WSSSPE3 Working Groups

Best Practices in Developing Sustainable Software

Sandra Gesing

Software Sustainability Education Governance Impact Science Working towards Sustainable Software for Science Careers Practice and Experiences Incentives Training Research WSSSPE Communities Development Policy Reuse Engineering

https://github.com/WSSSPE/WG-Best-Practices

BEST PRACTICES FOR DEVELOPING SUSTAINABLE SCIENTIFIC SOFTWARE

SANDRA GESING⁽¹⁾, ABANI PATRA⁽²⁾, DANIEL S. KATZ⁽³⁾, KYLE E. NIEMEYER⁽⁴⁾, SURESH MARRU⁽⁵⁾, DAN GUNTER⁽⁶⁾, TOM CRICK⁽⁷⁾, JEFFREY C. CARVER⁽⁸⁾,

2. Related Work

***Note: Leading author for Case Studies: ..., contributors: Kyle Niemyer (PeTSC)...

3. Case Studies

***Note: Leading author for Community Related Practices: ..., contributors: ...

4. Community-related Practices

***Note: Leading author for Government and Management: ..., contributors: ...

5. Government and Management

***Note: Leading author for Funding: ..., contributors: ...

6. Funding

***Note: Leading author for Metrics: Dan Katz, contributors: ...

7. Metrics

***Note: Leading author for Tools: ..., contributors: ...

8. Tools

9. CONCLUSION

Acknowledgments

Funding Research Programmer Expertise

James Hetherington

List of Research Software Groups

- Most Research Software Engineers are employed as Research Associates on individual research projects.
- But we are particularly interested in the ways in which research organisations bring research programmers together into larger teams.
- See http://www.rse.ac.uk/international.html
- Send a pull request to <u>https://github.com/UKRSE/UKRSE.github.io/blob/master/internation</u> <u>al.md</u>

Transition Pathways to Sustainable Software: Industry & Academic Collaboration

Nic Weber (Daniel S. Katz)

Transition Pathways: Industry & Academia

- Goal: better understand successful pathways for scientific software to "transition" from grant-funded research projects to industry sponsorship
 - Some software projects will begin their life being sponsored by industry, or result in collaboration between industry and academia
 - In such cases, there is still a need to understand how IP and how maintenance of the software is sustained over time
- Activities: Examine previous case studies; understand what has worked and not worked, and why; build generalized framework, including pathways other than academia→ industry
- Output: white paper
- Status: needs funded effort

Principles for Software Engineering Design for Sustainable Software

Colin Venters (Daniel S. Katz)

Principles for software engineering

- Ideas:
 - Principles for software engineering form the basis of methods, techniques, methodologies and tools
 - However, there is often a mismatch between software engineering theory and practice particularly in the fields of computational science and engineering, which can lead to the development of unsustainable software
 - Understanding and applying software engineering principles is essential in order to create and maintain sustainable software
- Discussion focused on identifying existing principles of software engineering design that could be adopted by the computational science and engineering communities.

Principles for Sustainable Software Actions

- Start with principles from the Karlskrona Manifesto on Sustainability Design, Tate (Sustainable Software Development: An Agile Perspective), and the Software Engineering Body of Knowledge (SWEBOK), then
- (1) Systematically analyze a number of example systems from different scientific domains with regards to the identified principles
- (2) Identify the commonalities and gaps in applying those principles to different scientific systems
- (3) Propose a set of guidelines on the principles and examine how they exemplarily apply to scientific software systems
- Preliminary work will be carried out through undergraduate or postgraduate student projects.

Useful Metrics for Scientific Software

Gabrielle Allen

Motivation

- No commonly used standard for collecting or presenting metrics
- No common set of metrics for research/scientific software
- No consensus on the value of metrics

Software Sustainability Education Governance Science Working towards Sustainable Software for Science Careers Practice and Experiences Incentives Research WSSSPE Communities Development Policy Reuse Engineering

WSSSPE4, September 12-14, Manchester, UK

WSSSPE3 Metric Group

- Collected and discussed related activities
- Formulated plan for surveying NSF SI2 PI community
- Made outline for white paper
 - Stalled, restart here?

WSSSPE4, September 12-14, Manchester, UK

WSSSPE4, September 12-14, Manchester, UK

Software Sustainability Education Governance Science Working towards Sustainable Software for Science Careers Practice and Experiences Incentives Research WSSSPE Communities Development Policy Reuse Engineering

Progress and Plans

- Progress:
 - SI2 initial survey completed
 - Emily Chen, Ray Idaszak, Dan Katz, Gabrielle Allen (Lightening Talk)
- Obstacles:
 - time and dedicated effort, would benefit from funding to engage e.g. graduate student with relevant interest and background
- Moving Forward:
 - Given results of initial survey, potentially expand or reformulate
 - Revisit white paper concept
 - Brainstorm funding possibilities or how to bring more effort



WSSSPE4, September 12-14, Manchester, UK

Training

Nick Jones (Daniel S. Katz)

Training

- Lots of groups providing elements of training for sustainable software
- Possible need for coordination
- Goal: Create a community of training organizations
- Via an initial physical or virtual workshop
 - And then later regular meetings
- Status: No progress, needs a champion with available time
 - And interest of groups in coordinating is partially assumed and partially unclear

Software Credit

Kyle Niemeyer

WSSSPE3 Software Credit Working Group

- Aim: ensure developers of scientific software receive credit for their efforts, like authors of scientific papers
 - First: standardize software citations
- At WSSSPE3: discussed related efforts, first on contribution taxonomy/dividing credit but mostly software citation
 - Discussion on standardized metadata needed for citation
 - Mechanism for citing software in publications
 - Indexing of software citations

WSSSPE3 Software Credit Working Group

- Done since: joined FORCE11 Software Citation Working Group: <u>https://www.force11.org/group/software-citation-working-group</u>
- Wrote software citation principles: Smith AM, Katz DS, Niemeyer KE, FORCE11 Software Citation Working Group. (2016) Software Citation Principles. *PeerJ Preprints* 4:e2169v4 <u>https://doi.org/10.7287/peerj.preprints.2169v4</u>
- Obstacles: community acceptance. Indexing of citations.
- Goal for WSSSPE4: shift focus back to credit

Publishing Software

Steve Brandt

Executable Papers/Journals

- 1. Verifiable
- 2. Mini Laboratories
- 3. Executable journals could be written around a framework
- 4. More Understandable No missing steps
- 5. More Metadata
- 6. More interaction/Upvotes?
- Effort to shine a light on existing efforts: https://www.software.ac.uk/resources/guides/where-can-i-publishexecutable-papers



Wallpaper from http://www.jasperfforde.com

Building Sustainable Communities

Dan Gunter & Ethan Davis (Daniel S. Katz)

User Communities

- User communities are lifeblood of sustainable scientific software; include
 - Developers, both internal and external
 - Users
 - Other software projects that depend on the software
 - Other groups that create or consume data that is specific to the software
- These groups provide:
 - Reason for sustaining the software
 - Requirements that drive its continued evolution and improvement

User Communities

- Working Group discussion:
 - What practices and circumstances may lead to having and maintaining a community?
 - How can funding help or hinder this process?
 - How can best practices be described and distilled into a document that can help new projects?
- Plans:
 - Create best practices document
 - Train software projects about best practices
- Status:
 - No progress; champion with available time needed