

## ISSUES IN RESEARCH SOFTWARE

# Report on the Second Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE2)

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This technical report records and discusses the Second Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE2). The report includes a description of the alternative, experimental submission and review process, two workshop keynote presentations, a series of lightning talks, a discussion on sustainability, and five discussions from the topic areas of exploring sustainability; software development experiences; credit & incentives; reproducibility & reuse & sharing; and code testing & code review. For each topic, the report includes a list of tangible actions that were proposed and that would lead to potential change. The workshop recognized that reliance on scientific software is pervasive in all areas of world-leading research today. The workshop participants then proceeded to explore different perspectives on the concept of sustainability. Key enablers and barriers of sustainable scientific software were identified from their experiences. In addition, recommendations with new requirements such as software credit files and software prize frameworks were outlined for improving practices in sustainable software engineering. There was also broad consensus that formal training in software development or engineering was rare among the practitioners. Significant strides need to be made in building a sense of community via training in software and technical practices, on increasing their size and scope, and on better integrating them directly into graduate education programs. Finally, journals can define and publish policies to improve reproducibility, whereas reviewers can insist that authors provide sufficient information and access to data and software to allow them reproduce the results in the paper. Hence a list of criteria is compiled for journals to provide to reviewers so as to make it easier to review software submitted for publication as a “Software Paper.”

**Keywords:** sustainability; software; research

### (1) Introduction

The Second Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE2)<sup>1</sup> was held on 16 November, 2014 in the city of New Orleans, Louisiana, USA, in conjunction with the International Conference for

High Performance Computing, Networking, Storage and Analysis (SC14).<sup>2</sup> WSSSPE2 followed the model of a general initial workshop, WSSSPE1<sup>3</sup> [1, 2], which co-occurred with SC13, and a focused workshop, WSSSPE1.1,<sup>4</sup> which was organized in July 2014 jointly with the SciPy conference.<sup>5</sup>

Progress in scientific research is dependent on the quality and accessibility of software at all levels. Hence it is critical to address challenges related to the development, deployment, maintenance, and overall sustainability of reusable software as well as education around software practices. These challenges can be technological, policy based, organizational, and educational, and are of interest to developers (the software community), users (science disciplines), software-engineering researchers, and researchers studying the conduct of science (science of team science, science of organizations, science of science and innovation policy, and social science communities). The WSSSPE1 workshop engaged the broad scientific community to identify challenges and best practices in areas of interest to creating sustainable scientific software. WSSSPE2 invited the community to propose and discuss specific mechanisms to move towards an imagined future practice for software development and usage in science and engineering. The workshop included multiple mechanisms for participation, encouraged team building around solutions, and identified risky solutions with potentially transformative outcomes. It strongly encouraged participation of early-career scientists, postdoctoral researchers, and graduate students, with funds provided to the conference organizers by the Moore Foundation and the National Science Foundation (NSF), to support the travel of potential participants who would not otherwise be able to attend, and young participants and those from underrepresented groups, respectively. These funds allowed 17 additional participants to attend, and each was offered the chance to present a lightning talk.

This report extends a previous report that discussed the submission, peer-review, and peer-grouping processes in detail [3]. It is also based on a collaborative set of notes taken with Google Docs during the workshop [4]. Overall, the report discusses the organization work done before the workshop (§2); the keynotes (§3); a series of lightning talks (§4), intended to give an opportunity for attendees to quickly highlight an important issue or a potential solution; a session on defining sustainability (§5). The report also gives summaries of action plans proposed by five breakout sessions, which explored in specific areas including sustainability (§6); software development experiences (§7); credit & incentives (§8); reproducibility, reuse, & sharing (§9); code testing & code review (§10). Lastly, the report also includes some conclusions (§11) and an incomplete list of attendees (**Appendix A**).

## (2) Submissions, Peer-Review, and Peer-Grouping

WSSSPE2 began with a call for papers [3]. Based on the goal of encouraging a wide range of submissions from those involved in software practice, ranging from initial thoughts and partial studies to mature deployments, but focusing on papers that are intended to lead to changes, the organizers wanted to make submission as easy as possible. The call for papers stated:

We invite short (4-page) **actionable** papers that will lead to improvements for sustainable software science. These papers could be a call to action, or could

provide position or experience reports on sustainable software activities. The papers will be used by the organizing committee to design sessions that will be highly interactive and targeted towards facilitating action. Submitted papers should be archived by a third-party service that provides DOIs. We encourage submitters to license their papers under a Creative Commons license that encourages sharing and remixing, as we will combine ideas (with attribution) into the outcomes of the workshop.

The call included the following areas of interest:

- defining software sustainability in the context of science and engineering software
  - how to evaluate software sustainability
- improving the development process that leads to new software
  - methods to develop sustainable software from the outset
  - effective approaches to reusable software created as a by-product of research
  - impact of computer science research on the development of scientific software
- recommendations for the support and maintenance of existing software
  - software engineering best practices
  - governance, business, and sustainability models
  - the role, operation, and sustainability of community software repositories
  - reproducibility, transparency needs that may be unique to science
- successful open source software implementations
  - incentives for using and contributing to open source software
  - transitioning users into contributing developers
- building large and engaged user communities
  - developing strong advocates
  - measurement of usage and impact
- encouraging industry's role in sustainability
  - engagement of industry with volunteer communities
  - incentives for industry
  - incentives for community to contribute to industry-driven projects
- recommending policy changes
  - software credit, attribution, incentive, and reward
  - issues related to multiple organizations and multiple countries, such as intellectual property, licensing, etc.
  - mechanisms and venues for publishing software, and the role of publishers
- improving education and training
  - best practices for providing graduate students and postdoctoral researchers in domain communities with sufficient training in software development
  - novel uses of sustainable software in education (K-20)
  - case studies from students on issues around software development in the undergraduate or graduate curricula

- careers and profession
  - successful examples of career paths for developers
  - institutional changes to support sustainable software such as promotion and tenure metrics, job categories, etc.

31 submissions were received; all but one used arXiv<sup>6</sup> or figshare<sup>7</sup> to self-publish their papers.

The review process was fairly standard. First, reviewers bid for papers. Then an automated system matched the bids to determine assignments. After the reviewers completed their assigned reviews (with an average of 4.9 reviews per paper and 4.1 reviews per reviewer), they used EasyChair<sup>8</sup> to record scores on relevance and comments. Finally, the organizers accessed the information to decide which papers to associate with the workshop and provided authors with the comments to help them improve their papers.

The organizers decided to list 28 of the papers as significantly contributing to the workshop, a very high acceptance rate, but one that is reasonable, given the goal of broad participation and the fact that the reports were already self-published.

The organizers wanted very interactive sessions, with the process of creating the sessions open to the full program committee, the paper authors, and others who might attend the workshop. In order to do this, the organizers used Well Sorted<sup>9</sup> with the following steps:

- (1) Authors were asked to create Well Sorted “cards” for the papers. These cards have a title (50 characters maximum) and a body (255 characters maximum).
- (2) Authors, members of the WSSPE program committee, and mailing list subscribers were asked to sort the cards. Each person dragged the cards, one by one, into groups. A group could have as many cards as the person wanted it to have, and it could have any meaning that made sense to that person.
- (3) Well Sorted produced a set of averages of all the sorts, with various numbers of card clusters.

The organizers then chose a sort that contained five groups that felt most meaningful. After that, they decided on names for the five groups:

- Exploring Sustainability
- Software Development Experiences
- Credit & Incentives
- Reproducibility & Reuse & Sharing
- Code Testing & Code Review.

Finally, since some of the papers were not represented by cards in the process, they were not placed in groups by the peer-grouping system. The authors of these papers were asked which groups seemed the best for their papers; these papers were then placed in those groups. Sections 6–10 discuss the breakout groups, including a list of the papers associated with each group.

### (3) Keynotes

The workshop featured two keynote addresses. In the opening keynote presentation, Kaitlin Thaney of the Mozilla Science Lab talked about her organization’s work and policy to enable and support sustainable and reproducible scientific research through the open web. The second keynote speaker was Neil Chue Hong of Software Sustainability Institute. He shed light on how scientific software is prevalently driving advances in many science and engineering fields. Both keynote speeches spawned further discussion among workshop participants on the crucial notion of software *sustainability* in the theme of our workshop.

#### 3.1 Kaitlin Thaney, Designing for Truth, Scale, and Sustainability [5]

Kaitlin Thaney is the Director of the Mozilla Science Lab (hereafter Mozilla), which is a non-profit organization interested in openness, news, website creation, and Science, all taking advantage of the open web.

Thaney started noting the unfortunate fact that many current systems suffer the unintended consequence of creating friction that hinders users, despite designers’ original purposes to do good. An example is the National Cancer Institute’s caBIG. A total of \$350 million was spent, including more than \$60 million for management. More than 70 tools were created, but caBIG is still seen as a failure.<sup>10</sup> Those that had the least investment were the most used; the most invested software were the least utilized.

Thaney emphasized that for efficient reproducible open research, we would need research tools (e.g., software repositories), social capital (e.g., incentives), and capacity (e.g., training and mentor-ship). Our systems would need to communicate with each other. A point was made by a member of the audience that as systems become less monolithic, it often becomes harder to sustain the links between them.<sup>11</sup>

Thaney spoke about Mozilla’s work around code citation, through a collaboration and prototype crafted between Mozilla, GitHub, figshare, and Zenodo. This work was presented at a closed meeting in May 2014 at the National Institutes of Health (NIH) around these issues, sparking a conversation from that meeting around what a *Software Discovery Index*<sup>12</sup> might look like. The meeting included a number of publishers, researchers, and those behind major scientific software efforts such as Bioconductor,<sup>13</sup> Galaxy,<sup>14</sup> and nanoHUB.<sup>15</sup> Ted Habermann in the audience commented that if the metadata is minimal, it would be less onerous for data providers, but more burdensome for users—it could be challenging to keep a balance between what have to be captured and what would be ideal if we do not want to lose user engagement, which he said he had experienced with the Harvard Dataverse [6] where a large amount (three pages) of metadata was requested, but often only the first four fields were filled out.

The speaker concluded her talk urging the audience to design scientific software with the general community,

not an individual, in mind; and to design to unlock latent potential of our systems. In addition, she encouraged everyone to rethink how we reward researchers and support roles.

### 3.2 Neil Chue Hong, We are the 92% [7]

Neil Chue Hong is the Director of the Software Sustainability Institute (SSI) in the United Kingdom (UK). The SSI was founded to support the UK's research software community by cultivating better, more sustainable research software to enable world-class research. Chue Hong's keynote started by making the point that the use of – and reliance on – software is pervasive in all areas of world-leading research, showing examples from disciplines as diverse as humanities and high-energy physics, quoting Kerstin Kleese Van Dam of the Pacific Northwestern National Laboratory via a petition campaign<sup>16</sup> at change.org, *“Today there are very few science areas left which do not rely on IT and thus software for the majority of their research work. More importantly key scientific advances in experimental and observational science would have been impossible without better software.”* He also cited Daniel Katz, Software Infrastructure for Sustained Innovation (SI2) Program Director of the NSF, *“Scientific discovery and innovation are advancing along fundamentally new pathways opened by development of increasingly sophisticated software. Software is an integral enabler of computation, experiment and theory, and directly responsible for increased scientific productivity and enhancement of researchers' capabilities.”*

Chue Hong drew attention to the issue that in the cyber-infrastructure and high-performance community, hundreds of thousands of researchers developing software are all too often disregarded or considered the long tail. Actually, the numbers point to the fact that they are the mainstream. He emphasized that software is no longer special; it is both essential to and common in scientific research. A 2014 survey<sup>17</sup> conducted by the SSI polled researchers from 15 research-intensive UK universities (406 respondents covering a representative range of funders, disciplines, and seniority). The survey reported that 92% respondents confirmed the use of research software and 89% affirmed that it would be impossible or difficult to conduct research without software. Nevertheless the British research community is just starting to understand the magnitude of the issue. Whilst many researchers make use of software such as MATLAB, SPSS, and Excel, data from the aforementioned SSI survey shows that over half (56%) of respondents developed their own research software (which equates to over 140,000 researchers if extrapolated across the UK) and yet 71% of all UK researchers had no formal software-development training, having to rely on their own coding skills.

Examining another aspect of the size of the research software community, Chue Hong noted that the costs of software-reliant research in the UK included £840 million of investment in the financial year 2013–2014, and this amount has risen by 3% on average over the past four years. About 30% of total research investment has been spent on research that relies on software over the last four financial

years. These numbers stemmed from an analysis by the SSI of data from 49,650 grant titles and abstracts published on Gateway to Research between years 2010 and 2014. A similar analysis of university jobs advertised in the same period discovered that despite this investment, only 4% of positions were software development related, and of these only 17% were explicitly named as a software developer or software engineer positions: the vast majority being advertised as research associate or research assistant positions. This in turn leads to the issue of career paths for those bridging the research and software worlds, who are essential to support the use and further development of research software, a point highlighted by a graphic showing UK STEM graduate career paths<sup>18</sup> showing that only 3.5% were able to secure permanent positions.

To conclude, Chue Hong led the audience in discussing the following questions: What are we going to do to help and benefit the 92% of researchers who rely on software? Who do we need to persuade? What are the incentives we need to put in place? Finally, he challenged the workshop participants to change the current deficient practices in research and academia.

## (4) Lightning Talks

Lightning talks were a new feature in WSSPE2. Since the workshop program was mostly dedicated to discussions, the organizers wanted to give the attendees a chance to also 'make a pitch' for an idea, either representing a contributed paper or something different. Eighteen attendees volunteered to participate in the lightning talks, each given only two minutes to speak and at most one slide to show. The talks were presented in reverse alphabetic order of speakers' last names. In the rest of this section, we highlight the gist of some of the speakers' messages.

- (1) **Colin C. Venters: The Nebuchadnezzar Effect: Dreaming of Sustainable Software through Sustainable Software Architectures [8].** Venters proposed that sustainable software is a composite, first-class, non-functional requirement (NFR) that is at a minimum a measure of a system's maintainability and extensibility, but may also include other NFRs such as efficiency (e.g., energy, cost), interoperability, portability, reusability, scalability, and usability. To achieve technically sustainable software, Venters suggested that software architectures are fundamental as they are the primary carrier of system NFRs, i.e., pre-system understanding; and influence how developers are able to understand, analyze, extend, test, and maintain a software system, i.e., post-deployment system understanding. In addition, Venters highlighted that sustainability of software architectures needs to be addressed to endure different types of change and evolution in order to mitigate architectural drift, erosion, and knowledge vaporization.
- (2) **Marlon Pierce: Patching It Up, Pulling It Forward [9].** Pierce discussed how open open source is. Open software needs a diverse, openly governed

community behind it, just as it needs open licensing and a public code repository. To probe the level of governance within open source projects, he and his co-authors (Marru and Mattmann) suggested a contest to encourage individual developers to submit patches and requests to projects that are important to them. This simple mechanism shall expose several governance mechanisms, such as how easy it is for independent developers to communicate with project leadership, how projects accept and license third-party contributions, and how projects make decisions such as granting source tree write access.

- (3) **John Peterson: Continuous Integration for Current MOOSE Framework and Application Development on GitHub [10].** Peterson from the Idaho National Laboratory reported that in March 2014, the MOOSE framework was released under an open source license on GitHub, significantly expanding and diversifying the pool of current active and potential future contributors on the project. The MOOSE team employs an extensive continuous integration test suite to ensure that both the framework and the applications based on the framework are verified before any code changes are accepted into the repository. They use a combination of built-in Git features such as branching and submodules, GitHub API integration capabilities, and in-house developed testing software to perform this verification and update the dependent applications in a relatively seamless manner for users.
- (4) **Abani Patra: Execute it [11].** Patra discussed the value of an easily accessible platform for executing scientific software, e.g., HUBzero to access XSEDE or other computing resources. Such a platform for executing benchmark problems (even at a small scale) allows the developer community access a reference implementation and provides an easy way to train the larger user community. A second idea of this talk was that for true usability, much more attention and support needs to be given to the integrated use of simulation tools inside complex workflows.
- (5) **Daniel S. Katz: Implementing Transitive Credit with JSON-LD [12].** Science and engineering research increasingly relies on activities that facilitate research but are not rewarded or recognized, such as: data sharing; developing common data resources, software and methodologies; and annotating data and publications. To promote and advance these activities, we must develop mechanisms for assigning credit, facilitate the appropriate attribution of research outcomes, devise incentives for activities that facilitate research, and allocate funds to maximize return on investment. Katz discussed the issue of assigning credit for both direct and indirect contributions by using JSON-LD to implement a prototype transitive credit system.
- (6) **Samin Ishtiaq: Daemons, Notifications and Sustaining Software.** The reproduction and replication of novel results has become a major issue in computer science, systems biology, and other computational disciplines. These include both the inability to re-implement novel algorithms and approaches, and lack of an agreement on how and what to benchmark these algorithms on. Ishtiaq from Microsoft Research Cambridge pointed out these problems and made several suggestions to address them.
- (7) **James Howison: Retract all Bit-Rotten Publications.** Howison sought to provoke discussion by proposing that papers whose workflows are not kept current with the changing software ecosystem should be automatically retracted. This would create an incentive for authors to keep their software current and usable, rather than the current situation in which every potential user has to do this individually. A softer version of the proposal would identify papers whose software workflow has become bit-rotten and allow others to keep the code up to date, either adding them as new authors of the paper or providing credit for their academic service in some other form.
- (8) **Robert Downs: Community Recommendations for Improving Sustainable Scientific Software Practices [13].** Robert Downs, of the Columbia University Center for International Earth Science Information Network (CIESIN), described a focus group study conducted with the Science Software Cluster (SSC) of the Federation of Earth Science Information Partners (ESIP). For the study, almost 300 attendees of the 2014 Summer ESIP Meeting were invited to participate in simultaneous roundtable discussions on sustainability of science software. Over two-thirds of the roundtable focus groups responded to a semi-structured survey that contained three sets of questions eliciting recommendations for near-term actions of the community to improve sustainable software practices. Initial analysis of the participants' responses to the questionnaire revealed several suggestions, which included improving community engagement and collaborative activities, increasing understanding and awareness, and creating incentives to motivate sustainable science software practices. The ESIP SSC plans to engage the community in the recommended activities for improving sustainable scientific software practices.
- (9) **Carl Boettiger: rOpenSci: Building Sustainable Software by Fostering a Diverse Community [14].** Boettiger described how the rOpenSci project has been successful by focusing not just on building software but also on building a community of researchers who learn and adopt their approaches to reproducible research and sustainable software practice. Through outreach, mentoring, workshops, and hackathons, they have not only reached new users, but also turned users into co-developers of robust software and good practices to support data science research across a growing set of disciplines.

(10) **Jakob Blomer: The Need for a Versioned Data Analysis Environment [15].** Large-scale scientific endeavors, such as the discovery of the Higgs boson at the Large Hadron Collider (LHC), often rely on complex software stacks. Maintaining thousands of dependencies of software libraries and operating system versions has shown that despite source code availability, the setup and the validation of a minimal usable analysis environment can easily become prohibitively expensive. In high-energy physics, CernVM-FS, a special-purpose, open-source, versioning, and snapshotting file system used to capture and distribute entire software stacks, proved to be useful for providing instant access to ready-to-run data analysis environments.

(11) **Alice Allen: Find it! Cite it!** The Astrophysics Source Code Library (ASCL) is an online registry of scientist-written software used in astronomy research. Their primary interest is rendering research more transparent by making this software more discoverable for examination. The ASCL is treated as a publication by an indexing resource for astronomy, the Astrophysics Data System (ADS). ADS tracks citations to what it indexes, including citations to ASCL entries. Increasing rewards for writing software, whether through citation, transitive credit or other methods, gives software authors a powerful reason to take the time to build sustainability into their software and is an excellent way to drive community change.

## (5) Defining Sustainability

In the first interactive session, the attendees divided themselves into groups to discuss software sustainability. They were asked to

- (1) discuss what the term “software sustainability” meant to them
- (2) determine three things they considered to be significant enablers of software sustainability
- (3) determine three things they considered to be significant barriers to software sustainability.

Once each group had come up with answers, all the answers were compiled, and the attendees voted on which they thought were important by a show of hands.

The general responses to what software sustainability meant were:

- keeping software scientifically useful
- separating techniques in code from knowledge in code
- that an adequately large community finds value in software and is willing to sustain it.

The enablers of and barriers to software sustainability, roughly ranked by attendee votes, are shown in **Figures 1** and **2**, respectively.<sup>19</sup>

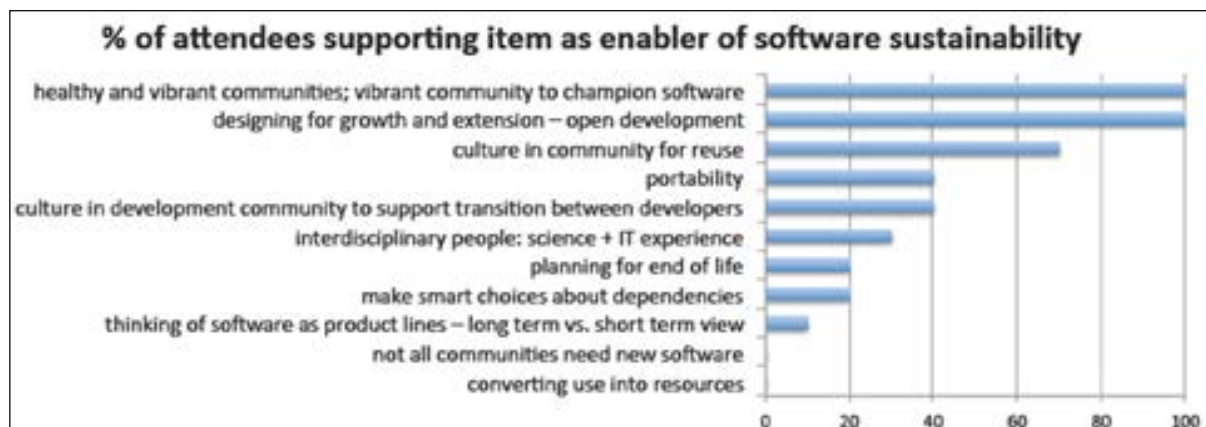
## (6) Exploring Sustainability

Six papers were categorized under the theme of Exploring Sustainability. The group included four of the authors from the six papers submitted and an additional number of participants who expressed an interest in the theme at the workshop. Each paper had a different perspective on the concept of sustainability, which ranged from the sustainment of communities to defining sustainability as a first-class, composite non-functional requirement.

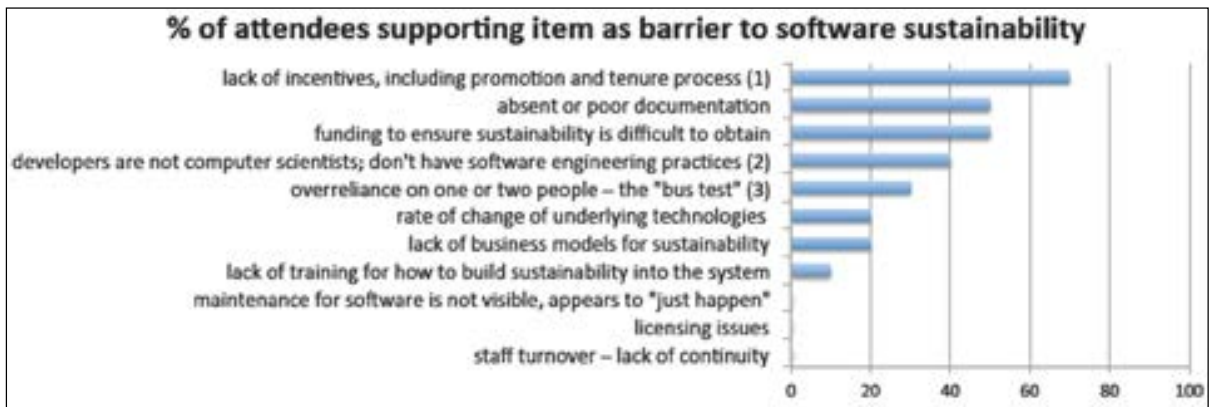
### 6.1 Discussion and Actions

#### 6.1.1 Discussion

Each author was invited to outline the key action from their paper as a potential discussion point for the group; where the authors were not present, the group facilitators outlined the actionable points from their papers. The key actions from the six papers included recommendations for improving practice in sustainable software engineering [16, 17]; development of *Software and Infrastructure as a Service* as a mechanism for fostering sustainable science communities [18]; developer incentives for code contributions to open source projects [19]; establishment of a set of software engineering principles based on scalability, reproducibility, and energy efficiency [20]; and applying software architectures as a mechanism for



**Figure 1:** Enablers of software sustainability, showing the fraction of attendees (rounded to the nearest 10%) who voted for an item as important.



**Figure 2:** Barriers to software sustainability, showing the fraction of attendees (rounded to the nearest 10%) who voted for an item as important.

- (1) This item also included the fact that that the promotion and tenure process in academic is incompatible with sustainability.
- (2) The software engineering practices were those in particular that are needed to scale-up projects to support and be developed by a large sustainable community.
- (3) The smallest number of key people a project would need to lose to become non-viable – the larger the number, the healthier the project.

architectural-level reasoning about sustainability [21]. The group took the position of viewing sustainability from the perspective of addressing the challenges related to the development, deployment, and maintenance of reusable software [2].

The principal focus of the initial discussion considered how to foster cultural change towards developing sustainable software in academic environments. It was suggested that a new requirement driven by the agencies funding research projects where software was an intrinsic part of enabling the research program would be an additional element within the grant proposal to provide a sustainability plan for sustaining the software. This type of initiative would provide the necessary incentive and motivation for researchers to consider how to sustain their software beyond the lifetime of the project.

The discussion then focused on a need for a common language and a definition on the concept of sustainability that moved beyond the current fuzzy definitions where time was the simple measurement of sustainment. It was suggested that there was a need to identify tangible actions that underpin sustainability that developers could incorporate into the development stream of their software. This prompted a debate regarding whether sustainability should be considered as a nonfunctional requirement or software quality as defined within ISO/IEC 25010 [22]. The focus of the discussion was based on the paper by Venters et al. [21], which suggested that sustainability is a first-class, composite, non-functional requirement composed of a number of sub-characteristics. It was generally agreed that maintainability and extensibility were key qualities underlying sustainability. In addition, the group also discussed what other non-functional requirements would contribute to the development of sustainable software, e.g., reusability and scalability. However, it was recognized that there was a need to identify appropriate metrics and measures.

The group also discussed whether the concept of sustainability itself was a barrier to achieving sustainable software. It was suggested that “the first rule of software sustainability is do not talk about software sustainability.” Instead there should be a focus on best software engineering practice. Playing devil's advocate, it was asked that if the focus on the concept of sustainability was ignored, what current software engineering practices and principles could be utilized by software developers and domain scientists to achieve sustainability? This raised the question of why existing software engineering knowledge, such as that contained in SWEBOK [23], was largely ignored and to what extent the environment has a strong influence on practice within the scientific and engineering community. As a result, there is a need to identify best practices and reach a consensus beyond the theories that underpin the discipline of software engineering. Similarly, how could we translate or distill some of the key building blocks that underpin software engineering practice?

A final key point of the discussion was the role that software design and patterns play before committing to writing a line of code. It was suggested that modeling must play a major role in attaining sustainable software. The point was raised that design involves making decisions and a mechanism would be necessary for capturing these decision points. This introduced the idea of software provenance that moved beyond commits in software repositories to how to capture and maintain relationships between sources and design decisions to prevent knowledge vaporization. Whether this could be achieved through software architectures is an open-research challenge.

### 6.1.2 Actions

The main action to come from the group was a proposal to identify the ten best software engineering practices similar to Philip Bourne's approach of Ten Simple Rules [24].

## 6.2 Papers

The papers that were discussed in the Exploring Sustainability group are:

- Mario Rosado de Souza, Robert Haines, and Caroline Jay. Defining sustainability through Developers' Eyes: Recommendations from an Interview Study [16].
- Robert Downs, W. Christopher Lenhardt, Erin Robinson, Ethan Davis, and Nicholas Weber. Community Recommendations for Sustainable Scientific Software [17].
- Abani Patra, Matthew Jones, Steven Gallo, Kyle Marcus, and Tefvik Kosar. Role of Online Platforms, Communications and Workflows in Developing Sustainable Software for Science Communities [18].
- Marlon Pierce, Suresh Marru, and Chris Mattmann. WSSPE2: Patching It Up, Pulling It Forward [19].
- Justin Shi. Seeking the principles of sustainable software engineering [20].
- Colin C. Venters, Michael K. Griffiths, Violeta Holmes, Rupert R. Ward, and David J. Cooke. The Nebuchadnezzar Effect: Dreaming of Sustainable Software through Sustainable Software Architectures [21].

## (7) Software Development Experiences

Of the short actionable papers that would lead to improvements for sustainable software science, 11 submissions were categorized in the Software Development Experiences group. Because of the large number, we split these into two subgroups prior to the event. Some common themes helped in this division. For example, several papers that addressed education and training issues, including best practices and case studies, were grouped together. Others discussed experiences with registries, developer collectives and specific examples of successful, sustainable software (including a valuable industry perspective).

### 7.1 Discussion and Actions

Subgroup A consisted of ten participants who discussed papers surrounding training and successful community software initiatives. Subgroup B had six participants who discussed four papers. Because of the nature of the papers, training emerged as a common theme. However the conversation was wide-ranging, including incentives, reproducibility, and funding to promote sustainability. In the end, both groups discussed training, though from somewhat different points of view and resulting in somewhat different suggested actions.

#### 7.1.1 Subgroup A Discussion

Group discussion started with a position statement by each person surrounding what they had learned from their software development experiences and how those lessons might be translated into actionable outcomes. Participants came from a range of backgrounds, and represented multiple software and training initiatives, including Software Carpentry, Data Carpentry, Open Science for Synthesis (OSS), the Community Surface Dynamics Modeling Systems group, ROpenSci, DataONE, the HDF Group, and others. Some of these software experiences

were focused on development of new products for use in the sciences (e.g., ROpenSci, CSDMS), and these recounted the difficulties of engaging with disciplinary scientists in writing software. Software was clearly utilized broadly across the various science disciplines represented, and it was developed within those disciplines as well. Some researchers created software for statistical analysis and modeling, while others used it to control instrumentation, collate data across networks, collect information from respondents, and many other uses. There was broad consensus that, within the disciplines represented, formal training in any type of software development or engineering was rare among the practitioners; most are self-taught, and develop software to get another job done. Any ancillary utility of the software outside of the specific science target was generally unplanned and few researchers would want to invest more time to make their own software more re-usable.

There was general agreement that this body of disciplinary software improvement needed to be understood in terms of the scientific productivity that could be achieved. A software maturity model is needed for science software, but it needs to be introduced in a way that fits the culture of science, which largely thinks of software as a tool, rather than a product itself. The group was in general consensus that more widespread training in software practice is needed within the domain sciences, and several of the participants were involved in efforts along these lines. Participants felt that projects that build a sense of community via training in software and technical practices would have the most success in changing practices in that community, but that there was a need for a managed introduction of these practices. Participants also recognized that these could not be one-time, one-off training opportunities, as software and technologies change rapidly over time. For example, while today Software Carpentry is focused on teaching version control via Git, there has been a rapid evolution from RCS to CVS to SVN to Git over a short time frame, and thus communities should expect the need to train for adaptability and a changing technology tool chain, rather than assume that these technologies will stay fixed. Thus, although short term training that introduces specific tools was considered highly valuable, these trainings were also not considered sufficient to engender the changes in software practice that were deemed necessary. Combining the need for changes in practice to be introduced incrementally with the need to minimize the divergence of training from direct science goals and the difficulties of training for a rapidly evolving technology space, participants concluded that multiple training efforts that targeted different parts of the spectrum were needed. Short-term courses introducing immediately useful skills needs to be offered alongside more in-depth courses on software engineering and practice that allow students to adapt to a changing landscape.

Finally, after agreeing that these complementary training models were needed, the group discussed sustainability of training, and how the leading groups in this space are teaching only a small fraction of the community that needs and wants training. Most graduate programs in the



sciences do not currently incorporate these approaches in their graduate curricula, although there is an increasing number of quantitatively oriented courses around analysis and modeling. These still, however, generally omit engineering practices such as version control, unit and regression testing, and software modularity and abstraction, often because the instructors themselves in the domain sciences are not familiar with these techniques. Thus, students who are being trained in these approaches are doing so through short 2–3 day training workshops such as Software and Data Carpentry, rather than through semester-long graduate education courses at their universities, which tend to focus on statistical and modeling techniques. Hybrid programs like the three-week Open Science for Synthesis (OSS) training that combine the three (science, quantitative techniques, and software engineering) into an holistic course serve part of the need but reach only a few researchers at this time. Thus, the group concluded that significant strides needed to be made in coordinating these trainings so that they are complementary, on increasing their size and scope, and on better integrating them directly into graduate education programs.

### 7.1.2 Subgroup B Discussion

The statement “applied computer science is being attempted in academia without any formal training” kicked off our discussion. The group brought expertise in several different training models, from a two-day Software Carpentry workshop, a three-week Open Science for Synthesis (OSS) program, to semester-long programs. We discussed the pros and cons of different training approaches, touching on informal learning, for example, where people learn the necessary skills by asking questions of cross-disciplinary people (“boundary scientists”) in their work environments.

Some papers explored gaps in training of early-career scientists. Industry participants in our group confirmed this observation. We asked ourselves, “Are traditional courses failing?” We think yes. Changes to undergraduate curricula requirements are difficult. But as programming models become more complex, we have to raise the skill levels. Skills must be improved not only in traditional programming – learning languages and algorithms – but also around professional software development. We want to get to a point where “Everyone has a new minimum now – everyone knows Git.” Developers also need training on licensing choices. Just because some source code is on Git does not mean that it is open.

“How do you get people to look for the training they need?” wondered one participant. People seek out opportunities like Software Carpentry to augment skills. While some instructions can be done in institutional curricula, independent groups (non-profits, institutes) have more flexibility. Some asked whether Silicon Valley would be interested in funding training so that people are better prepared to enter the workforce. Some felt that companies were reluctant to deliver training for fear that their employees might then leave them. While others felt that pushing all training to industry could lead to good technical people “getting on the Google bus” and leaving sciences.

“How will we know when people are trained effectively in these new skills?” We discussed certification. It can be hard to build the recognition of Java or database certifications among all technologies. OSS offers badges to those completing training. However we need to demonstrate proficiency, not just completion. Google Summer of Code is a big CV augmentation for participants—can we create something similar?

The group also discussed how to fund training. On participant observed that NYU runs a six-week data-science training; companies grab the graduates and pay for those they hire. OSS also used the NSF Software Institutes program as a vehicle to fund training activities. Software Carpentry uses a collaborative teaching approach where people publish open teaching materials and receive credits for their use.

We then discussed career paths for those supporting sustainable software. While tenure track is not the only option for graduate students, the challenges for those who remain in academia can be large. Research scientists are entirely dependent on soft money, which can be unpredictable. Postdocs and those who do pursue tenure track positions need to publish and see no rewards in software development. These challenges were all identified at WSSPE1. What actions would we recommend to improve things? Altmetrics and download statistics may slowly change the system and improve a developer’s ability to receive credits for time invested in software development. NSF’s recognition of scientific products including datasets, software, and publications is also helping.

We asked ourselves, “Are there examples of things that are changing because of this and how can we build momentum?” One example demonstrates change over time. In 2007, nanoHUB listed the academic reward structure as a problem in an EDUCAUSE report where the authors note, “In the future, nanoHUB researchers are hoping to change the research culture. While they recognize that young faculty members are unlikely to get tenure based on their nanoHUB contributions, they hope to encourage faculty to think beyond their own research needs to consider publishing tutorials and other content in their fields on the nanoHUB site.” Fast forward to seven years later where, in a 2014 iSGTW article, quote nanoHUB Principal Investigator (PI) Gerhard Klimeck, “A former student of mine published eight tools on nanoHUB, serving over 6,000 people with his tools. He then joined a university as a professor and introduced nanoHUB. Use of the gateway from that university skyrocketed; he used nanoHUB in existing classes, created new classes, and infused it in his research. Ultimately, the professor’s department head attributed his two-year rise to tenure with the reputation and innovation he gained through nanoHUB.”

The group also discussed “attribution trees,” an idea put forward by Dan Katz and Arfon Smith where a chain of attributions can, for example, give credit to those developing libraries and building blocks that other pieces of software use. The group considered potential journals and medium to push the application of this idea. One participant noted that Dryad<sup>20</sup> works with journals. If a paper is accepted to one of those journals, the supporting data

must be submitted to Dryad. The group also discussed reproducibility as a component of the journal review process and “active papers,” with immediate links to the data and software.

We then discussed variations among scientific domain areas and wondered “Are some communities more or less open than others?” To some members of the group, biology seems to be more open, while physics less so. Some felt, with the more recent development of bioinformatics as a field, there were fewer historical practices to undo in biology. Physics has preprint philosophy to overcome. Environmental sciences may be mixed. The group felt that the biomedical area, however, was very competitive and closed. One participant mentioned blueprints for going open source (like NWChem recently did) where authors outline how this helps, what you do and what the next steps are.

We then moved beyond our training discussion to address funding that encourages sustainable software – funding of both people and projects that create a true system to support sustainability. We called this “institutionalized serendipity.” As science is increasingly reliant on software, one participant observed that “software development can have much broader impact than publishing individual research, but it is not viewed that way.” Because of this centrality, one participant mentioned that training ought to be called Science Carpentry rather than Software Carpentry. We felt we were beginning to see changes in the research community as a result of the NSF’s data management plan requirements. PIs are thinking more about data and some university libraries are offering data repositories. We wondered if a software management plan might be effective. “How might funding programs need to adapt to reward good software development practices?” we asked ourselves. We thought about best practices such as version control, test harnesses, mailing lists, bug tracking, community contribution, and reuse where appropriate. We thought about measuring success through usage statistics (downloads, altmetrics). “Should funders demand reproducibility?” we wondered. In order for results to be reproduced, software would need to be carefully curated.

Again, our industry participants contributed unique viewpoints. Partnering with industry was seen as one path to sustainability. The unique partnerships Kitware engages in promote academic freedom while creating an income stream from certain portions of the software. This type of approach to sustainable software frees researchers from performing tasks that do not offer the rewards their institutions value. We also discussed about successful models for industry partnerships that preserve open science. Participants noted that there are some NSF programs that prohibit partnerships with for-profit companies (but there are other programs in which this is encouraged).

### 7.1.3 Subgroup A Actions

Three main actions were identified by Subgroup A that would be of interest to participants and benefit the research community. These focused on the desire to amplify the current community efforts in training and software

engineering by connecting the current training initiatives (e.g., Software and Data Carpentry, rOpenSci, OSS) that are of different durations at appropriate stages. Generally it was felt that a modicum of interaction between short term workshops (SwC, DC), medium term trainings (e.g., OSS), and longer-term courses (e.g., BIDS Data Science) would benefit from coordinating curriculum, discussing and aligning prerequisites, and coordinating timing of courses. A training coordination effort would go a long way towards amplifying the value of the individual efforts and make them all more effective.

- **Action 1:** Create a roadmap of research software training initiatives. Such a roadmap would provide a taxonomy of training opportunities: what they deliver, and what attendees need to know going in (prerequisites). It would also show which recommended roadmap actions will have a clear and immediate payoff, and which will have long-term payoffs. The training roadmap would emphasize time savings and efficiency gains to be had from each training.
- **Action 2:** Build a report card characterizing use of best practices in scientific software. Generally, people felt that researchers would be very willing to migrate practices if they could identify where they needed to improve. Such a report card would ask simple questions to characterize use of best practices in science software, and could be structured similarly to Joel Spolsky’s Software Maturity questionnaire (also known as the Joel Test [25]). The survey would create a report card that shows areas where a project could improve, and then link those areas to specific training offerings from the training taxonomy from Action 1.
- **Action 3:** Create a science software review forum. It was generally acknowledged that a little code review can have a tremendous impact on the quality of software in a project, but that sites for science code review are lacking. While people can ask questions on the Stack Exchange sites, they are generally not open to questions of style, approach, or appropriateness, as they try to avoid subjective commentary. Instead, we need a site where code gets discussed/summarized/described (in small bites) by the science software community. The target audience would be graduate and undergraduate students in the sciences, and there would need to be mechanisms to keep the review positive and constructive, and not get pedantic or judgmental. This could be tied to a software registry (such as the nascent GeoSoft project), or to language repositories like R’s CRAN repository, and could lead to the report card discussed in Action 2.

### 7.1.4 Subgroup B Actions

Subgroup B then focused on actions it could take. It discussed development of a white paper that describes a matrix approach to training (multi-day, multi-week, semester). The white paper might include a survey of existing techniques. There are many, some dating back many years, for example the Interuniversity Consortium for

Political and Social Research (ICPSR) and various summer institutes. The white paper could include a call for a comprehensive assessment of these techniques. We need to think carefully about the right venue for such a white paper, where it would have the most impact. The subgroup believes it would need to approach editors directly to ascertain this.

The group felt that training in techniques that promote sustainability has a range of benefits: career paths, educated reviewers, reproducible science, and more. There is some information on how that has been approached and assessed, but more is needed. The group felt that this training is undervalued and that it is important to communicate the return on investment (ROI) – both individual ROI (skills that make scientists more effective and more marketable) and funder ROI (better use of taxpayer funds, research more likely to be reproducible because sustainable software exists, better trained reviewers).

## 7.2 Papers

The papers that were discussed in the Software Development Experiences Subgroup A are:

- Michael R. Crusoe and C. Titus Brown. Channeling community contributions to scientific Software: A Hackathon Experience [26]
- Marcus Hanwell, Patrick O’Leary, and Bob O’Bara. Sustainable software ecosystems: Software Engineers, Domain Scientists, and Engineers Collaborating for Science [27]
- W. Christopher Lenhardt, Stanley Ahalt, Matt Jones, J. Aukema, S. Hampton, S. R. Hespanh, R. Idaszak, and M. Schildhauer. ISEES-WSSI Lessons for Sustainable Science Software from an Early Career Training Institute on Open Science Synthesis [28]
- Jory Schossau and Greg Wilson. Which Sustainable Software Practices do Scientists Find Most Useful? [29]

The papers that were discussed in the Software Development Experiences Subgroup B are:

- Jordan Adams, Sai Nudurupati, Nicole Gasparini, Daniel Hobley, Eric Hutton, Gregory Tucker, and Erkan Istanbuluoglu. Landlab: Sustainable Software Development in Practice [30]
- Alice Allen and Judy Schmidt. Looking before Leaping: Creating a Software Registry [31]
- Carl Boettiger, Ted Hart, Scott Chamberlain, and Karthik Ram. Building Software, Building Community: Lessons from the ROpenSci Project [32]
- Yolanda Gil, Eunyoung Moon, and James Howison. No Science Software Is an Island: Collaborative Software Development Needs in Geosciences [33]
- Ted Habermann, Andrew Collette, Steve Vincena, Werner Bengler, Jay Jay Billings, Matt Gerring, Konrad Hinsén, Pierre de Buyl, Mark Könnecke, Filipe Rnc Maia, and Suren Byna. The Hierarchical Data Format (HDF): A Foundation for Sustainable Data and Software [34]

- Eric Hutton, Mark Piper, Irina Overeem, Albert Kettner, and James Syvitski. Building Sustainable Software – The CSDMS Approach [35]
- James S. Spencer, Nicholas S. Blunt, William A. Vigor, Fionn D. Malone, W. M. C. Foulkes, James J. Shepherd, and Alex J. W. Thom. The Highly Accurate N-DEterminant (HANDE) Quantum Monte Carlo Project: Open-source Stochastic Diagonalisation for Quantum Chemistry [36]

## (8) Credit & Incentives

This group, with just three papers but a large amount of interest and participation from attendees, focused on the institutional, social, and cultural mechanisms that encourage the creation and maintenance of shared software, in the context of what now exists, what mechanisms are desired, and how we might achieve them.

### 8.1 Discussion and Actions

In the first discussion session, this group decided to break into two smaller groups, each independently working through the same general topic: credit and incentives.

#### 8.1.1 First breakout discussion: Group A

The first sub-group discussed issues around the current system for credit and incentives, which it called “hacking the incentive structure.” The group considered four potential points of leverage:

First, that we currently have systems that collect information, and these could be modified to collect different information, then map that information to actions. We could initially build a proof-of-concept for a new use of a given system, then determine what actions would be needed to make this use more common.

Second that we could create entirely new systems, perhaps because the existing systems are too tied to what they measure, and modifying them is not practical.

Third that we could change academic culture, rather than worrying about the systems. This was mostly focused on citations, because they matter for hiring, promotion, and tenure decisions. The group discussed how we could weigh the citations within papers better than we now do. How could we identify the five citations that really matter for a paper, distinguishing them from the related works and general background that are also cited? Perhaps we could break these out in the reference list, working with publishers to implement this. Or maybe we could also break out categories of citations, such as the most important software used, the previous publication that we are building from, the data that we actually used, etc. The Moore Foundation’s award in data science was given as an example, asking proposers: What are the five canonical citations that are most important to your work? [37] This would be a way of giving credit and assigning importance to these works, differently from how we just count citations today. A possible action that the group discussed was conducting a longitudinal study of most useful software, data, etc. in a discipline.

Fourth, that we could change the ways funders make decisions, and use these funding policies as incentives.

After this discussion, group A brainstormed about incentives, with the following items suggested:

- running programming contests, creating bounties for contributing to open source software, etc.
- augment author lists to give credit to people who do not now get credit (and making them machine readable)
- developing a microcitation standard and mechanism (for both software and data)
- developing a well-defined standard for author contribution – what level of contribution rises to the level of authorship?
- leveraging social media for citation and reviewing of content – then using social media to bring more people into the review process than is traditional
- determining where else software can be cited and recorded (e.g., acknowledgments sections of papers)
- developing a taxonomy of contributors (e.g., Project Credit [38]) tied to places that these metrics are already stored (e.g., ORCID [39])
- making metadata easier to add for software, creating incentive for providing software metadata – note that this cannot be centralized
- creating something like the h-index that tenure committees can make use of – simplify a way of measuring and documenting the overall credit given to an individual over different projects
- thinking about publishing software versus journal – software does not have to be novel
- determining guidelines for recommending software characteristics for tenure – perhaps draft guidelines then get ACM or IEEE agreement.

### 8.1.2 First breakout discussion: Group B

This group started by discussing who should be incentivized, thinking of two categories of people: those in science (who could be incentivized to do better, more shareable, more sustainable work), and those in industry but interested in science (who could be incentivized to contribute to science.) It was pointed out that we are not yet clear enough on exactly what we want to incentivize, suggesting that we need to have a clearer picture of “good computational work” and what sort of contributions are truly generative for science.

The discussion of incentivizing those in science acknowledged that the publications system was far from perfect for incentivizing good software work. Nonetheless, the discussion focused on bringing software people into publications. There were two main suggestions. The first is to focus on end users of software and encourage them to cite software the “right” way. James Howison suggested that his research showed that few projects were making a formal request for citation (but that authors weren’t necessarily following those suggestions anyway) [40]. He suggested making access to the software conditional on a license that requires citation. Others found this “too confrontational”

and preferred to concentrate on making it easier to do the right thing. The second was focusing on those leading software projects, and the group was more enthusiastic about “forcing” PIs to include their “software people” on publications, although there were few ideas on how exactly to do this. Another technique mentioned was that when scientific software projects are hosted in organizations like Apache, the scientific contributors can benefit from building their reputations, perhaps yielding job offers that they can use to negotiate better job and career packages.

The discussion on incentivizing those outside science focused on accessing the well of affection that those working in software have for scientific research. How can the interest and skills of this group be marshaled towards sustainable contributions? There is evidence that the migration of scientific software projects to the Apache Software Foundation (ASF) has created opportunities for those not employed in the scientific center to contribute to projects initiated by scientists (especially where there is cross-over with industry needs, such as provenance and workflow).

The group also discussed developing “software prizes” arguing that while it is hard to “mint” other new sources of reputation, prizes are possible without getting too many others on board. The prize criteria can form a template for describing what we mean by scientific contributions made through software, particularly focusing on building active communities, not only writing great code.

### 8.1.3 Group merger and redivision

After the first breakout session, the groups A and B came together and discussed a rollup of the ideas from the subgroups at a high level:

- citation ecosystem – traces of usage (metrics)
- taxonomy of contributorship, understanding roles
- prizes
- new metrics (for people’s activities in software)
- guidelines for evaluating scientific contribution through software (perhaps using new metrics).

In the remaining discussion sessions, the group chose to split into three subgroups to discuss a version of these topics: *citation ecosystems*, *taxonomy of contributorship/guidelines for software for tenure review*, and *prizes*. The subgroups were asked to clearly identify

- the problem to be solved
- steps towards a solution.

### 8.1.4 Remaining breakout discussions: Citation ecosystems

This group defined its goal as creating a low-barrier-of-entry method for recording names and roles (and in a second phase, optionally including weights) of contributors (coders and other intellectual contributions) to a software package in a machine readable way (to be called a credit file), then encouraging the scientific community to adopt this practice.

The following general points were initially discussed:

- The FLASH [41] project was suggested as an example of how something like this has been done.
- This data could be a file that can be associated with a citation to the software, either through use of a DOI (digital object identifier) for the credit file, or by uploading the credit files as associated with the paper.
- This idea could also be applied to data.
- The credit file should be part of the metadata that are freely available to those who have not paid for access to the journal, like citations are now in most cases.
- It was suggested that there should also be a *separate* file to track software dependencies.

The group came up with the following actions to be performed:

- (1) Build a tool that can automatically determine who the contributors are (from a Git or other repository), then allows the user to manually edit the output to add/remove people, define roles.
- (2) Work with repositories to encourage them to provide the information we need based on what they already store.
- (3) Define what a citation file should look like and what it should be called.
- (4) Test adoption with a substantial scientific organization such as the Lawrence Berkeley National Laboratory (LBNL).
- (5) Create credit file for a set of software.
- (6) Build a validator (and perhaps a visualizer) for credit files.
- (7) Write a tool to collect files and visualize/output interconnections (which software is used with which), based on an existing project.
- (8) When we (the group members) write papers, we should track the software we use, and encourage the software developers to make their software citable and create credit files.
- (9) Build a tool to export the credit file to BibTeX and other citation styles.
- (10) Make sure the BibTeX entries (exported from internal data) are somewhat standardized so that they can be imported into papers. Also make sure that standard LaTeX style files understand and accept these entries.

#### **8.1.5 Remaining breakout discussions: Taxonomy of contributorship/guidelines for software for tenure review**

At the start of the discussion, the breakout group brought forth the important observation of the wide disparity in commonly accepted habits of publication in different research fields. In domains which have, historically, relied on large groups of researchers collaborating towards a common goal (e.g., high-energy physics, astronomy), publications often have tens or even hundreds of co-authors (with some papers in experimental particle physics having over 3000). In other domains, the number of co-authors is

typically much smaller with, in some cases, even a preference for single-author papers. Similarly, the various platforms for publication are valued differently in different domains. Most commonly, publications in peer-reviewed scientific journals are regarded as the most important and most impactful. However, in certain domains, especially in Computer Science, many researchers typically regard conference proceedings as their prime publication target. It is often suggested that this difference is due to the rapid developments in information technology, a pace that cannot be upheld by traditional peer-reviewed journals. Whatever the causes, any useful taxonomy of contributorship or guideline for tenure review should take such differences into account.

Despite these differences, and despite the fact that software often has taken the role of a proper, albeit less tangible, scientific research instrument, neither the software nor its creators are commonly credited as part of a scientific publication. The group acknowledged the need for more recognition for the creators of such software instruments, and indicated a number of possible pathways. First and foremost, domain scientists must be made aware of the important role of software, and include the developers as co-authors of papers. A second approach is to fully embrace an open badging infrastructure (such as Mozilla's Open Badges), where a *badge* is a free, transferrable, evidence-based indicator of an accomplishment, skill, quality, or interest. A third approach is for the scientific community to support the increasing momentum of peer-reviewed journals specialized in the open source/open access publication of scientific research software, such as Computer Physics Communication, F1000 Research, Journal of Open Research Software, and SoftwareX.

Recognizing publication of research software as a proper scientific contribution raises several important but currently unsolved questions, however. For example, is the number of users of the software a relevant measure of impact? What standards of coding quality must be followed in order to justify publication and hence recognition? Should the release of a new version of the software be eligible for a new publication; if so, under what conditions? And above all: should software publications be valued in the same way as traditional scientific publications? Or is there a need for new measures of productivity and impact?

In part, the answers will come from the scientific community at large, as a natural consequence of growing awareness and mindset change. Some of the answers, however, also should be based on decades of experience in (and developing standards for) implementing, maintaining, refactoring, documenting, testing, and deploying software instruments in scientific research. Care should be taken, however, not to impose such standards for all domains in equal ways right from the start. Forerunners should serve as an example, but should not scare away domains that have based their progress on much less advanced methods of *software carpentry*. Nevertheless, proper guidelines are needed, which eventually should be followed across all domains. The group also recognized that funding bodies,

universities, and publishers eventually should demand that research projects follow such guidelines, and to implement a proper software sustainability plan.

To enable a form of standardized crediting for developers of research software, the group proposed to work towards a taxonomy for software-based contributorship. The taxonomy should be derived from, or extend, existing taxonomies for research impact and contributorship such as defined by CASRAI (in particular based on the Wellcome-Harvard contributorship taxonomy,<sup>21</sup> VIVO, or ISNI. An interesting measure of impact raised by the group was the *betweenness centrality*, an indicator of a person's centrality (and hence, importance) in a scientific collaboration. It is expected that developers of research software often play such a central role.

The group defined the following actions to be performed:

- (1) Investigate existing taxonomies for roles and contributorships.
- (2) Investigate prototype badging initiatives.
- (3) Investigate journals focusing on publishing peer-reviewed research software.
- (4) Investigate guidelines and checklists of best practices.
- (5) Communicate the results of the above investigations to the WSSSPE community and decision-making bodies (funders, publishers, universities, and tenure committee representatives).
- (6) Ensure engagement of the broader research community in this discussion.

### 8.1.6 Remaining breakout discussions: Prizes

This group discussed the idea of prizes. Prizes are expected to reframe software as “instrument building” but will prizes be good or bad, and how can we make sure there are no negative affects and the process cannot be gamed?

Prizes in different categories were discussed (like Academy Awards), for example: best contribution (non-founder), broadest diversity of contributions, best tutorials or documentation, best leadership transition (award ex-leader and new leader), best generalization (taking something that was limited and making it more general), and best mentorship of contributors (bringing others into the community).

Other (non-prize) forms of incentives are

- Converting reputation by joining the ASF, Google, etc.
- Inviting ASF and open source people to contribute to scientific code (at least in areas where there is overlapping interest).
- Template for assessing scientific contributions made through software.

The group suggested that to determine who should give out prizes, perhaps we should find those who we think would be awarded prizes, then ask them who they would want to receive a prize from, and subsequently contact those organizations to see if they are willing to be involved in the process.

One of the group's ideas was to create a funding program for disciplines or other organizations to create a

prize program. We would provide a framework and a set of requirements, for example: awards to individuals; must award in 5 or 6 areas; must have a jury that includes senior/junior domain experts and technologists (and should have objective criteria); must have the recipients awarded at a relevant event; and must provide citations that explain why the prizes should be awarded. Different organizations could then decide to sign up to the framework and give out awards under this general brand. However, there was a concern that having many organizations award prizes may reduce the impact of the prizes.

Possible groups that might give out awards, either under our framework, or more generally, are AAAS, Nature Publishing Group, ACM, IEEE, Astro, Ecology Society of America, etc. Perhaps this could be a joint technology/science partnership, for example, the [Apache | Mozilla]-[AAAS | disciplinary society] prize.

Some potential criteria for prizes the group suggested are: community engagement, helping out others; number of unique contributors; adding new pieces of functionality to software; integrating software into broader ecosystem; championing broad principles of sustainability, open science, open source, etc.; improving accessibility to software, to scientific software (perhaps championing inclusiveness or making software accessible?); documentation; tutorials; commits/patching; leadership transition; and best contribution by a non-founder.

The group discussed if there should be different criteria for “established” members of the community versus junior members, and if prizes should be restricted to junior members, but left these as open questions.

A point the group considered important is that we do not want to give prizes just to reward people who are really good at this one thing, but rather we want to reward people who are building the culture we want as scientists.

## 8.2 Papers

The papers that were discussed in the Citation & Incentives group are:

- James Howison. Retract Bit-rotten Publications: Aligning Incentives for Sustaining Scientific Software [42]
- Daniel S. Katz and Arfon M. Smith. Implementing Transitive Credit with JSON-LD [43]
- Ian Kelley. Publish or Perish: The Credit Deficit to Making Software and Generating Data [44]

## (9) Reproducibility & Reuse & Sharing

This group discussed five papers with a wide variety ideas of how to support reproducibility and reuse. It focused on identifying concrete practices that the attendees could work together on, which would have a positive effect on the community.

### 9.1 Discussion and Actions

In the first discussion session, this group broke up into two smaller groups working on different topics: Reproducibility, and Reuse and Sharing. In the second discussion session, three subgroups worked on creating specific pieces of guidance.

### 9.1.1 First breakout discussion: Reproducibility group

The first group discussed ways in which reproducibility of papers could be improved. A consensus surrounded the provision of examples: demonstrating to others how to achieve reproducibility. Major public funding investments go into research that heavily relies on reproducible software, hence the lack thereof is raising major concerns.

Two main avenues could be used to implement policy that would improve reproducibility and drive top-down culture change:

- Funders can aim to get more software expertise on to funding review panels and provide more guidance on what is required of software related to research (cf. data management plans)
- Journals can define and publish journal policies to improve reproducibility, and reviewers can insist that authors provide sufficient information and access to data and software to allow them reproduce the results in the paper. Stronger policies even for some high-impact journals have recently come into place, for example Nature Publishing journals.

If journals do enforce greater reproducibility constraints, it is important to lower the barriers to reviewers attempting to verifying the correctness of the software used to generate the results. A major issue is that a lot of software only builds on certain systems. Should journals provide more tools/support for reviewers, and if so, what is it? An idea that came from the groups was to define a set of support services that should be available to software paper reviewers. Another was to provide the ability for reviewers to flag the requirement for a 'software verification,' similar to the ability to flag that a paper needs to be seen by a statistician.

Other discussion focused on ways in which researchers themselves could improve the reproducibility of research. One way would be to establish tracks at conferences that subject papers to reproduction, which for those that pass would lend them an additional badge (similar to OOPSLA). Another is simply to get more people to use your software: for instance by outreach to high school students – can your software be used by them? Finally, there is a role for community-curated benchmarks to validate the performance and capabilities of tools.

### 9.1.2 First breakout discussion: Reuse and Sharing group

The second group discussed ways in which software could be more easily reused and shared. From the perspective of both user and developer, any solutions must be 1) easy; 2) cheap; 3) not too time-consuming.

Reuse and sharing were considered to be distinct but linked. In many cases, pre-existing software does not exist, so new software is written but even then it is not shared afterwards. The principal barriers to reuse are the difficulty of finding out what software is available, understanding if it is usable, and then of installing and running software if it is located.

Discovery of relevant software is still a fundamental issue: we need standard vocabularies and metadata, better tools, and approaches that are sustainable. Publications are an easy entry point for locating suitable software, but should the publishers lead the way, or is this the responsibility of "the community?" Some communities have had significant initiatives to improve software discovery, e.g., the NIH Software Discovery Index.<sup>22</sup> Likewise, there were examples of journals which had made software more discoverable: ACM Transactions on Software offers a reproducibility review; the Journal of Biostatistics has an opt-in to provide code and a certification mark if it can be run; the Journal of Open Research Software requires software to be deposited in suitable repositories and referenced.

An issue around the sustainability of software catalogues is that their usefulness often depends on the domain. For instance, in the biosciences, there is more homogeneous data and standard shared code. In areas like ecology, code is often very specific to a problem, meaning that the level of re-use might be at a general statistical level of abstraction, but then every research use is highly customized.

Finally, it was clear from the discussion that there were many ways in which software could be made available in more reusable ways than just a tarball sitting on a personal website. Using code repositories like GitHub<sup>23</sup> gets you an archived, shared platform and improve the reusability of your software incrementally, for instance by adding a license or by archiving (with a DOI) in Figshare<sup>24</sup> or Zenodo.<sup>25</sup> Docker<sup>26</sup> might be a solution to the issue of dependencies, to allow binaries and libraries to be bundled in a more lightweight fashion than a virtual machine image.

The key enabler for reuse and sharing was to get domain scientists more effectively connected with programmers/analysts. Both have skills and experience which is necessary to make the right decisions for improving the reusability and discoverability of software, and to apply community pressure to change practice.

### 9.1.3 Second breakout discussion: Categorization of software journals

This group aimed to come up with a categorization of journals which published software papers. Starting from the list of journals<sup>27</sup> maintained by the Software Sustainability Institute, the group chose seven journals and looked at their advice to authors and reviewers. These were the Journal of Open Research Software,<sup>28</sup> PLoS ONE,<sup>29</sup> Journal of Statistical Software,<sup>30</sup> Methods in Ecology and Evolution,<sup>31</sup> Transactions of Mathematical Software,<sup>32</sup> GigaScience,<sup>33</sup> and PLoS Computational Biology.<sup>34</sup> From these a set of common categories were synthesized, against which all journals could be compared:

- Journal Policies
  - Accessibility of papers
    - \* Open access
    - \* "Freely" available
  - Repositories
    - \* Provides suggestions for recommended repositories
    - \* Provides its own repository

- Review
  - \* Reviewing software is mandatory
    - Must check that software runs
    - Must check quality of code
    - Must check performance of code if paper makes claims on relative performance
- Supporting data
  - \* Must be publicly available
  - \* Must be in an open access repository
  - \* must have a DOI
- Article processing charge (APC)
  - \* APC charge is transparent
  - \* APC waiver program
- Paper Policies
  - Required sections
  - Keywords
    - \* Paper provides keywords to help describe software
  - Papers can be updated when new releases of software are made
    - \* At no extra cost/at significantly reduced cost
- Software Policies
  - Software must have a license
    - \* Software must have an open source license
  - Availability
    - \* Software must be openly available and accessible
  - Deposit policies
    - \* Software should be in a public repository
      - Of particular stature/with a preservation plan
    - \* Software should have a permanent identifier
    - \* Software deposit doesn't count as a prior publication
  - Runnability and dependencies
    - \* Provide documentation to understand how to run
    - \* Provide sample data
    - \* Provide dependency information

The follow-up actions to this work are to use this set of categories on all the journals in the list, refining the categories if necessary, then identify if any of the categories are seen to be more useful to promote reproducibility, reuse and sharing.

#### **9.1.4 Second breakout discussion: What should journals provide reviewers of software papers?**

This group discussed whether they could come up with a list of things that a journal should provide its reviewers to make it easier to review software submitted for publication as a “Software Paper.”

Journals should provide guidelines about what to consider when reviewing a software submission. A good example for a relatively comprehensive guidelines for reviewers (and thus in turn authors) are those of JORS.<sup>35</sup> Journals might also learn from organizations such as the ASF as to what is good practice for software submissions. Guidance is needed on what constitutes an incremental improvement that is significant enough to qualify

for publication, otherwise this assessment can be very subjective.

Journals should provide mechanisms to enable and track communication between reviewers and authors. For anonymous peer review journals, anonymity of reviewers should be maintained. If communication is necessary, that may mean that software is not that well documented. Journals should also provide a set of simple metrics for software evaluation that reviewers can use for ratings, similar to Consumer Reports.

Journals should provide guidelines about requirements for documentation of code: both in-lined in code, and manuals/web pages, etc. Journal editors could provide documentation checks before it goes out for review. This should include a requirement for good Use Cases specified for the software, with references to executable test cases that demonstrate each use-case is met (at least in the form of the test case).

Journals should support mechanisms to run software. Sometimes this may be very hard to accomplish, despite best efforts. Journals could provide an execution environment for any software submitted for review, perhaps via a Docker container or a virtual machine. If not, instructions must be adequate to compile and execute the software; to interpret the results (output files, formats, etc.); and the full source code must be accessible to the reviewer. Mechanisms to quantify what has changed compared to a previously published version would assist version comparison. However, this cannot simply take lines of code into account. For example, a speedup of an algorithm may not result in a huge code difference, but may nonetheless provide a breakthrough. Journals should require software submissions to also provide ‘test materials’ – sample data, parameters to validate that code is working as intended. In certain cases, well-selected benchmark datasets may be required to assess performance and accuracy.

Journals should ensure minimal metadata are provided, similarly as is already the case for certain kinds of data (though the latter is often enforced by data repositories) – Dublin core-ish (creator, owner), and more specific (platform and compiler dependencies, sample benchmarks of performance, etc.). Journals should provide guidance or constraints as to software licensing conditions.

The follow-up actions to this work are to work with journals and reviewers to identify whether any of these suggestions can be easily provided, perhaps for a range of journals.

#### **9.1.5 Second breakout discussion: Reproducibility Meta-track toolkit**

This group worked on defining a “toolkit” for running a reproducibility meta-track at a conference. They decided to take the work done during the workshop and publish it as a paper.

## **9.2 Papers**

The papers that were discussed in the Reproducibility & Reuse & Sharing group are:



- Jakob Blomer, Dario Berzano, Predrag Buncic, Ioannis Charalampidis, Gerardo Ganis, George Lestaris and Ren e Meusel. The Need for a Versioned Data Analysis Software Environment [45]
- Ryan Chamberlain and Jennifer Schommer. Using Docker to Support Reproducible Research [46]
- Neil Chue Hong. Minimal Information for Reusable Scientific Software [47]
- Tom Crick, Benjamin A. Hall, and Samin Ishtiaq. "Can I Implement your Algorithm?": A Model for Reproducible Research Software [48]
- Bryan Marker, Don Batory, Field G. Van Zee, and Robert van de Geijn. Making Scientific Computing Libraries Forward Compatible [49]
- Stephen Piccolo. Building Portable Analytical Environments to Improve Sustainability of Computational-Analysis Pipelines in the Sciences [50]

## (10) Code Testing & Code Review

This group began by recognizing that they knew what the problems of code testing and code review are, so the purpose of the group was really to think about concrete things that people in the group would be willing to commit to, in order to improve the sustainability of software.

### 10.1 Discussion and Actions

The consensus of the group was that small, concrete actions would have the greatest chance of proper follow-through by members of the group. An example of this approach was the Architecture of Open Source Applications book [51], containing contributed chapters on open source software. The group contemplated creating an analogous book or web resource for testing of scientific software.

A key point of discussion was that there are two major challenges to software testing in science. The first is convincing developers to incorporate testing. This challenge is both social and technical. We need to communicate the value of testing and also teach developers how to choose and use testing frameworks. The second challenge—and the one that the group felt was more difficult—is choosing appropriate tests for scientific software. This is the difference between learning how to use, say, Python unittest and knowing how to test that one's code correctly implements, for example, a Lattice-Boltzmann model in computational fluid dynamics.

#### 10.1.1 Choosing and implementing testing frameworks

There was general consensus that once a developer has been exposed to a testing framework in a nontrivial fashion, he/she will subsequently insist upon using a framework for further work. The acknowledged challenge was how to create that crucial first exposure to such frameworks.

Within the group, there were several different paths by which participants had their first exposure to code testing:

- Formal tutorials at conferences (for example, a test driven development (TDD) at a Software Developers

Best Practices conference): These often require self-learning following a tutorial, but it can be hard to find a tutorial that matches the programming language and/or the domain of the participant.

- As a way to be confident in other software: When breaking out pieces of software from a larger application, a developer wants to ensure the software works as expected. These types of tests may be ephemeral though, living long enough to give the author of the test confidence in the code, but not handed on and made available to next user. These experiences can lead to more systematic testing.
- Through experience with coding: As you write more software, your confidence in code is reduced and the importance of testing becomes clearer. Attendees joked that they started testing "when their skepticism/guilt became larger than their arrogance."
- From other projects: When building on top of projects with good testing frameworks, you realize that you should also adopt those good software engineering habits.

The two non-self-taught paths were direct learning and indirect through other software (learning by example). The group recognized that teaching about testing needs to start early in projects and careers. We need to teach people how to test short bits of code, rather than waiting until they have thousands of lines of code and being surprised when they don't write tests. The group generated a set of practical suggestions for improving adoption of code testing. Established software projects can encourage the latter through a simple rule of accepting only software patches with associated tests and through good documentation of testing practices and requirements.

Simpler, standard ways of setting up appropriate testing infrastructure will be important for adoption by scientists. Jenkins<sup>36</sup> was suggested as a common open-source solution, but the initial configuration was considered to be challenging for typical scientists.

Teach testing by beginning with a (smallish) piece of code that lacks appropriate tests and develop an exercise that involves refactoring the code into a more presentable form through creating/deriving unit tests. Students would extract unit-tests through reverse-engineering and/or questioning a partner who is a developer/expert.

This led into a more general discussion about whether programming courses should be part of the standard curriculum for science students and the challenges of fitting additional material into university curricula. This is the reasons that short workshops such as Software Carpentry and others exist.

Ironically, Software Carpentry no longer teaches testing [52]. This boils down to two issues. First, that scientific computing doesn't (yet) have the cultural norms for error bars that experimental sciences have, and second, that there is a breathtaking diversity of scientific code; scientific research is highly specialized, which means that the tests scientists write are much less transferable or reusable than those found in other fields.

### 10.1.2 Writing tests for scientific software

The second major discussion thread in the group addressed the issues identified by Software Carpentry – the difficulties in writing tests appropriate for scientific software: What tests are appropriate to ensure that a complex method is working correctly? When is the result of a numerical computation ‘close enough’ to pass a test?

Several members of the group indicated that while they valued the concept of software testing in theory, they were unaware of how to test certain kinds of software. Or, more importantly, they lacked relevant examples of software testing that would be suitable for new members of their teams. As an example, the group asked if it could produce a 100-line example of how to test neutron transport (or other specific scientific examples) targeted at a sophomore? This would be a demonstration of “How do I do this right?”

Another question was “How do I test so that I know that the code is not the source of my problems?” A common challenge is that of stripping things down to an appropriate level for tests. The group recognized that the difficulty is different for so-called software infrastructure than for numerical/scientific layers of software applications. There is some discussion of the issue in the computer science literature [53, 54] but less in domain-specific journals. Some lessons on multiphysics software verification can be found in a recent paper [55].

Two important pieces of the barrier are a) picking/ implementing testing frameworks (a technical barrier) and b) deciding what are the actual tests that I need to write? A possible method to solve the latter is to ask students “how is what you are doing different from typing random keys on the keyboard?” and then, turn their answer into the concept of tests. That is to say, expand the process of creating code from one that is solely about “how?” into one that also includes “why?”

Another point of discussion is that many scientists are not aware that “testing the code” and “testing the science” are distinct issues. A related question that came up is “How do you know that your method produces a result that is ‘close enough’?”

The group then decided that a useful action would be to create a set of scientific codes with associated tests. They developed the following basic structure for these examples and sketched out six specific examples:

- (1) A paragraph or two explaining the scientific problem the code addresses
- (2) The size of the simplest piece of relevant, interesting code (i.e., an estimate of lines of code)
- (3) A point-form list of the test cases you would use.

The follow-up actions from this work include creating a compilation of testing examples in scientific software. Some of the examples from the workshop have become the starting seed of a collaborative book (<https://github.com/swcarpentry/close-enough-for-scientific-work>) in which scientists provide concrete examples of testing scientific software. The goal is a set of testing examples, aimed

at sophomores in science and engineering, that cover a broad range of domains and problems and could be easily incorporated into other workshops or courses.

### 10.2 Papers

The papers that were discussed in the Code Testing & Code Review group are:

- Thomas Clune, Michael Rilee, and Damian Rouson. Testing as an Essential Process for Developing and Maintaining Scientific Software [56]
- Marian Petre and Greg Wilson. Code Review for and by Scientists [57]
- Andrew E. Slaughter, Derek R. Gaston, John Peterson, Cody J. Permann, David Andrs, and Jason M. Miller. Continuous Integration for Concurrent MOOSE Framework and Application Development on GitHub [58]

## (11) Conclusions

The WSSSPE2 workshop continued our experiment from WSSSPE1 in how we can collaboratively build a workshop agenda, and we began a new experiment in how to build a series of workshops into an ongoing community activity.

The differences in workshop organization in WSSSPE2 from WSSSPE1 are in using an existing service (EasyChair) to handle submissions and reviews, rather than an ad hoc process, and using an existing service (Well Sorted) to allow collaborative grouping of papers into themes by all authors, reviewers, and the community, rather than this being done in an ad hoc manner by the organizers alone.

The fact remains that contributors also want to get credit for their participation in the process. And the workshop organizers will want to make sure that the workshop content and their efforts are recorded. Ideally, there would be a service that would index the contributions to the workshop, serving the authors, the organizers, and the larger community. Since there still isn’t such a service today, the workshop organizers are writing this initial report and making use of arXiv as a partial solution to provide a record of the workshop.

WSSSPE actively used the online social network Twitter, with hashtag “#WSSSPE”. There were substantially more tweets (messages) during the days of the workshops WSSSPE2, WSSSPE1.1, and WSSSPE1. Out of about 670 tweets as of Apr 18, 2015, more than 225 were about WSSSPE2 and about 180 were posted during the day of the workshop. Some of the main points and highlights in the meeting are shown in **Table 1**, which summarizes the top #WSSSPE tweets from the day of workshop, selected by the metrics that number of retweets or favorites larger than five and the sum of two measures greater than ten.

In terms of building community activities, we wanted to focus primarily on working groups, which we were able to do, as discussed above, but we also wanted to make sure that attendees felt they had a chance to get their ideas across to the whole group, which was the purpose of the lightning talks. Overall, this seemed to be successful at the time, in terms of both the lightning talks and the breakout

Author	Tweet	Retweets	Favorites
Neil P Chue Hong	Here's @SoftwareSaved guidance on Writing and using a software management plan used by EPSRC software grants <a href="http://www.software.ac.uk/resources/guides/software-management-plans">http://www.software.ac.uk/resources/guides/software-management-plans</a>	7	4
Neil P Chue Hong	@jameshowison as well as software plans <a href="http://www.software.ac.uk/resources/guides/software-management-plans">http://www.software.ac.uk/resources/guides/software-management-plans</a> we provide a software evaluation tool: <a href="http://www.software.ac.uk/online-sustainability-evaluation">http://www.software.ac.uk/online-sustainability-evaluation</a>	4	7
Tom Crick	56% of UK researchers develop their own software → 140, 000 UK researchers write research software w/out any formal training	14	8
Karthik Ram	OH: "Institutionalize metadata before metadata institutionalizes you"	8	6
Josh Greenberg	@jameshowison: "1. retract any paper with bitrotten dependencies" *mic drop* "2. add anyone who fixes bitrot as an author" *mic drop*	13	8
Ethan White	"@rOpenSci is all about community... our measures of success [include] how many faces are up on our community page"	9	3
Ethan White	Daniel Katz talking about implementing transitive credit for software <a href="http://arxiv.org/abs/1407.5117">http://arxiv.org/abs/1407.5117</a> Work with @arfon	9	7
Kaitlin Thaney	Great point by @tracykteal about planning for "end of life" with scientific software projects and sustainability.	4	8
Aleksandra Pawlik	Lack of training as one of the main barriers for sustainable software at @Supercomputing. @swcarpentry @datacarpentry can fix that!	10	4
Kaitlin Thaney	My slides from this morning's keynote at WSSSPE on Designing for Truth, Scale + Sustainability: <a href="http://www.slideshare.net/kaythaney/designing-for-truth-scale-and-sustainability-wssspe2-keynote">http://www.slideshare.net/kaythaney/designing-for-truth-scale-and-sustainability-wssspe2-keynote</a>	11	12
Neil P Chue Hong	@kaythaney shout out for @swcarpentry @datacarpentry @rOpenSci @stilettofiend around open training activities for sustainability	9	4
Neil P Chue Hong	For those interested in Github – Figshare/Zenodo integration, but want SWORD/DSpace/Fedora/ePrints see: <a href="http://blog.stuartlewis.com/2014/09/09/github-to-repository-deposit/">http://blog.stuartlewis.com/2014/09/09/github-to-repository-deposit/</a>	5	12
Hilmar Lapp	Re: adopting the unix philosophy, consider signing the Small Tools in Bioinformatics Manifesto: <a href="https://github.com/pjotrp/bioinformatics">https://github.com/pjotrp/bioinformatics</a>	7	6
Andre Luckow	"Traditions last not because they are excellent, but because influential people are averse to change..." C. Sunstein	12	3
Tom Crick	"Can I Implement Your Algorithm?": A Model for Reproducible Research Software <a href="http://arxiv.org/abs/1407.5981">http://arxiv.org/abs/1407.5981</a>	9	8
Mozilla Science Lab	At a loose end this Sunday? Care about reproducibility, software + #open-science? Follow the #WSSSPE hashtag for more, live from New Orleans.	10	5
Kaitlin Thaney	I'm in New Orleans at #WSSSPE, speaking at 9:50 ET on scientific software + sustainability. Tune in! Live stream: <a href="http://ustre.am/17ddh">http://ustre.am/17ddh</a>	9	9
Daniel S. Katz	#WSSSPE Agenda (Sunday): <a href="http://wssspe.researchcomputing.org.uk/wssspe2/agenda/">http://wssspe.researchcomputing.org.uk/wssspe2/agenda/</a> URL for live stream of keynotes & lightning talks: <a href="http://ustre.am/17ddh">http://ustre.am/17ddh</a>	10	1

**Table 1:** Top tweets tagged #WSSSPE on Nov 16, 2014.

groups, and the discussion of sustainability also led to interesting and useful results. However, the challenge that we have discovered since WSSSPE2 is that it is very hard to continue the breakout groups' activities. The WSSSPE2 participants were willing to dedicate their time to the groups while they were at the meeting, but afterwards, they have gone back to their (paid) jobs. We need to determine how to tie the WSSSPE breakout activities to people's jobs, so that they feel that continuing them is a higher priority than it is now, perhaps through funding the participants, or through funding coordinators for each activity, or

perhaps by getting the workshop participants to agree to a specific schedule of activities during the workshop.

### Competing Interests

The authors believe that solving the issues discussed in this paper would have beneficial impacts on the development and use of software in science and engineering, including benefits to their own institutions and careers as parts of the overall community, but other than this general interest, they declare that they have only the following competing interest: Chue Hong is Editor-in-Chief of

the Journal of Open Research Software; he did not participate in the review process for this article.

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### Appendix A. Attendees

The following is a partial list of workshop attendees who registered on the collaborative notes document [4] that was used for shared note-taking at the meeting, or who participated in a breakout groups and were noted in that group's notes.

Jordan Adams	Tulane University	Samin Ishtiaq	Microsoft Research Cambridge, UK
Alice Allen	Astrophysics Source Code Library (ASCL)	Matt Jones	University of California Santa Barbara
Gabrielle Allen	University of Illinois Urbana-Champaign	Nick Jones	New Zealand eScience Infrastructure, University of Auckland
Pierre-Yves Aquilanti	TOTAL E&P R&T USA	Daniel S. Katz	University of Chicago & Argonne National Laboratory
Wolfgang Bangert	Texas A&M University	Ian Kelley	National Evolutionary Synthesis Center (NESCent) & Duke University
David Bernholdt	Oak Ridge National Laboratory	Hilmar Lapp	University of Saarland
Jakob Blomer		Christopher Lenhardt	Louisiana State University
Carl Boettiger	University of California Santa Cruz & rOpenSci	Richard Littauer	Rutgers
Chris Bogart	ISR/CMU	Frank Löffler	Istanbul Technical University
Steven R. Brandt	Louisiana State University	Andre Luckow	University at Buffalo
Neil Chue Hong	Software Sustainability Institute & University of Edinburgh	Berkin Malkoc	The University of Texas at Austin
Tom Clune	NASA GSFC	Kyle Marcus	Indiana University
John W. Cobb		Bryan Marker	Data to Insight Center/Libraries, Indiana University
Dirk Colbry	Michigan State University	Suresh Marru	Indiana University
Karen Cranston	NESCent	Robert H. McDonald	Whitehead Institute
Tom Crick	Cardiff Metropolitan University, UK	Rupert Nash	University at Buffalo
Ethan Davis	UCAR Unidata	Andy Nutter-Upham	Software Sustainability Institute
Robert R Downs	CIESIN, Columbia University	Abani Patra	Idaho National Laboratory
Anshu Dubey	Lawrence Berkeley National Laboratory	Aleksandra Pawlik	Idaho National Laboratory
Nicole Gasparini	Tulane University, New Orleans	Cody J. Permann	University of Mississippi
Yolanda Gil	Information Sciences Institute, University of Southern California	John W. Peterson	Brigham Young University, Utah
Kurt Glaesemann	Pacific northwest national lab	Benjamin Pharr	Indiana University
Sol Greenspan	National Science Foundation	Stephen Piccolo	NCSA, University of Illinois Urbana-Champaign
Ted Habermann	The HDF Group	Marlon Pierce	Georgia State University, Atlanta
Marcus D. Hanwell	Kitware	Ray Plante	Berkeley Institute for Data Science, University of California Berkeley & rOpenSci
Sarah Harris	University of Leeds		NASA/GSFC & Rilee Systems Technologies
David Henty	EPCC, The University of Edinburgh	Sushil Prasad	Foundation for Earth Science
James Howison	University of Texas	Karthik Ram	NCEAS, Univ. California, Santa Barbara
Maxime Hughes			Michigan State University
Eric Hutton	University of Colorado	Mike Rilee	Netherlands eScience Center
Ray Idaszak	RENCI/UNC	Erin Robinson	Rice University
		Mark Schildhauer	Temple University
		Jory Schossau	University of Nottingham
		Frank Seinstra	EPCC, The University of Edinburgh
		James Shepherd	Purdue University
		Justin Shi	Imperial College London
		Ardita Shkurti	Data Carpentry
		Alan Simpson	Mozilla Science Lab
		Carol Song	NCSA, University of Illinois Urbana-Champaign
		James Spencer	University of Huddersfield
		Tracy Teal	
		Kaitlin Thaney	University of Florida/Utah State University
		Matt Turk	San Diego Supercomputer Center, University of California San Diego
		Colin C. Venters	Software Carpentry
		Nathan Weeks	
		Ethan White	
		Nancy Wilkins-Diehr	
		Greg Wilson	

## Notes

- <sup>1</sup> <http://wssspe.researchcomputing.org.uk/wssspe2/>
- <sup>2</sup> <http://sc14.supercomputing.org>
- <sup>3</sup> <http://wssspe.researchcomputing.org.uk/wssspe1/>
- <sup>4</sup> <http://wssspe.researchcomputing.org.uk/wssspe1-1/>
- <sup>5</sup> <https://conference.scipy.org/scipy2014/participate/wssspe/>
- <sup>6</sup> <http://arxiv.org>
- <sup>7</sup> <http://figshare.com>
- <sup>8</sup> <http://easychair.org/>
- <sup>9</sup> <http://www.well-sorted.org>
- <sup>10</sup> Report Blasts Problem-Plagued Cancer Research Grid, <http://tinyurl.com/maf6dz2>
- <sup>11</sup> See, for example, <http://tinyurl.com/l76tba2>.
- <sup>12</sup> Software Discovery Index, <http://softwarediscoveryindex.org/report/>
- <sup>13</sup> Bioconductor, <http://www.bioconductor.org>
- <sup>14</sup> Galaxy, <http://galaxyproject.org>
- <sup>15</sup> nanoHUB, <https://nanohub.org>
- <sup>16</sup> <http://tinyurl.com/nkn5tnv>
- <sup>17</sup> <http://tinyurl.com/ooajs7m>
- <sup>18</sup> Source: The Scientific Century, Royal Society, 2010 (revised to reflect first stage clarification from “What Do PhD’s Do?” study)
- <sup>19</sup> A few other items were suggested as barriers, but were not voted on due to lack of time in the session: layering up dependencies; using software past its sustainable life; using software past its usable life; inertia for accepted answers versus wrong or right answers; monolithic or poor code; and need to restructure code when hardware/software/libraries change
- <sup>20</sup> The Dryad Digital Repository, <http://datadryad.org>
- <sup>21</sup> Project CRediT, <http://credit.casrai.org/>
- <sup>22</sup> NIH Software Discovery Index: <http://softwarediscoveryindex.org/>
- <sup>23</sup> GitHub: <http://github.com/>
- <sup>24</sup> FigShare: <http://figshare.com/>
- <sup>25</sup> Zenodo: <http://zenodo.org/>
- <sup>26</sup> Docker: <http://www.docker.com/>
- <sup>27</sup> <http://www.software.ac.uk/resources/guides/which-journals-should-i-publish-my-software>
- <sup>28</sup> <http://openresearchsoftware.metajnl.com/about/editorialPolicies#peerReviewProcess>
- <sup>29</sup> <http://www.plosone.org/static/guidelines#software>
- <sup>30</sup> <http://www.jstatsoft.org/instructions>
- <sup>31</sup> <http://www.methodsinecologyandevolution.org/view/0/authorGuidelines.html>
- <sup>32</sup> <http://toms.acm.org/Authors.html>
- <sup>33</sup> <http://www.gigasciencejournal.com/about>
- <sup>34</sup> <http://www.ploscompbiol.org/static/guidelines#software>
- <sup>35</sup> <http://openresearchsoftware.metajnl.com/about/editorialPolicies>
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