the context of software sustainability. For example, should a project ensure that it uses an OSI-approved license so that software products can outlive any single entity if they remain important.

Because part of the Policy panel (§5) was about modeling sustainability, and modeling requires defining what will be modeled, this panel saw particular attention to the questions surrounding the definition of sustainability. Two papers, Venters et al. [44] and Katz and Proctor [46], specifically discuss the issue.

According to Venters et al. [44], sustainability is a rather ambiguous concept, and the lack of an accepted definition hampers integrating the concept into software engineering. They suggest that sustainability falls under the category of non-functional requirements, and that a software's sustainability is a consequence of a set of central software architecture quality attributes, including extensibility, interoperability, maintainability, portability, reusability, and scalability. They also propose an evaluation framework with which quality and sustainability could be measured at the architectural level.

Katz and Proctor [46] propose a set of questions that could be used to measure software sustainability:

- Will the software continue to provide the same functionality in the future, even if the environment (other parts of the infrastructure) changes?
- Is the functionality and usability clearly explained to new users?
- Do users have a mechanism to ask questions and to learn about the software?
- Will the functionality be correct in the future, even if the environment changes?
- Does it provide the functionality that existing and future users want?
- Will it incorporate new science, theory, or tools as they develop?

Despite their phrasing, these questions are not intended to be given simplistic yes or no answers, and it is the complete set rather than any individual one that would determine where in the range of sustainability a software falls.

7.2 Career Paths for Scientific Software Developers

Career path issues also came up repeatedly, starting in the first keynote (§3.1), where Phil Bourne used the term "the Google Bus" to describe the issue of well-trained software development staff in academic labs choosing to leave science and to work instead for technology firms, especially Google, which happens in large enough numbers that Google operates a bus every day to its nearest offices (and hence staff who leaves academia in this way do not even have to physically move).

The career path issue emerged repeatedly across panels because for scientific software to be(come) sustainable, projects trying to create sustainable software need to be able to recruit and retain software developers trained in the various requisite software engineering facets. However, a career path in research means faculty at most universities, and as was noted repeatedly in discussions, faculty are hired based on their scientific qualifications, not on their software development skills or track record. Consequently, developing special software development skills is unlikely to further a career in science at a university, although national laboratories were acknowledged as a different case. Loffler et al. [70], one of the papers in the Communities panel (§6), brought the problem to the point:

> "The most severe problem for developers in most computational sciences currently is that while most of the work is done creating hopefully well-written, sustainable software, the academic success is often exclusively tied to the solution of the scientific problem the software was designed for. Tasks that from a software engineering standpoint are essential, e.g., high usability, well-written and updated documentation, or porting infrastructure to new platforms, are not rewarded within this system." [70]

Clearly, improving the recognition of software engineering work is connected to addressing the career path problem. As was noted in the Developing and Supporting Software (§4) and the Policy (§5) panel discussions, there are encouraging signs of improvement, including some altmetric services (such as Impactstory, http://impactstory.org) collecting metrics for software source code, and the fact that NSF now asks to list "products" rather than their "publications" in an investigator's biosketch or results from prior NSF support. However, how software, let alone parts of software are reused by others can be very difficult to measure, and better recognizing software products for principle investigators by itself does not create career paths for specialist software developers working as part of a university research group. Huang and Lapp [59], a contribution to the Policy panel, offer one possible solution in which a software engineering center of excellence offers a career path for a correspondingly trained workforce, and increased recognition of the resulting more sustainable software would in a virtuous cycle heighten the value of the center's services.

7.3 Licensing and Software Patents

Issues related to licensing and patents primarily was discussed in the Communities session, but licensing was also a concern of many of the other contributors in other sessions. Software is no longer just open or closed (only binaries available), but also licensed and patented, which clearly also impacts software sustainability. While many papers briefly discussed licensing issues, Elster [81] directly discussed the impact of software licenses on obtaining industrial funding for scientific software projects. In particular, she described her experiences with researchers unwilling to utilize GPL (copyleft) code, as it adds restrictions to reuse that they themselves as well as some industries find unacceptable for future commercialization. (This was discussed by Hanwell et al. [25] as well.)

US information technology companies funding academics will thus often insist on BSD licensing on software since they then can legally include the code into their commercial codes. On the other hand, there are companies that fund larger GPL-licensed software projects [30] and insist that the university projects they fund also produce code with GPL licensing. They do not accept BSD-like licenses since they argue that other companies then may choose to build closed commercial codes on they software they funded, rather than encouraging the community to contribute freely and thus ensuring software sustainability for the community. In either case, the university researchers are not given much choice if they want these much sought after funds in a increasingly competitive grant world.

Another obstacle to sustainability identified by Elster include patenting of software. Most countries place some limits on software patents. The European Union outright forbids them, while US patent law excludes "abstract ideas", which has been used to refuse some software patents. Further obstacles to sustainability include a lack of open access, and even more broadly, a lack of open source codes even in open access journals. Finally, a lack of awareness on the part of scientific software developers of commodity libraries for common tasks reduces their ability to reuse code.

8 Case Studies

In this section, we discuss some of the software projects as case studies to better understand the points discussed during the workshop and described in the previous sections, and to find how they are affected by sustainability issues in practice. Most of the software projects discussed here were publicly launched 10 or more years ago. We generally note the original release (o.r.) year of each project in parenthesis in its first mention.

We classify the software projects discussed in the workshop in two broad categories. First, the *utility* software, comprising of general purpose software. Utility software is often used as enabler or facilitator for the development of other tools and techniques to carry out scientific work. This includes the software developed to efficiently utilize new research infrastructures. Second, the *scientific* software, comprising the software that was originally developed with an aim to solve a specific scientific problem. This classification is motivated by our argument that the two kinds of software projects wildly vary in factors such as scope, purpose and usage. The development and management of each kind is significantly different. Consequently, the sustainability challenges faced by them differ and must be treated separately. For instance, the challenges faced by a gateway software development project such as CIPRES (o.r. 2007) or visualization software products such as VisIT (o.r. 2001) or ParaView (o.r. 2002) are distinct to a niche software for *ab initio* modeling and simulation such as VASP (o.r. 1992) or Quantum Espresso (o.r. 2001).

8.1 Utility Software

Software developed with a potentially wider audience and general purpose usage in mind is utility software. Utility software typically does not address fundamental research problems for a given scientific domain. Examples are collaborative development frameworks such as GitHub (o.r. 2008) and Bitbucket (o.r. 2008), distributed workflow and generic computing frameworks such as Galaxy (o.r. 2006), HUBzero (o.r. 2010), SimGrid (o.r. 2001), Swift (o.r. 2007), Globus (o.r. 2000) and VisTrails (o.r. 2007), and visualization frameworks such as VTK, VisIT, and ParaView.

Development is often a high risk/reward undertaking exploring uncharted territories and is largely influenced by (re)usability factors. Owing to a relatively large number of features, the development and prototype process is also lengthy which poses a significant survival risk. Challenges on a class of utility software for new architectures is well discussed in [83].

On the other hand, utility software presents opportunities to be usable by a larger community making its undertaking and development an attractive pursuit. It is generally more visible in community which in turn leads to a broader and deeper participation. For instance, it helps promoting collaborations across the breadth (e.g., different departments) and depth (e.g., stakeholders within a department) of community, one of the key ingredients of a sustainable process. Successful utility projects reap high rewards and have a longer usage span. Development process becomes user-driven and self-sustaining.

One such example is the Galaxy project [61]. It follows agile software development practices and implements standards such as test-driven development and socialized bug managing practices via trello. Galaxy *histories* and *toolshed* offer easy community sharing of data and tools further promoting a collaborative environment. The project closely follows the guidelines described in Carver and Thiruvathukal [84] and many from Prlić and Procter [41]. Many utility software projects are often developed aiming better utilizing a particular, new infrastructure and architecture, e.g., MVAPICH (o.r. 2002), VisIT, ParaView. Similarly, to leverage the power of emerging architectures such as accelerators, new code and libraries are required. The experience of one such effort as described in Ferenbaugh [83] which met with a limited success but nonetheless with many invaluable lessons were learned about influential cultural and technical aspects in sustainable software development practices.

A relatively new paradigm in utility software is the software delivered as service over the web. With increasing popularity of cloud-based storage and computational environments, many users are leaning towards tools used as services. GitHub and Bitbucket can be argued to be such tools, catering to collaborative development. For scientific users Globus-based tools are a case of service-based utility software discussed during the workshop. The data movement and sharing services offered by Globus can be easily used over the web by collaborating researchers.

8.2 Scientific software

Scientific software consists primarily of special-purpose software that was purpose-built for a target use-case scenario, fixed requirements in mind, or solving a specific problem. Software projects pertaining to specific scientific domain tend to be in a niche and the user community tends to be small to medium. They are mostly driven by the science and specific needs of a research group. Specific needs such as numerical accuracy and algorithmic optimization are some of the paramount requirements of most scientific software.

Long-term sustainability of scientific software is often a significant challenge and face radically different issues compared to utility software. Many submissions reported that software is practically considered a "byproduct" of the actual research. Others contended that the software was not the main funded part of their research. A smaller codebase and fixed requirements result in stability, ease of installation, and configuration. Many such projects mature and are treated as libraries to be integrated into larger systems such as some of the utility software discussed in the previous section. While the software can stay stable and require relatively low maintenance, the responsibility is often on the shoulders of a few developers who are often not specialists in software development. Development tends to be linear and simplistic with a limited scope to follow software best practices.

Some examples of such software discussed as part of the workshop are DUNE (o.r. 2008), R/qtl (o.r. 2002), Kitware (o.r. 1998), PETSc (o.r. 1995), and MINRES-QLP (o.r. 2007), most of which are focused on one scientific or applied mathematics domain. However, sometimes such projects grow beyond the initial vision of developers. One such example is Kitware, which while being a software product specializing in the scientific process, has a core focus of developing communities around software processes. Another instance of this process is the development of the CMake build utility, which started out as a building tool for ITK but grew to become a generic build utility for C++ projects. Similarly, PETSc is growing towards becoming a general purpose utility system usable for solving a variety of scientific problems.

8.3 Distinctions

In conclusion, we find that there are distinctions in the characteristics and challenges faced between utility and scientific software projects. We find that the utility software packages are more likely to use the best practices discussed during the workshop. Often, sustainability of scientific software projects is achieved by the fact that the core developer or team heavily utilizes the software for their own science, e.g., R/qtl, PETSc. Furthermore, the development of scientific software requires more scientific background compared with utility software, thus in many cases, the bulk of development is carried out by a domain scientist. For these reasons, we believe that separate guidelines and sustainability principles could be defined for these two software categories.

9 Conclusions

To conclude, we highlight what we have learned from the workshop, and what we plan to do going forward.

9.1 Issues and lessons

Three major issues came up repeatedly in different parts of the workshop:

(1) The need for a definition of sustainability such that the community can get behind it. Although some had hoped that at least an initial consensus could be reached in the course of the workshop, this proved elusive. However, in the absence of such a definition it will remain difficult to define

exactly what the goals should be towards achieving, or even only improving software sustainability, and hence what practices should be followed and implemented when. As described in the next subsection (§9.2), the workshop organizers have begun an effort to address this.

(2) The need for academic career paths for scientific software developers. Unfortunately, it is not clear how to ensure that these career paths become available, other than repeatedly talking about this issue. The recent Moore and Sloan initiative in data science [85] are trying to address this, to some extent, by providing funds and incentives to universities in the US that work towards this goal.

(3) The need for recognition of scholarship in scientific software over research articles. This need probably is the most addressed of the three, today, with efforts underway such as the Mozilla Science Lab, GitHub, and figshare "Code as a research object" project [86] among others.

In addition, licensing and patents, and how they impact research funding for software development, were also discussed.

Discussion sessions

Two strong lessons came out of the three discussion sessions:

(1) Use of shared repositories in the development of collaborative projects facilitates collaboration, reproducibility, and sustainability in computational science. However, it represents a barrier in some scientific fields and has yet to be more widely adopted.

(2) A sustainability model for scientific software is to build a pipeline from construction to consumption, as found in the most efficient information technology enterprises.

Use cases

Two distinct class of scientific software projects and products were discussed in the workshop: 1) generic, large-scale utility software and 2) niche, medium- and small-scale scientific software. Each class faces different and significant challenges. New undertakings should recognize the differences in advance and identify such challenges within the development and sustaining efforts. In particular, the dynamics associated with developers, scope, life cycle, users-community, (re)usability, funding support, and career paths vary widely among the two classes of software.

Workshop process

The WSSSPE workshop can be viewed as an experiment in how we can collaboratively and inclusively build a workshop agenda, without asking a large number of people to submit papers that will be rejected so that the workshop can have a low acceptance rate.

Contributors also want to get credit for their participation in the process. And the workshop organizers want to make sure that the workshop content and their efforts are recorded. The methods used in the WSSSPE1 workshop were successful: we had good participation; contributors have a report they can cite; the record of the workshop is open and available through the self-published reports, the workshop website and notes site, and this paper. In addition, many additional papers are being created that will include the discussions at the workshop, including extended versions of many of the self-published reports such as those that are in this special issue.

Ideally, there would be a service that would be able to index the contributions to the workshop, serving the authors, the organizers, and the larger community.

9.2 Future activities

The organizers of the workshop have begun a survey to understand how the community define software sustainability. It is expected that this survey will gather one or more consensus definitions, and lead to a short paper discussing them, as well as the level of consensus.

Additional activities that are being planned include two additional WSSSPE workshops at the 2014 SciPy and SC14 conferences. The SciPy workshop (WSSSPE1.1) will focus on how some software projects from the SciPy community have dealt with software sustainability issues, both successfully and unsuccessfully, while the SC14 workshop (WSSSPE2) will be more general, and will likely focus on determining and publicizing specific activities that the overall scientific software community can take to move forward. In addition, there will be a two-session minisymposium on "Reliable Computational Science" at the 2014 Society for Industrial and Applied Mathematics Annual Meeting (SIAM AN14, http://meetings.siam.org) to further explore some of the key issues raised here.

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Supporting Information

Appendix A: Call for Papers (PDF)
Appendix B: Papers Accepted and Discussed at WSSSPE1 (PDF)
Appendix C: Attendees (PDF)

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