FIRST WORKSHOP ON SUSTAINABLE SOFTWARE FOR SCIENCE: PRACTICE AND EXPERIENCES (WSSSPE): SUBMISSION AND PEER-REVIEW PROCESS, AND RESULTS

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Abstract. This technical report discusses the submission and peer-review process used by the First Workshop on on Sustainable Software for Science: Practice and Experiences (WSSSPE) and the results of that process. It is intended to record both this alternative model as well as the papers associated with the workshop that resulted from that process.

1. Introduction

The First Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE) will be held on Sunday, 17 November 2013, in conjunction with the 2013 International Conference for High Performance Computing, Networking, Storage and Analysis (SC13).

Progress in scientific research is dependent on the quality and accessibility of software at all levels and it is now critical to address many challenges related to the development, deployment, and maintenance of reusable software. In addition, it is essential that scientists, researchers, and students are able to learn and adopt software-related skills and methodologies. Established researchers are already acquiring some of these skills, and in particular a specialized class of software developers is emerging in academic environments who are an integral and embedded part of successful research teams. The WSSSPE workshop was intended to provide a forum for discussion of the challenges, including both positions and experiences. The short papers and discussion were archived to provide a basis for continued discussion, and the workshop was intended to feed into the collaborative writing of one or more journal publications.

2. Submissions

The workshop call for paper included:

In practice, scientific software activities are part of an ecosystem where key roles are held by developers, users, and funders. All three groups supply resources to the ecosystem, as well as requirements that bound it. Roughly following the example of NSF’s Vision and Strategy for Software (http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf12113), the ecosystem may be viewed as having challenges related to:

• the development process that leads to new software
  – how fundamental research in computer science or science/engineering domains is turned into reusable software
  – software created as a by-product of research

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http://wssspe.researchcomputing.org.uk
http://sc13.supercomputing.org
impact of computer science research on the development of scientific software
- the support and maintenance of existing software, including software engineering
  - governance, business, and sustainability models
  - the role of community software repositories, their operation and sustainability
- the role of open source communities or industry
- use of the software
  - growing communities
  - reproducibility, transparency needs that may be unique to science
- policy issues, such as
  - measuring usage and impact
  - software credit, attribution, incentive, and reward
  - career paths for developers and institutional roles
  - 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
- education and training

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, the organizers wanted to make submission as easy as possible. The call for papers stated:

We invite short (4-page) position/experience reports that will be used to organize panel and discussion sessions. These papers will be archived by a third-party service, and provided 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. An interactive site will be created to link these papers and the workshop discussion, with options for later comments and contributions. Contributions will be peer-reviewed for relevance and originality before the links are added to the workshop site; contributions will also be used to determine discussion topics and panelists. We will also plan one or more papers to be collaboratively developed by the contributors, based on the panels and discussions.

58 submissions were received, and almost all submitters used either arXiv\(^3\) or figshare\(^4\) to self-publish their papers.

3. Peer-Review

A peer review process followed the submissions, where the 58 papers received 181 reviews, an average of 3.12 reviews per paper. Reviews were completed using a Google form, which allowed reviewers to provide scores on relevance and comments to the organizers, which were used to decide which papers to associate with the workshop, and comments to the authors, which were provided back to the authors to allow them to improve their papers.

The organizers decided to list 54 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 papers were also grouped into 3 areas, each of which will be associated with a panel and discussion at the workshop.

4. Results

The contributed papers that will be discussed at the workshop follow, listed by area.

\(^3\)http://arxiv.org
\(^4\)http://figshare.com
4.1. Developing, Deploying and Supporting Software.

4.1.1. Development Experiences.

- Mark C. Miller, Lori Diachin, Satish Balay, Lois Curfman McInnes, Barry Smith. Package Management Practices Essential for Interoperability: Lessons Learned and Strategies Developed for FASTMath [35]
- Karl W. Broman, Thirteen years of R/qtl: Just barely sustainable [4]
- Charles R. Ferenbaugh, Experiments in Sustainable Software Practices for Future Architectures [19]
- Eric G Stephan, Todd O Elsethagen, Kerstin Kleese van Dam, Laura Riihimaki. What Comes First, the OWL or the Bean? [44]
- Derek R. Gaston, John Peterson, Cody J. Permann, David Andrs, Andrew E. Slaughter, Jason M. Miller, Continuous Integration for Concurrent Computational Framework and Application Development [21]
- Anshu Dubey, B. Van Straalen. Experiences from Software Engineering of Large Scale AMR Multiphysics Code Frameworks [17]
- Markus Blatt. DUNE as an Example of Sustainable Open Source Scientific Software Development [3]
- David Koop, Juliana Freire, Cláudio T. Silva, Enabling Reproducible Science with VisTrails [31]
- Sean Ahern, Eric Brugger, Brad Whitlock, Jeremy S. Meredith, Kathleen Biagas, Mark C. Miller, Hank Childs, VisIt: Experiences with Sustainable Software [11]
- Sou-Cheng (Terrya) Choi. MINRES-QLP Pack and Reliable Reproducible Research via Staunch Scientific Software [9]
- Michael Crusoe, C. Titus Brown. Walking the talk: adopting and adapting sustainable scientific software development processes in a small biology lab [15]
- Dhabaleswar K. Panda, Karen Tomko, Karl Schulz, Amitava Majumdar. The MVAPICH Project: Evolution and Sustainability of an Open Source Production Quality MPI Library for HPC [38]
- Eric M. Heien, Todd L. Miller, Becky Gietzel, Louise H. Kellogg. Experiences with Automated Build and Test for Geodynamics Simulation Codes [25]

4.1.2. Deployment, Support, and Maintenance of Existing Software.

- Henri Casanova, Arnaud Giersch, Arnaud Legrand, Martin Quinson, Frédéric Suter. SimGrid: a Sustained Effort for the Versatile Simulation of Large Scale Distributed Systems [8]
- Erik Trainer, Chalalai Chaithirunkarn, James Herbsleb. The Big Effects of Short-term Efforts: A Catalyst for Community Engagement in Scientific Software [49]
- Jeremy Cohen, Chris Cantwell, Neil Chue Hong, David Moxey, Malcolm Illingworth, Andrew Turner, John Darlington, Spencer Sherwin. Simplifying the Development, Use and Sustainability of HPC Software [12]
- Jaroslav Slawinski, Vaidy Sunderam. Towards Semi-Automatic Deployment of Scientific and Engineering Applications [43]

4.1.3. Best Practices, Challenges, and Recommendations.

- Andreas Plić, James B. Procter. Ten Simple Rules for the Open Development of Scientific Software [42]
- Anshu Dubey, S. Brandt, R. Brower, M. Giles, P. Hovland, D. Q. Lamb, F. Loffler, B. Norris, B. O’Shea, C. Rebbi, M. Snir, R. Thakur, Software Abstractions and Methodologies for HPC Simulation Codes on Future Architectures [16]
- Jeffrey Carver, George K. Thiruvathukal. Software Engineering Need Not Be Difficult [7]
- Craig A. Stewart, Julie Wernert, Eric A. Wernert, William K. Barnett, Von Welch. Initial Findings from a Study of Best Practices and Models for Cyberinfrastructure Software Sustainability [45]
4.2. Policy.

4.2.1. Modeling Sustainability.

- Coral Calero, M. Angeles Moraga, Manuel F. Bertoa. Towards a Software Product Sustainability Model [6]
- Colin C. Venters, Lydia Lau, Michael K. Griffiths, Violeta Holmes, Rupert R. Ward, Jie Xu. The Blind Men and the Elephant: Towards a Software Sustainability Architectural Evaluation Framework [51]
- Marlon Pierce, Suresh Marru, Chris Mattmann. Sustainable Cyberinfrastructure Software Through Open Governance [40]
- Daniel S. Katz, David Proctor. A Framework for Discussing e-Research Infrastructure Sustainability [20]
- Christopher Lenhardt, Stanley Ahalt, Brian Blanton, Laura Christopherson, Ray Idaszak. Data Management Lifecycle and Software Lifecycle Management in the Context of Conducting Science [32]
- Nicholas Weber, Andrea Thomer, Michael Twidale. Niche Modeling: Ecological Metaphors for Sustainable Software in Science [52]

4.2.2. Credit, Citation, Impact.

- Matthew Knepley, Jed Brown, Lois Curfman McInnes, Barry Smith. Accurately Citing Software and Algorithms Used in Publications [30]
- Jason Priem, Heather Piwowar. Toward a comprehensive impact report for every software project [11]
- Daniel S. Katz. Citation and Attribution of Digital Products: Social and Technological Concerns [28]
- Neil Chue Hong, Brian Hole, Samuel Moore. Software Papers: improving the reusability and sustainability of scientific software [11]

In addition, the following paper from another area will also be discussed in this area.

- Frank Lößler, Steven R. Brandt, Gabrielle Allen and Erik Schnetter. Cactus: Issues for Sustainable Simulation Software [33]

4.2.3. Reproducibility.

- Victoria Stodden, Sheila Miguez. Best Practices for Computational Science: Software Infrastructure and Environments for Reproducible and Extensible Research [46]

4.2.4. Implementing Policy.

- Randy Heiland, Betsy Thomas, Von Welch, Craig Jackson. Toward a Research Software Security Maturity Model [26]
- Brian Blanton, Chris Lenhardt. A User Perspective on Sustainable Scientific Software [2]
- Daisie Huang, Hilmar Lapp. Software Engineering as Instrumentation for the Long Tail of Scientific Software [27]
- Rich Wolski, Chandra Krintz, Hiranya Jayathilaka, Stratos Dimopoulos, Alexander Pucher. Developing Systems for API Governance [54]

4.3. Communities.
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- L. Christopherson, R. Idaszak, S. Ahalt. Developing Scientific Software through the Open Community Engagement Process [10]
- Reagan Moore. Extensible Generic Data Management Software [36]
- Karen Cranston, Todd Vision, Brian O’Meara, Hilmar Lapp. A grassroots approach to software sustainability [14]
- J.-L. Vay, C. G. R. Geddes, A. Koniges, A. Friedman, D. P. Grote, D. L. Bruhwiler. White Paper on DOE-HEP Accelerator Modeling Science Activities [50]
- Marlon Pierce, Suresh Marru, Mark A. Miller, Amit Majumdar, Borries Demeler. Science Gateway Operational Sustainability: Adopting a Platform-as-a-Service Approach [39]
- Lynn Zentner, Michael Zentner, Victoria Farnsworth, Michael McLennan, Krishna Madhavan, and Gerhard Klimeck, nanoHUB.org: Experiences and Challenges in Software Sustainability for a Large Scientific Community [55]
- Andy Terrel. Sustaining the Python Scientific Software Community [48]
- Frank Löffler, Steven R. Brandt, Gabrielle Allen and Erik Schnetter. Cactus: Issues for Sustainable Simulation Software [33]
- Ketan Maheshwari, David Kelly, Scott J. Krieder, Justin M. Wozniak, Daniel S. Katz, Mei Zhi-Gang, Mainak Mookherjee. Reusability in Science: From Initial User Engagement to Dissemination of Results [34]
- Nancy Wilkins-Diehr, Katherine Lawrence, Linda Hayden, Marlon Pierce, Suresh Marru, Michael McLennan, Michael Zentner, Rion Dooley, Dan Stanzione. Science Gateways and the Importance of Sustainability [59]
- Edmund Hart, Carl Boettiger, Karthik Ram, Scott Chamberlain. rOpenSci – a collaborative effort to develop R-based tools for facilitating Open Science [24]

In addition, the following paper from another area will also be discussed in this area.
- Marcus Hanwell, Amita Perera, Wes Turner, Patrick O’Leary, Katie Osterdahl, Bill Hoffman, Will Schroeder. Sustainable Software Ecosystems for Open Science [23]

4.3.2. Industry & Economic Models.
- Anne C. Elster. Software for Science: Some Personal Reflections [18]
- Ian Foster, Vas Vasiadiis, Steven Tuecke. Software as a Service as a path to software sustainability [20]
- Marcus Hanwell, Amita Perera, Wes Turner, Patrick O’Leary, Katie Osterdahl, Bill Hoffman, Will Schroeder. Sustainable Software Ecosystems for Open Science [23]

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- Andy Terrel. Sustaining the Python Scientific Software Community [48]

4.3.3. Education & Training.
- Ivan Girotto, Axel Kohlmeyer, David Grellscheid, Shawn T. Brown. Advanced Techniques for Scientific Programming and Collaborative Development of Open Source Software Packages at the International Centre for Theoretical Physics (ICTP) [22]
- Thomas Crawford. On the Development of Sustainable Software for Computational Chemistry [14]

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5. Conclusions

The WSSSPE workshop has begun an experiment in how we can collaboratively build a workshop agenda. However, contributors also want to get credit for their participation in the process. And the workshop organizers want to make sure that the workshop content and their efforts are recorded. Ideally, there would be a service that would be able to index the contributions to the workshop, serving the authors, the organizers, and the larger community. But since there 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.

After the workshop, one or more additional papers will be created that will include the discussions at the workshop. These papers will likely have many authors, and may be submitted to peer-reviewed journals.

REFERENCES

[1] Sean Ahern, Eric Brugger, Brad Whitlock, Jeremy S. Meredith, Kathleen Biagas, Mark C. Miller, and Hank Childs. VisIt: Experiences with sustainable software. Technical Report 1309.1796, arXiv, 2013. http://arxiv.org/abs/1309.1796
[2] Brian Blanton and Christopher Lenhardt. A user perspective on sustainable scientific software. Technical Report 789028, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.789028
[3] Makus Blatt. DUNE as an example of sustainable open source scientific software development. Technical Report 1309.1783, arXiv, 2013. http://arxiv.org/abs/1309.1783
[4] Karl W. Broman. Thirteen years of r/qtl: Just barely sustainable. Technical Report 1309.1192, arXiv, 2013. http://arxiv.org/abs/1309.1192
[5] Jed Brown, Matthew Knepley, and Barry Smith. Run-time extensibility: anything less is unsustainable. Technical Report 791571, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.791571
[6] Coral Calero, M. Angeles Moraga, and Manuel F. Bertoa. Towards a software product sustainability model. Technical Report 1309.1640, arXiv, 2013. http://arxiv.org/abs/1309.1640
[7] Jeffrey C. Carver and George K. Thiruvathukal. Software engineering need not be difficult. Technical Report 830442, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.830442
[8] Henri Casanova, Arnaud Giersch, Arnaud Legrand, Martin Quinson, and Frédéric Suter. SimGrid: a sustained effort for the versatile simulation of large scale distributed systems. Technical Report 1309.1630, arXiv, 2013. http://arxiv.org/abs/1309.1630
[9] Sou-Cheng T. Choi. MINRES-QLP Pack and reliable reproducible research via staunch scientific software. Technical Report 791562, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.791562
[10] Laura Christopherson, Ray Idaszak, and Stan Ahalt. Developing scientific software through the open community engagement process. Technical Report 790723, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.790723
[11] Neil Chue Hong, Brian Hole, and Samuel Moore. Software papers: improving the reusability and sustainability of scientific software. Technical Report 795303, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.795303
[12] Jeremy Cohen, Chris Cantwell, Neil Chue Hong, David Moxey, Malcolm Illingworth, Andrew Turner, John Darlington, and Spencer Sherwin. Simplifying the development, use and sustainability of HPC software. Technical Report 1309.1101, arXiv, 2013. http://arxiv.org/abs/1309.1101
[13] Karen Cranston, Todd Vision, Brian O’Meara, and Hilmar Lapp. A grassroots approach to software sustainability. Technical Report 790739, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.790739
[14] T. Daniel Crawford. On the development of sustainable software for computational chemistry. Technical Report 790757, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.790757.

[15] Michael Crusoe and C. Titus Brown. Walking the talk: adopting and adapting sustainable scientific software development processes in a small biology lab. Technical Report 791567, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.791567.

[16] A. Dubey, S. Brandt, R. Brower, M. Giles, P. Hovland, D.Q. Lamb, F. Löffler, B. Norris, B. OShea, C. Rebbi, M. Snir, and R. Thakur. Software abstractions and methodologies for HPC simulation codes on future architectures. Technical Report 1309.1780, arXiv, 2013. http://arxiv.org/abs/1309.1780.

[17] A. Dubey and B. Van Straalen. Experiences from software engineering of large scale AMR multiphysics code frameworks. Technical Report 1309.1781, arXiv, 2013. http://arxiv.org/abs/1309.1781.

[18] Anne C. Elster. Software for science: Some personal reflections. Technical Report 1309.2357, arXiv, 2013. http://arxiv.org/abs/1309.2357.

[19] Charles R. Ferenbaugh. Experiments in sustainable software practices for future architectures. Technical Report 1309.1428, arXiv, 2013. http://arxiv.org/abs/1309.1428.

[20] Ian Foster, Vas Vasiliadis, and Steven Tuecke. Software as a service as a path to software sustainability. Technical Report 791604, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.791604.

[21] Derek R. Gaston, John Peterson, Cody J. Pernamb, David Andrés, Andrew E. Slaughter, and Jason M. Miller. Continuous integration for concurrent computational framework and application development. Technical Report 790755, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.790755.

[22] Ivan Girotto, Axel Kohlmeyer, David Grellscheid, and Shawn T. Brown. Advanced techniques for scientific programming and collaborative development of open source software packages at the ICTP. Technical Report 796439, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.796439.

[23] Marcus Hanwell, Anitha Perera, Wes Turner, Patrick O'Leary, Katie Osterdahl, Bill Hoffman, and Will Schroeder. Sustainable software ecosystems for open science. Technical Report 790756, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.790756.

[24] Edmund Hart, Carl Boettiger, Karthik Ram, and Scott Chamberlain. ropensci - a collaborative effort to develop r-based tools for facilitating open science. Technical Report 791569, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.791569.

[25] Eric M. Heien, Todd L. Miller, Becky Gietzel, and Louise H. Kellogg. Experiences with automated build and test for geodynamics simulation codes. Technical Report 1309.1199, arXiv, 2013. http://arxiv.org/abs/1309.1199.

[26] Randy Heiland, Betsy Thomas, Von Welch, and CraigJackson. Toward a research software security maturity model. Technical Report 1309.1787, arXiv, 2013. http://arxiv.org/abs/1309.1787.

[27] Daisie Huang and Hilmar Lapp. Software engineering as instrumentation for the long tail of scientific software. Technical Report 791560, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.791560.

[28] Daniel S. Katz. Citation and attribution of digital products: Social and technological concerns. Technical Report 791606, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.791606.

[29] Daniel S. Katz and David Proctor. A framework for discussing e-research infrastructure sustainability. Technical Report 790767, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.790767.

[30] Matthew G. Knepley, Jed Brown, Lois Curfman McInnes, and Barry Smith. Accurately citing software and algorithms used in publications. Technical Report 785731, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.785731.

[31] David Koop, Juliana Freire, and Cláudio T. Silva. Enabling reproducible science with VisTrails. Technical Report 1309.1784, arXiv, 2013. http://arxiv.org/abs/1309.1784.

[32] Christopher Lenhardt, Stanley Ahalt, Brian Blanton, Laura Christopherson, and Ray Idaszak. Data management lifecycle and software lifecycle management in the context of conducting science. Technical Report 791561, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.791561.

[33] Frank Löffler, Steven R. Brandt, Gabrielle Allen, and Erik Schnetter. Cactus: Issues for sustainable simulation software. Technical Report 1309.1812, arXiv, 2013. http://arxiv.org/abs/1309.1812.

[34] Ketan Maheshwari, David Kelly, Scott J. Krieder, Justin M. Wozniak, Daniel S. Katz, Mei Zhi-Gang, and Mainak Mookherjee. Reusability in science: From initial user engagement to dissemination of results. Technical Report 1309.1813, arXiv, 2013. http://arxiv.org/abs/1309.1813.

[35] Mark C. Miller, Lori Diachin, Satish Balay, Lois Curfman McInnes, and Barry Smith. Package management practices essential for interoperability: Lessons learned and strategies developed for fastmath. Technical Report 789055, figshare, 2013. http://dx.doi.org/10.6084/m9.figshare.789055.

[36] Reagan W. Moore. Extensible generic data management software. Technical Report 1309.5372, arXiv, 2013. http://arxiv.org/abs/1309.5372.

[37] National Science Foundation. A vision and strategy for software for science, engineering, and education: Cyberinfrastructure framework for the 21st century, 2012. NSF 12-113, http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf12113.
