

# Better Scientific Software https://bssw.io

So your code will see the future.

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December 6, 2017

In webinar series: Best Practices for HPC Software Developers



## Better Scientific Software (BSSw)

Scientific software has emerged as an essential discipline in its own right. Because computational models, computer architectures, and scientific software projects have become extremely complex, the Computational Science & Engineering (CSE) community now has a unique opportunity-and an implicit mandate-to address pressing challenges in scientific software productivity, quality, and sustainability.

## https://bssw.io

Collaborative content development on general topics topics related to developer productivity and software sustainability for CSE

We want and *need* contributions from the community ... Join us!

2

Site Overview

Intro To CSE

Intro To HPC



## Dedicated to improving developer productivity and software sustainability for CSE

## https://bssw.io

- New <u>community-based resource</u> for scientific software improvement exchange
- Clearinghouse to gather, discuss, and disseminate experiences, techniques, tools, and other resources to improve software productivity and sustainability for computational science and engineering (CSE)

## Goals:

- Raise awareness of the importance of good software practices to scientific productivity and to the quality and reliability of computationally-based scientific results
- Raise awareness of the increasing challenges facing CSE software developers as high-end computing heads to extreme scales

## Site users can:

- Find information on scientific software topics
- Propose to curate or create new content based on their own experiences. The backend enables collaborative content development using standard GitHub tools and processes.

## **BSSw** site history ... And an invitation: Join us!

- BSSw site launch at SC17
  - BOF on Software Engineering and Reuse in Computational Science and Engineering
    - <u>https://swe-cse.github.io/2017-11-sc17-bof</u>
- Seeking contributions from the international CSE community
  - Researchers, practitioners, and stakeholders from national laboratories, academic institutions, and industry ... share your resources, experiences, etc.
- Over time: Collaborate to build the site to a vibrant community resource
  - Content and editorial processes provided by volunteers throughout the CSE community
  - We need your contributions!

## Initiative of the IDEAS Software Productivity Project

- Support from DOE Office of Advanced Scientific Computing Research, DOE Exascale Computing Project
- Thank you to DOE program mangers Thomas Ndousse-Fetter, Paul Bayer, and David Lesmes for encouragement and support





Site snapshot: Content organized in 6 categories

# Resources For Developer Productivity And Software Sustainability

#### Better Planning

Strategies for planning in order to improve software productivity, quality, and sustainability.

#### Better Development

Aspects of scientific software development that should be systematically addressed in order to improve software productivity, quality, and sustainability.

#### Better Performance

Approaches for developing code that is efficient, scalable, and portable—from laptops to emerging extreme-scale architectures.

#### Better Reliability

Methods for testing and verification to ensure that software is robust and produces reliable results.

#### Better Collaboration

Ways to facilitate and distribute work across teams, promote partnerships via software, and contribute to stronger communities.

#### Better Skills

Ways to improve productivity and sustainability from an individual perspective.

# **Resource topics**

#### **Better Performance:**

- High-performance computing
- Performance at LCFs
- Performance portability



#### Personal productivity and sustainability **Better Planning: Online** learning Requirements Performance Design . Planning Skills Software **Software** interoperability **Productivity & Better Collaboration: Sustainability Better Development:** Licensing • Strategies for more effective **Documentation** ٠ Collaboration **Development** Version control teams Reliability Funding sources and programs Configuration and builds ٠ Projects and organizations Deployment Software publishing and citation Issue tracking **Better Reliability:** Discussion forums, Q&A sites Refactoring Testing Software engineering Continuous integration testing **Development tools** Reproducibility

Debugging

**Better Skills:** 

Site content spans a broad range of topics.

## **Resource examples**

**Curated links:** A brief article that highlights other web-based articles or content. Your article should describe why the CSE community might find value.

## An Introduction To Software Licensing

Share f 🎔 in %

This tutorial provides a brief introduction to software copyright and licensing for researchers in computational science and engineering. Explains the difference between closed and open source software, and copyleft and permissive open source licenses. Outlines a variety of factors researchers might want to consider when selecting a software license. Provides links to some key web resources as a starting point for deeper exploration.

#### Prerequisites

#### What Is Software Intellectual Property?

PUBLISHED JUNE 20, 2017 CONTRIBUTOR DAVID BERNHOLDT

Tutorial presented at SIAM CSE17: CSE Collaboration through Software: Improving Productivity and Sustainability.

A recording of this tutorial presentation is available at https://www.pathlms.com/siam/courses /4150/sections/5826/video\_presentations/42639

https://bssw.io/resources/an-introduction-to-software-licensing

## Planning For Better Software: PSIP Tools

Share f 🍠 in 🗞

Scientific software teams are typically focused on the creation of a new set of features that will enable the next set of computational experiments. Teams seldom have the time to stop development and focus solely on improving productivity or sustainability. However, teams can incorporate improvements *on the way* to developing new science capabilities.

#### Prerequisites

#### **CSE Software Requirements?**

#### What Are Strategies For More Effective Teams?

PUBLISHED NOVEMBER 21, 2017 CONTRIBUTOR MIKE HEROUX

The Productivity and Sustainability Improvement Planning (PSIP) process recognizes that productivity and sustainability improvements for scientific software benefit from an incremental, iterative approach. The PSIP-Tools GitHub repo is a collection of documents that enable the adoption and use of PSIP for a software team. The PSIP-Tools repo contains everything from a template for the first introduction letter to a complete interview guide, interview prompts and expected timeline.

The PSIP process has been successfully used to help scientific software teams acheive incremental, sustainable process improvement, while still achieving their science goals.

#### https://bssw.io/resources/planning-for-better-software-psip-tools

### **Communities Overview**

The Better Scientific Software umbrella encompasses a rich variety of communities who are working to advance the methods, practices, and processes of CSE software.



Community-specific landing pages, tailored to unique perspectives and priorities, provide a variety of starting points for using the BSSw site and promote a shared understanding of CSE software issues. Curators of a community landing page can customize content to serve the needs community members through highlighted resources and other custom content.

#### Better Scientific Software Communities:

- Exascale Computing Community
- Scientific Libraries Community
- Community of Supercomputing Facilities and Their Users
- Software Engineering Community
- Environmental System Science Community

We want your input and perspectives. Please contact us if you would like to start a community-specific landing page.

# Community landing pages

Infor	mation For 🔺	Contribute To BSSw	Receive	Our Email D	)igest
>	Environment Community	al System Science		out	Q
>	Exascale Cor	mputing Community			
>	Scientific Lib	oraries Community			×

Featured Resources for the Environmental System Science Community

Planning For Better Software: PSIP Tools TOPICS REQUIREMENTS AND STRATEGIES FOR MORE EFFECTIVE TEAM

Test Driven Development In Scientific Software: A Survey

TOPICS TESTING, RELIABILITY, AND REPRODUCIBILITY

# **BSSw current status**

- BSSw site now includes a sampling of resources
  - But many topics need content!
- Current site is a starting point for **CSE community collaboration** to share information on developer productivity and software sustainability
- Over time, build up rich content resources



#### Contributors

We thank all BSSw contributors for sharing information and perspectives on issues in software productivity and sustainability.

Below is an alphabetized list of contributors thus far. We welcome your input to the site, too; see Contribute to BSSw for information on how to get started



Github profile pics

and links of all

go here.

site contributors

















9

## We want and *need* contributions scientific software from the community .... Join us!

• "What Is" document: Define terms and concepts in a particular topic area.



- "How To" document: A document that describes a process for improving productivity and sustainability.
- **Original experience:** An original article to inform the CSE community about how to improve developer productivity and software sustainability.
- **Blog article:** An original article in the form of a blog of 250 500 words. We will solicit contributions from thought leaders in the community and welcome proposals from anyone.
- **Curated links:** A brief article that highlights other webbased articles or content. Your article should describe why the CSE community might find value.
- **Event:** A brief description of an event relevant to better scientific software.

### **In-scope Content**

- General issues in productivity and sustainability that overlap with common challenges faced in the CSE software community.
- General tools for productivity and sustainability that can be widely used by CSE developers.
- Characterization of challenges and solutions that may be particularly valuable to the CSE community.

## **Highlight Connections to CSE**

- How your topic intersects with themes that are of particular interest to CSE, for example MPI, Fortran, C++, architectures, modeling and simulation.
- Why your topic could be of particular interest to CSE.

### Ease of Adoption and Use

- Address how easy or hard it is to benefit from your topic.
- Address who would be particularly interested in the topic.



# Promoting collaborative content creation through Github back-end

## **BSSw Software Platform**

Component		Frontend	
Technology	Google Docs	GitHub	<b>Ruby on Rails</b>
Location	Google Drive	betterscientificsoftware GitHub organization	https://bssw.io
Purpose	<ul> <li>Rapid collaborative content development</li> <li>Multi-user typing, suggest edits, comments</li> </ul>	<ul> <li>Content creation, refinement, management (from Google Drive)</li> <li>Content packaging for use with bssw.io</li> </ul>	<ul> <li>User-facing portal</li> <li>Polished backend content</li> <li>Blogs</li> <li>Mailing lists</li> </ul>
Contributors	Community subject matter experts	Community subject matter experts, BSSw staff	BSSw staff. Web development experts
Consumers	BSSw GitHub Backend	BSSw Frontend	CSE community
Content Notes	Content migrates to GitHub after it stabilizes	Content managed in git repos, markdown	Content from Backend

**Contribute!** Share your insights on CSE software practices and processes:

- https://github.com/betterscientificsoftware/betterscientificsoftware.github.io/blob/master/README.md
- Or search "github betterscientificsoftware"

11

# https://bssw.io: Site details

- Site content (backend): Managed using a public GitHub repository
  - Enables a growing community of content contributors using <u>Markdown</u> files; ensures site history and version control
- Frontend: A custom <u>Ruby on Rails</u> content management system automatically imports, updates, and formats content from GitHub
- Images: Optimized using <u>Cloudinary</u>; the <u>Bootstrap 3.0</u> framework is used in displaying the site across all browsers and devices
- Partnership:
  - <u>IDEAS project team</u>: Conceived of the site, oversaw its creation and production. The team continues to curate site content, with growing participation from the broader CSE community.
  - <u>Sandbox Studio, Chicago</u>: Visual brand, interface design, site strategy
    - Sandbox Studio is an interactive design, UX, branding, and web development firm
    - Erica Dreisbach assisted Sandbox in front-end development
  - Parallactic Consulting: Custom content management system and GitHub integration developed with Ruby on Rails
    - Parallactic is a small web development & data architecture company

# We need your input! Contribute to BSSw!





## Site: https://github.com/betterscientificsoftware/betterscientificsoftware.github.io

14



**Goal:** Foster and promote practices, processes, and tools to improve developer productivity and software sustainability of scientific codes.

**Application process:** Includes the proposal of a funded activity that promotes better scientific software.

**Awards:** We select three Fellows\* per year. Each Fellow is awarded up to \$10,000 for an activity that promotes better scientific software. Activities can include organizing a workshop, preparing a tutorial, or creating content to engage the scientific software community.



15

# **BSSw Fellowship application process**

# We are looking for applications from people with the following characteristics:

- Passionate about scientific software.
- Interested in contributing powerful ideas, tools, methodologies, and more that improve the quality of scientific software.
- Able to use the fellowship to broadly benefit the scientific software community.
- Willing to participate as an alum in subsequent years to guide selection of future fellows and promote better scientific software in their community.

Jan 5, 2018: Application deadline

BSSw Fellowship Application Form

#### **Question Summary**

## **Experience:**

- Describe your work relevant to scientific software (1000 1500 characters).
- Describe your background and experience relevant to being a BSSw Fellow (1000 1500 characters).

## **Proposed work and impact:**

- What would you do as a BSSw Fellow? (1000 1500 characters).
- What impact do you foresee from your efforts? (1000 1500 characters).



# Screen-shots from Github walk-through, done live during webinar.

# What to contribute: Content types

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GitHub, Inc.

Developer productivity and software sustainability efforts for computational science and engineering (CSE) benefit from communicating the experiences, reasoned insights, and curated content from a broad spectrum of community members.

Content Types

Types of content can include:

- "What Is" document: A document that defines terms and concepts in a particular topic area. For example, the article
  could describe terms and concepts related to automated testing. This kind of document is often helpful as
  background for "How To" documents that describe testing processes.
  - folder: Articles
- "How To" document: A document mat describes a process for improving productivity and sustainability.
  - folder: Articles
- Original experience: An original article (brevity is appreciated) to inform the CSE community about how to improve developer productivity and software sustainability.

• folder: Articles

• Blog article: An original article in the form of a blog of 250 - 500 words. We will solicit contributions from thought leaders in the community and welcome proposals from anyone.

folder: Articles/Blog

- Curated links: A brief article that highlights other web-based articles or content. Your article should describe why the CSE community might find value in the linked content.
  - folder: CuratedContent
- Event: A brief description of an event (such as a workshop, conference, or tutorial) relevant to better scientific software.

folder: Events

Content Scope

The exact scope of relevant content will evolve as we learn about community interests. However, presently we believe the following guidelines should be useful:

Several types of contributions can be made, from original content articles, to blogs, to pointers for other content you find useful.

Events announcements are also welcome.

# What to contribute: Content scope

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#### **Content Scope**

The exact scope of relevant content will evolve as we learn about community interests. However, presently we believe the following <u>guidelines</u> should be useful:

GitHub, Inc.

#### In scope Content

- General issues in productivity and sustainability that overlap with common challenges faced in the CSE software community.
- . General tools for productivity and sustainability that can be widely used by CSE developers.
- Characterization of challenges and solutions that may be particularly valuable to the CSE community.

#### **Highlight Connections to CSE**

- How your topic intersects with themes that are of particular interest to CSE, for example MPI, Fortran, C++, architectures, modeling and simulation.
- Why your topic could be of particular interest to CSE.

#### Ease of Adoption and Use

- Address how easy or hard it is to benefit from your topic.
- Address who would be particularly interested in the topic.

#### **Out-of-scope Content**

- Narrow scope, focused on a particular CSE subcommunity.
- Tools, processes and practices that have little in common with CSE.
- Content that is deemed incomplete or biased, as determined by the BSSW leaders.

#### Qoes your idea seem to fic?

If you have an idea that might work, continue to the How To Contribute page.

We are looking for content that has CSE focus, is accessible and generally helpful. Before investing in writing a lot of content, open a GitHub Issue describing what you want to do.

## How to contribute: Pre-steps

ability to work with the website as a Citi tub repository, and the possibility to create scripting tools that can extract, create and test content in this repository, we encourage contributors to the BSSw project to use the following processes.

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#### Before creating your content

- 1. Is your content a good fit? If you have doubts, please see What To Contribute. If you are still unsure, contact the DSSw team.
- 2. Ready to contribute? Please set up a GitHub Issue (New to GitHub Issues? See this intro):
- 3. Go to the BSSw GitHub Issues page.
- 4. Tap on green New issue button.
- 5. Enter a descriptive title and a longer comment about the work you will do.
- 6. (BSSw non-members) Wait for confirmation from the BSSw team that your proposed contribution is a good fit. Once this is confirmed, continue to Create Your Contribution.
- 7. (2SSw members)
- 8. If you have site permissions, you can assign the issue to yourself or someone else.
- 9. Assign appropriate labels. Common choices are:

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- blog Tell us what is on your mind about Better Scientific Software. Keep it short and to the point.
- curated link Did you find an article you want to share with the BSSw community? Describe it and include a link.
- howto Did you write instructions for how to accomplish a useful task? Write a How To.
- short article Like a blog, but more fact than experience.
- what is A What Is describes terms and concepts, especially useful as background for a How To.
- event A workshop, tutorial, conference, or other event with activities related to software productivity and sustainability.
- 1. Assign issue to a milestone, if you want to commit to a deadline.
- 2. Create your contribution!

20 Create Your Contribution

Before investing in writing a lot of content, open a GitHub Issue describing what you want to do.

# How to contribute: Creating content



BSSw content creation is possible with any standard Git/GitHub workflow. Most content is in markdown (.md files). The GitHub web portal is very useful for this kind of writing.

#### Style Guide

See the BSSw Style Guide for guidance on naming conventions, descriptive text, and metadata.

## Example: Contribute "Team of Teams": Find a similar article

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I want to create a curated article, briefly describing the "Team of Teams" content collection. This article is similar in type to a curated article on Google's High Performance Teams, located in the *CuratedContent* folder.

Also, a generic starting point for curated articles is: *ResourceTemplate.Basic.md* 

2 days ago

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When viewing the article you want to use as a template, select *Raw* as the viewing mode. This mode will show the markdown text and some important meta-data that we use to construct the bssw.io website.

# Raw: GoogleHighPerfTeams.md

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<pre># High Performing Teams at Google What makes for a high performing team? [This interv Performing Teams at Google") of [Matt Sakaguchi](htt lists items that have little to do with technical to structure &amp; clarity, meaning and impact. #### Contributed by [Mike Heroins](https://github.com &lt;1 Publish: yes</pre>	view podcast](https://www.infoq.com/podcasts/ tps://qconsf.com/sf2016/sf2016/users/matt-sak opics and everything to do with people and cu n/maherou)	matt-sakaguchi aguchi.html "} lture: psychol	article text. You can use it as a reference for how to format links, create bold and italics text, and format the meta-data (see next box).
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# Create markdown file: TeamOfTeams.md

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# **TeamOfTeams preview**



#### Team of Teams: Strategies for large organizations

Numerous CSE projects (The DOE Exascale Computing Project, Square Kilometer Array, Blue Brain Project and Energy Exascale Earth System Model - Formerly ACME to name a few) are large, hierarchical organizations that produce and manage scientific software in a complex environment. The Team of Teams body of work provides a collection of books, online resources and lectures on concepts and strategies for this kind of project. A first resource from this collection is the book Team of Teams: New Rules of Engagement for a Complex World

Key concepts include the goals of:

- Shared consciousness: Establishing a common conceptual model and big picture understanding of the comprehensive project.
- Empowered execution: Fostering authority of sub-teams and individuals to act without explicit senior leadership consultation. These resources can be useful for anyone engaged in large projects where requirements are multiscale and emergent or, in other words, complex.

#### **Contributed by Mike Heroux**

## **Propose new file**



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## High Performing Teams At Google

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What makes for a high performing team? This interview podcast of Matt Sakaguchi from Google lists items that have little to do with technical topics and everything to do with people and culture: psychological safety, dependability, structure & clarity, meaning and impact.

#### Prerequisites

#### What Are Strategies For More Effective Teams?

PUBLISHED JUNE 20, 2017 CONTRIBUTOR MIKE HEROUX

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New resource for TeamOfTeams.md will also appear on the frontend, after the webinar demo.

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