Better Scientific Software

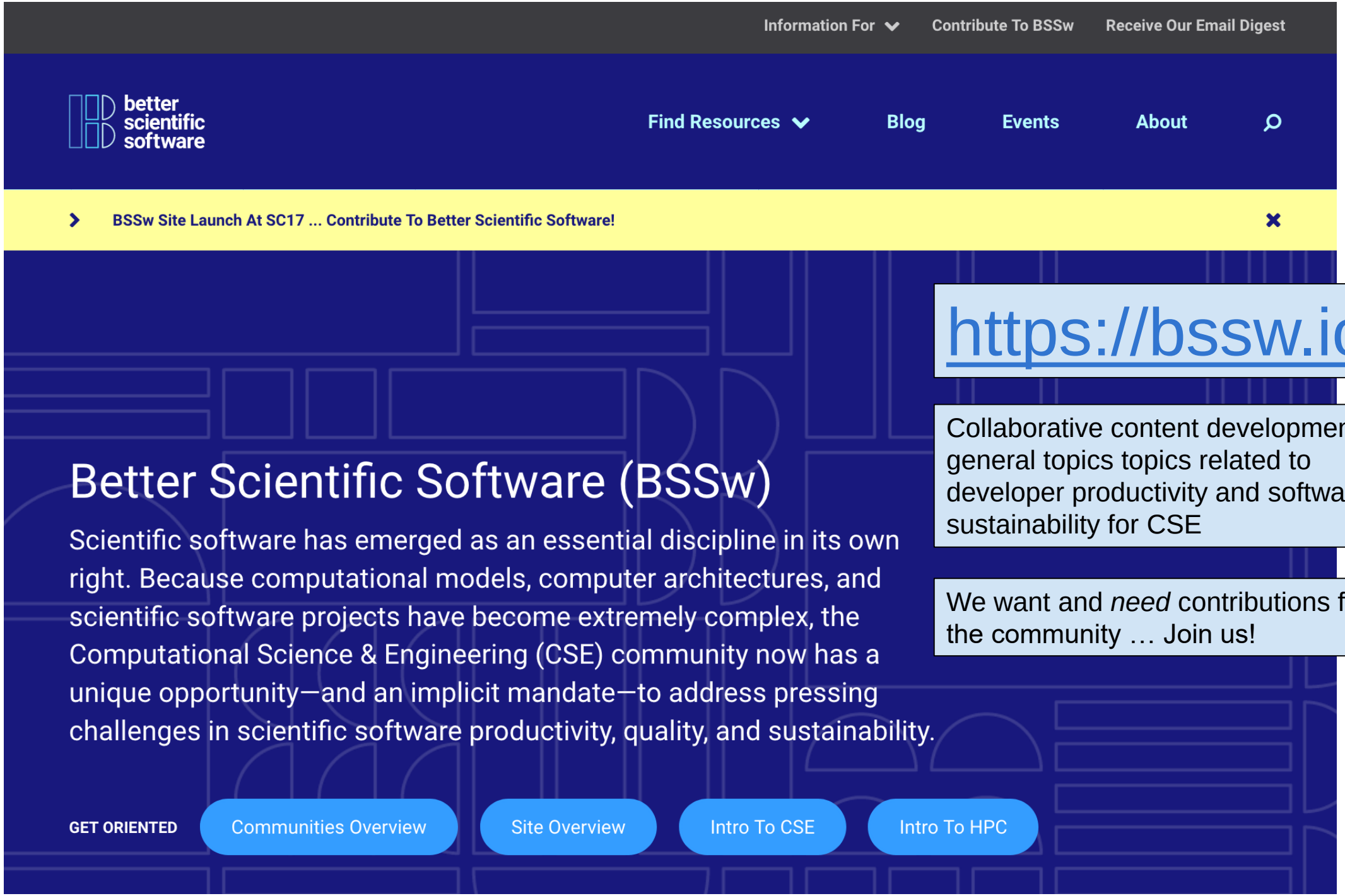
https://bssw.io

So your code will see the future.

Mike Heroux (SNL) and Lois Curfman McInnes (ANL)

December 6, 2017

In webinar series: Best Practices for HPC Software Developers



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!

Dedicated to improving developer productivity and software sustainability for CSE

https://bssw.io

- **New community-based resource 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***
    - https://swe-cse.github.io/2017-11-sc17-bof
- **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

U.S. DEPARTMENT OF ENERGY | Office of Science

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.

View All Resources

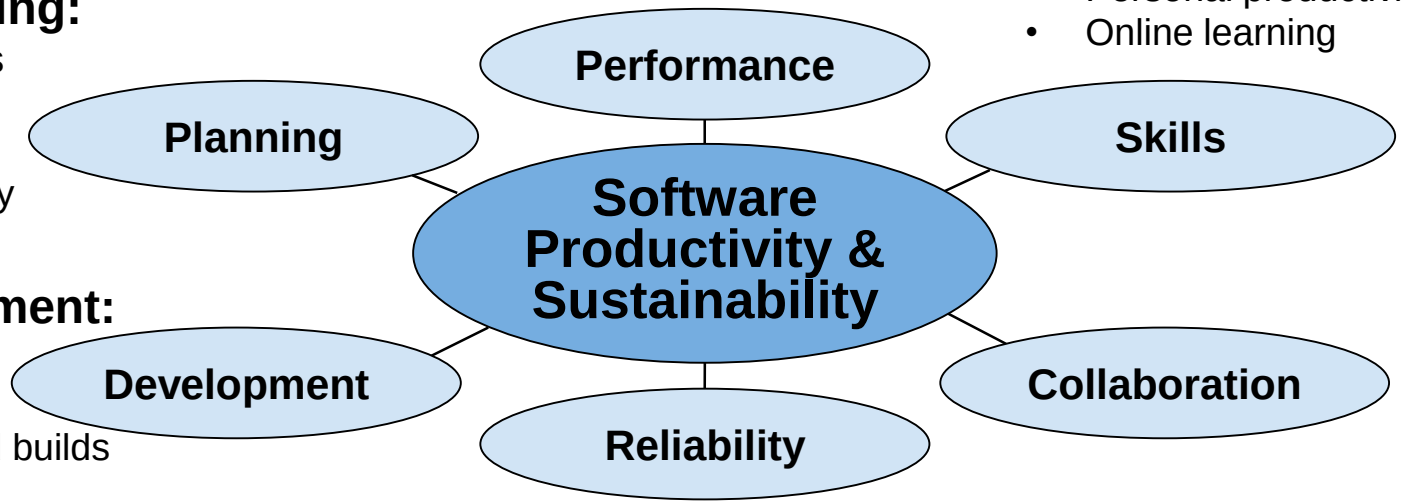
Resource topics

better scientific software

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

Better Planning:
- Requirements
- Design
- Software interoperability

Better Skills:
- Personal productivity and sustainability
- Online learning



Better Development:
- Documentation
- Version control
- Configuration and builds
- Deployment
- Issue tracking
- Refactoring
- Software engineering
- Development tools

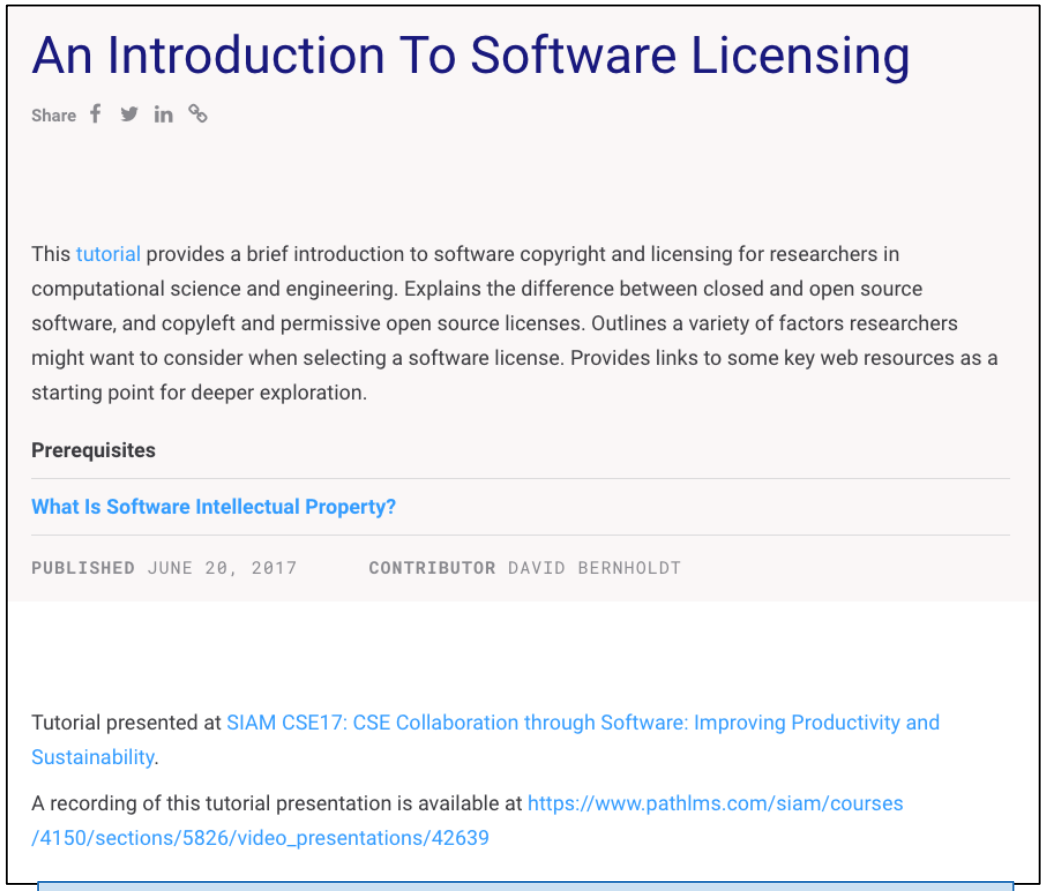
Better Collaboration:
- Licensing
- Strategies for more effective teams
- Funding sources and programs
- Projects and organizations
- Software publishing and citation
- Discussion forums, Q&A sites

Better Reliability:
- Testing
- Continuous integration testing
- Reproducibility
- Debugging

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

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

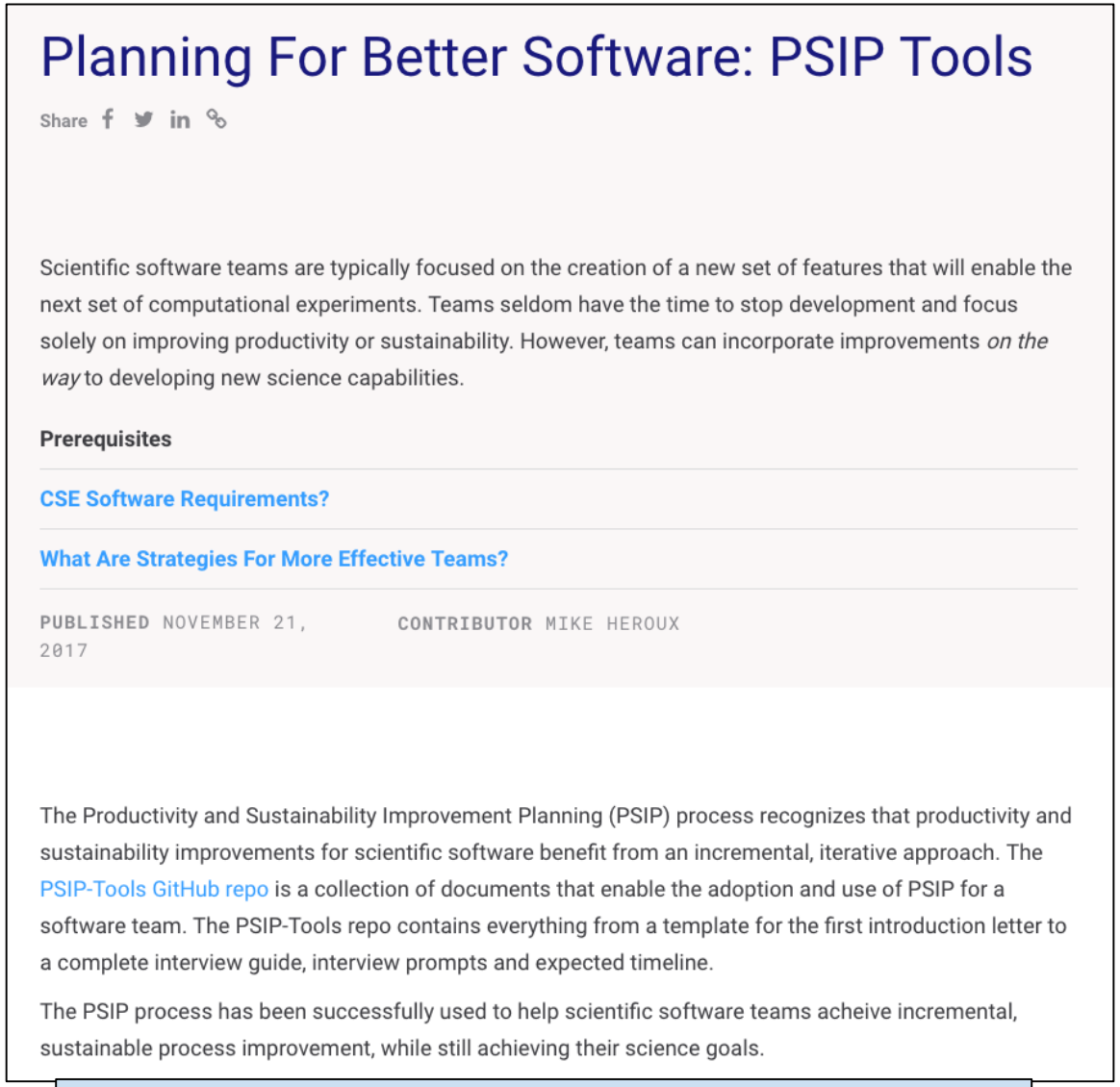
What Is Software Intellectual Property?

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

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?

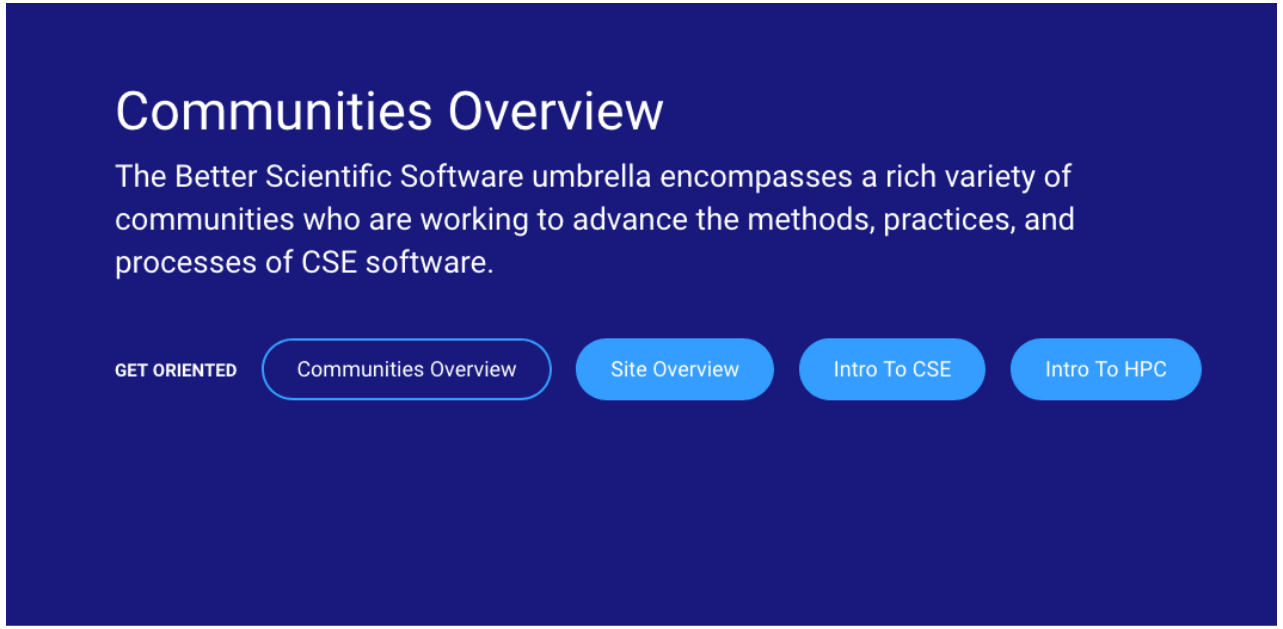
PUBLISHED NOVEMBER 21, 2017 CONTRIBUTOR MIKE HEROUX

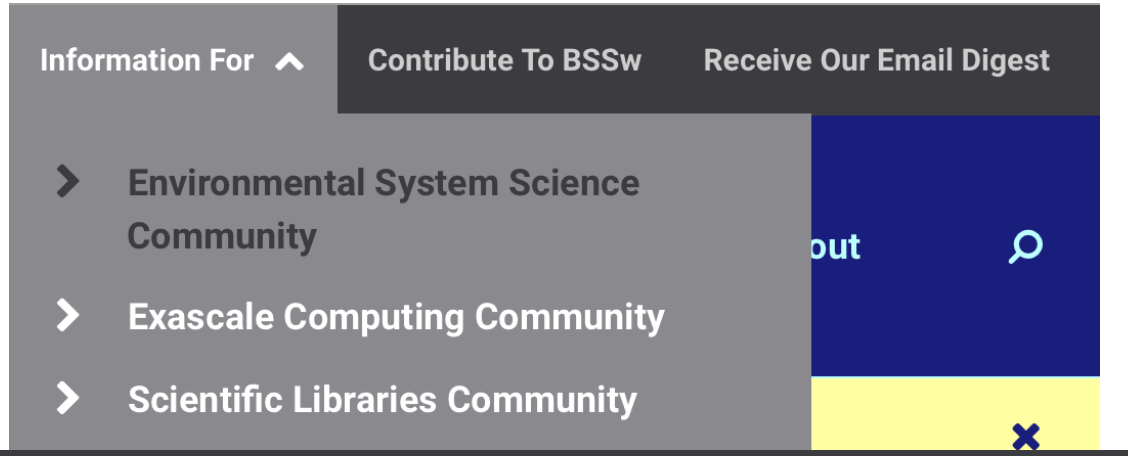
The Productivity and Sustainability Improvement Planning (PSIP) process recognizes that productivity and sustainability improvements for scientific software benefit from an incremental, iterative approach. The PSIP-Tools GitHub repo is a collection of documents that enable the adoption and use of PSIP 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

Community landing pages



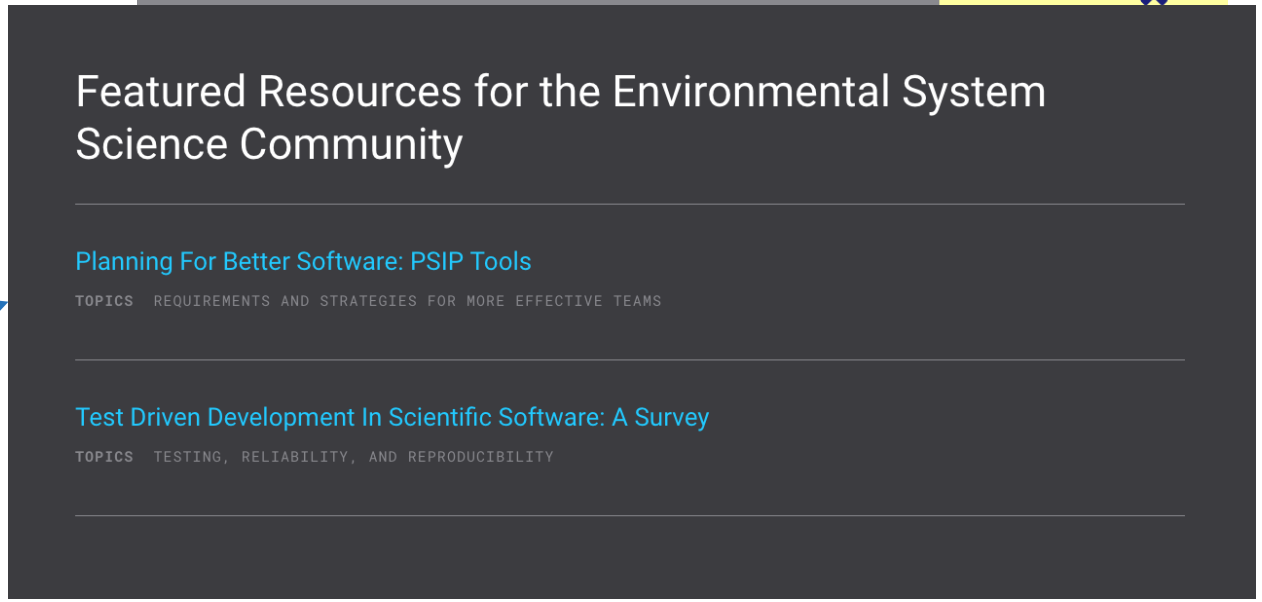


Community-specific landing pages, tailored to unique perspectives and priorities, provide a variety of starting points for using the BSSw site and promote a shared understanding of CSE software issues. Curators of a community landing page can customize content to serve the needs community members through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

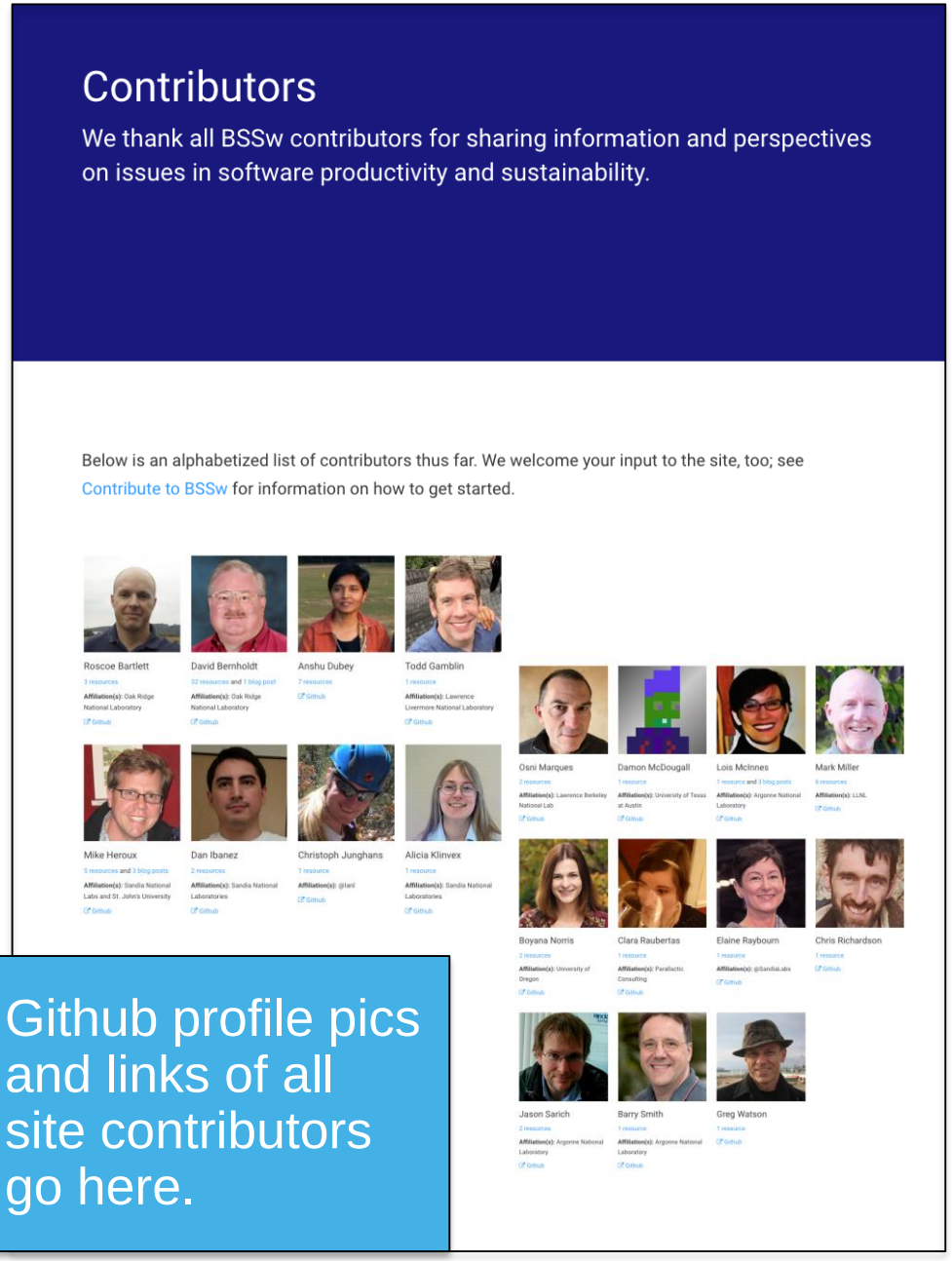
We want your input and perspectives. Please contact us if you would like to start a community-specific landing page.



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

We need your contributions!



Github profile pics and links of all site contributors go here.

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

Types of Content

- **"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 web-based 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	**Backend**		**Frontend**
Technology	**Google Docs**	**GitHub**	**Ruby on Rails**
Location	Google Drive	betterscientificsoftware GitHub organization	https://bssw.io
Purpose	• Rapid collaborative content development • Multi-user typing, suggest edits, comments	• Content creation, refinement, management (from Google Drive) • Content packaging for use with bssw.io	• User-facing portal • Polished backend content • Blogs • Mailing lists
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

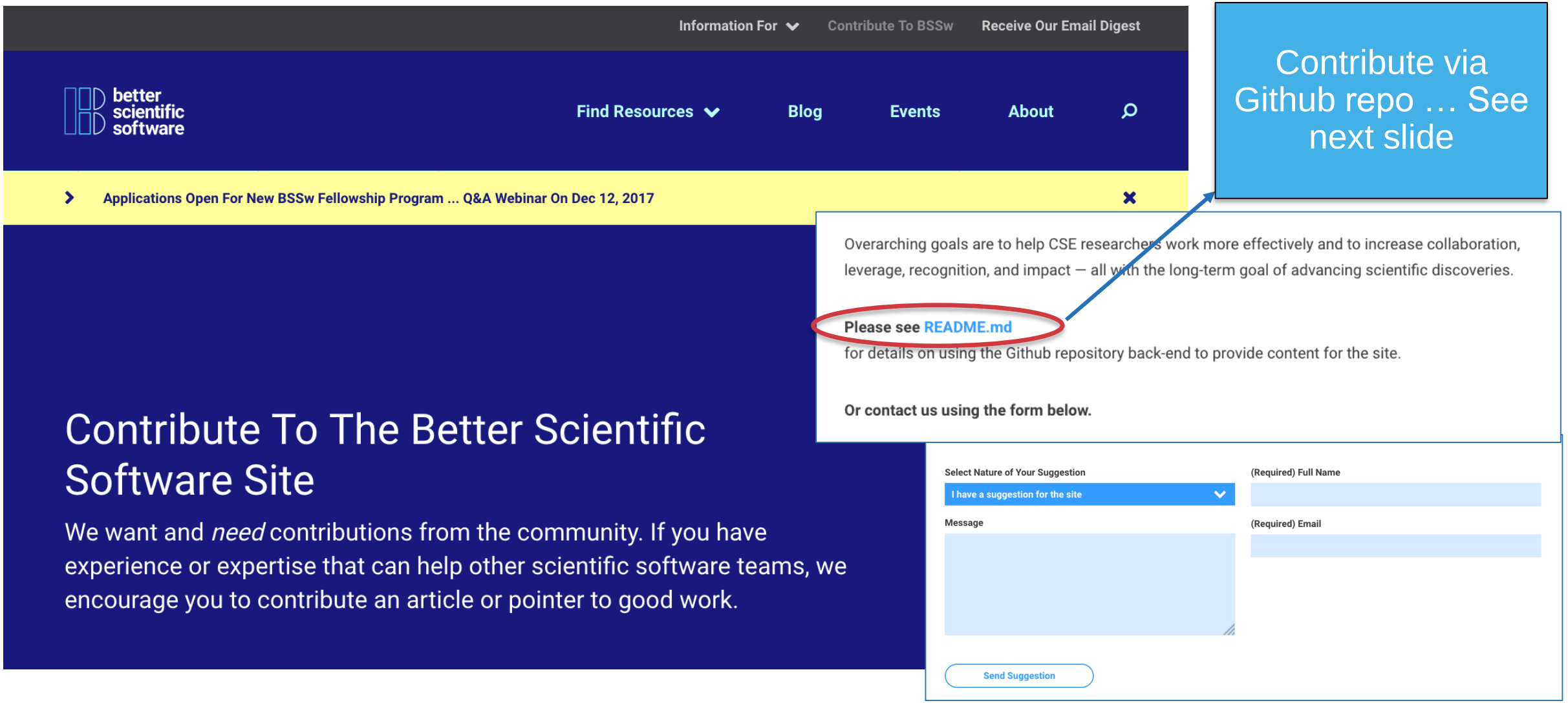
Contribute! Share your insights on CSE software practices and processes:

- https://github.com/betterscientificsoftware/betterscientificsoftware.github.io/blob/master/README.md
- Or search “github **b**etter**s**cientific**s**oftware”

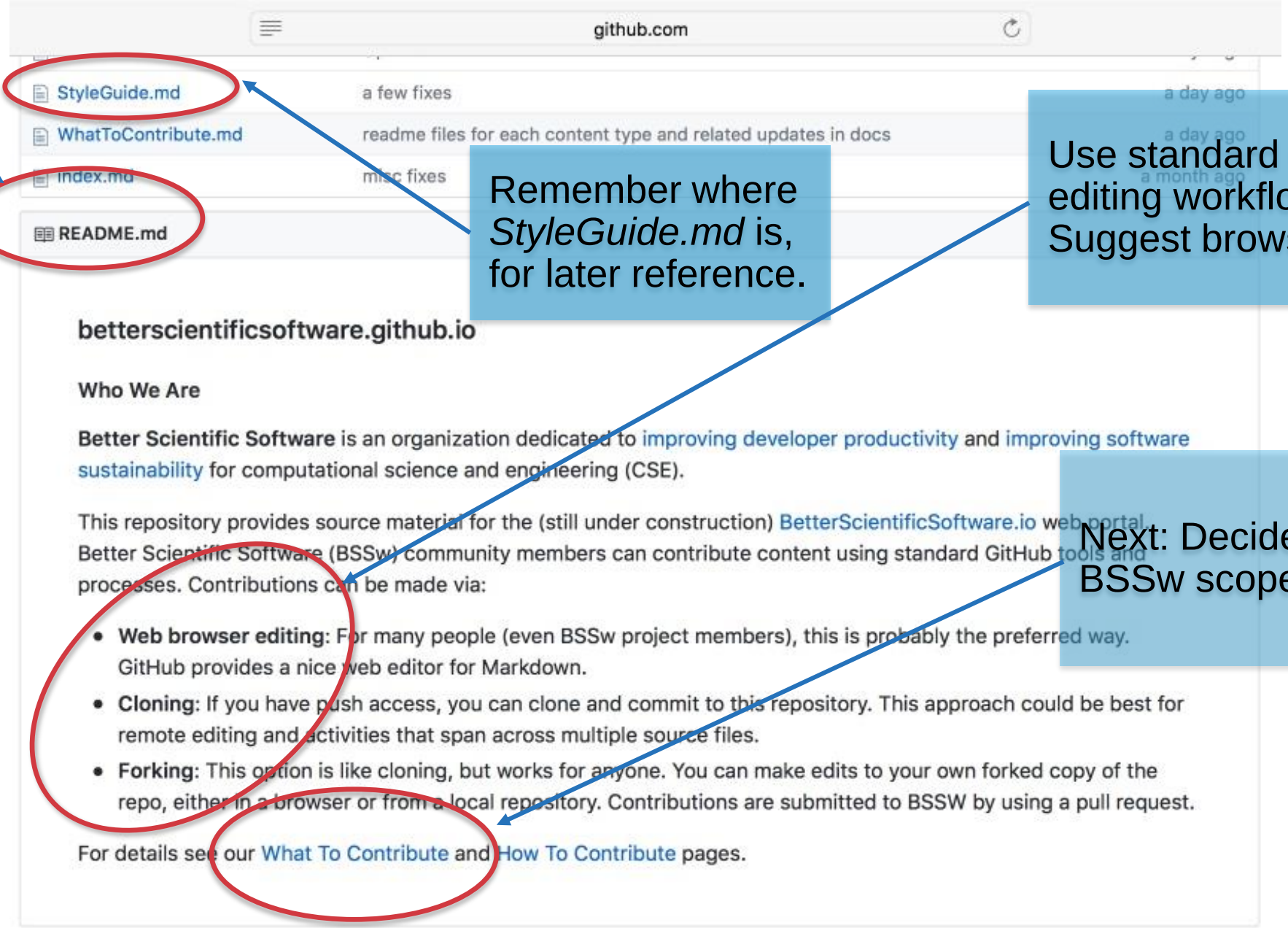
https://bssw.io: Site details

- **Site content (backend):** Managed using a public GitHub repository
  - Enables a growing community of content contributors using Markdown files; ensures site history and version control
- **Frontend:** A custom Ruby on Rails content management system automatically imports, updates, and formats content from GitHub
- **Images:** Optimized using Cloudinary; the Bootstrap 3.0 framework is used in displaying the site across all browsers and devices
- **Partnership:**
  - IDEAS project team: Conceived of the site, oversaw its creation and production. The team continues to curate site content, with growing participation from the broader CSE community.
  - Sandbox Studio, Chicago: 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!



Start Here



Remember where *StyleGuide.md* is, for later reference.

Use standard GitHub editing workflows. Suggest browser editing.

Next: Decide if idea fits BSSw scope.

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

BSSw Fellowship Program

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.

* BSSw Fellows must be affiliated with a U.S.-based institution that is able to receive funding from the U.S. Department of Energy.

Details: https://bssw.io … Click on ***BSSw Fellowship Program*** … in the footer area

Coming soon …

Timeline

- **Dec 12, 2017, 4:30 pm EST:** Fellowship webinar, Q&A. Subscribe to the BSSw mailing list to be notified about details
- **Jan 5, 2018:** Application deadline
- **Jan 12, 2018:** Notification of 2018 BSSw Fellows
- **Feb 6 - 8, 2018:** Fellows announced at DOE ECP Annual Meeting in Knoxville, TN
- **Feb 2018 – Jan 2019:** Period of performance for 2018 BSSw Fellows

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).

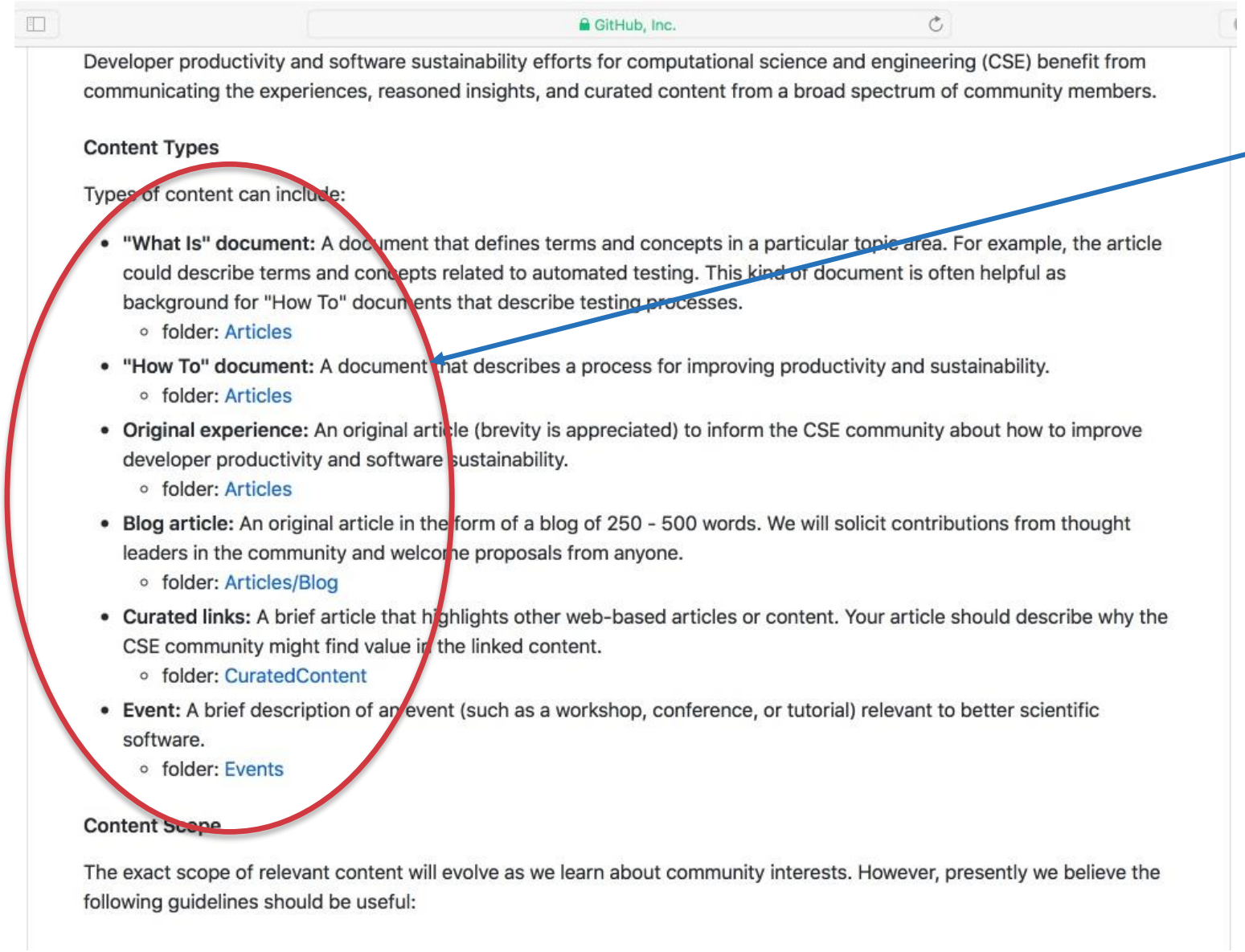
Proposed work and impact:

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

Appendix:

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

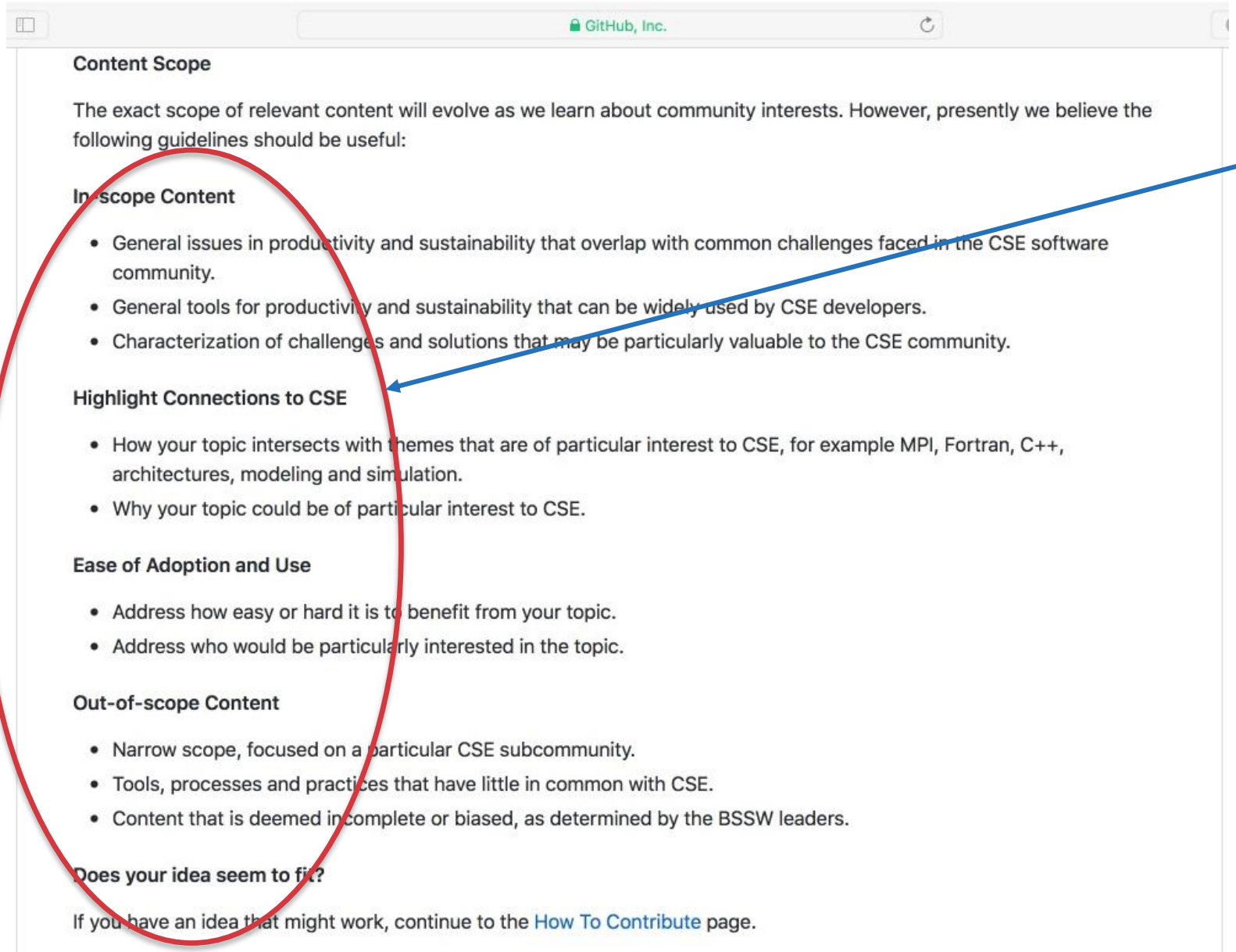
What to contribute: Content types



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

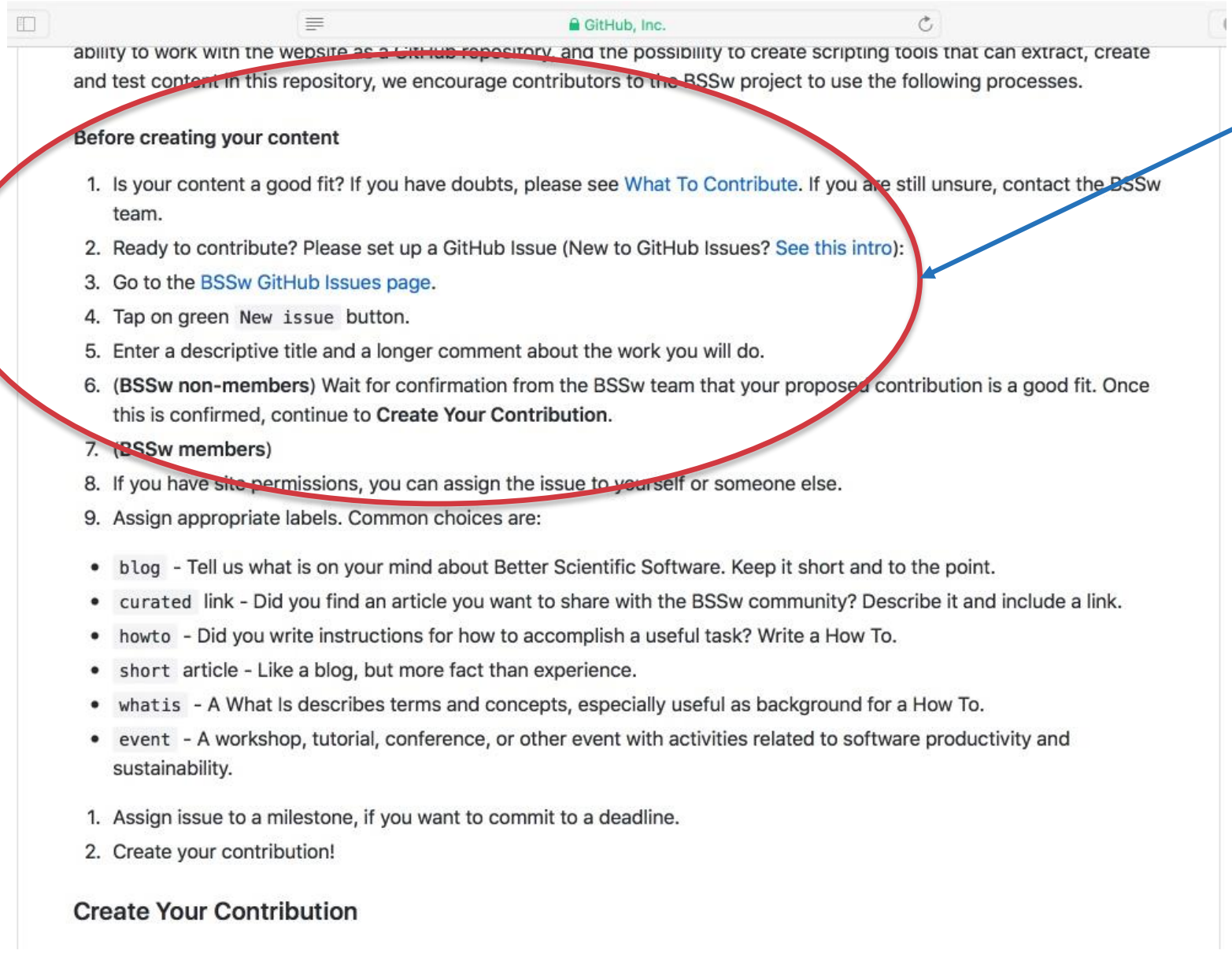
Events announcements are also welcome.

What to contribute: Content scope



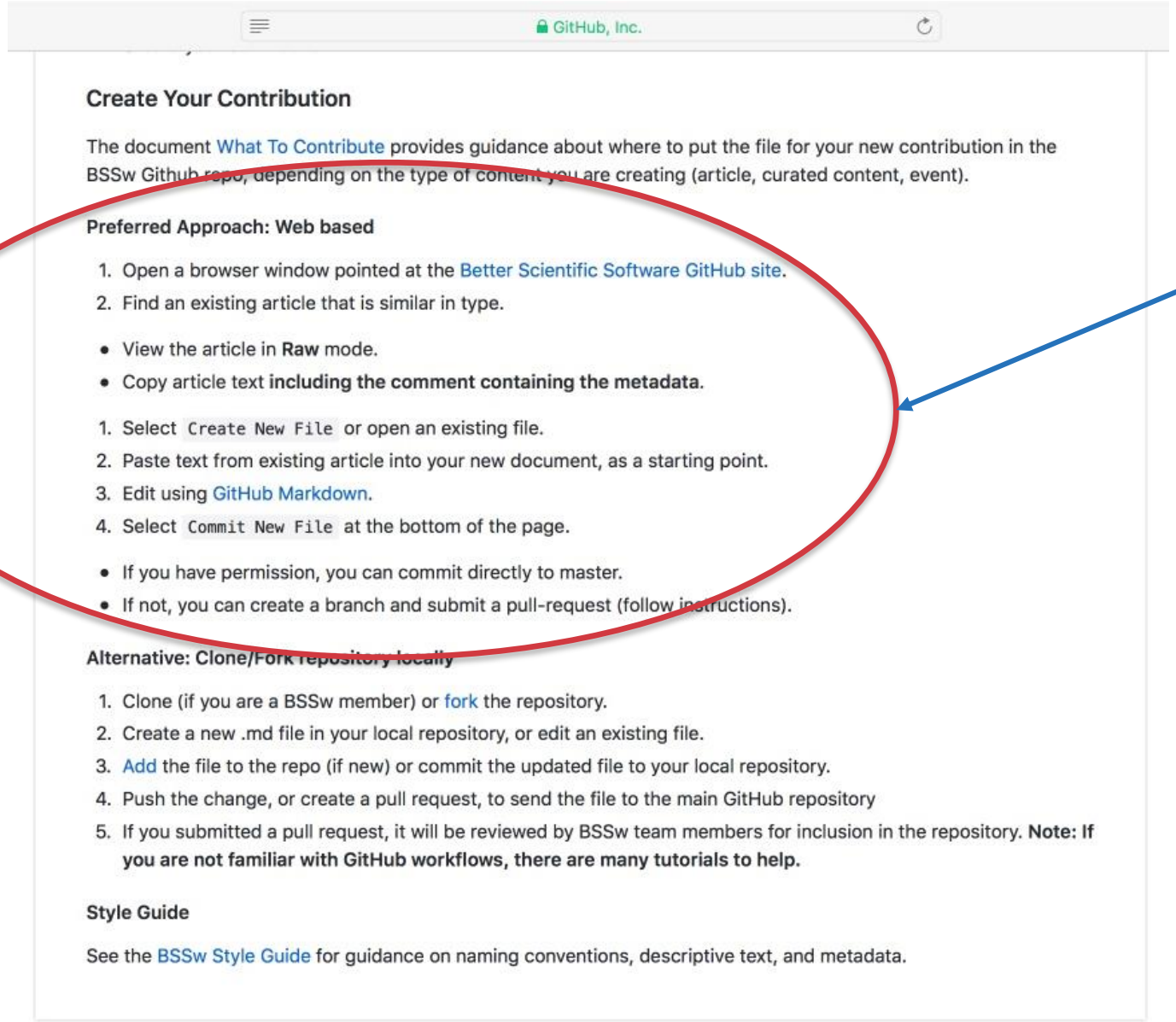
We are looking for content that has CSE focus, is accessible and generally helpful. Before investing in writing a lot of content, open a GitHub Issue describing what you want to do.

How to contribute: Pre-steps



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

How to contribute: Creating content

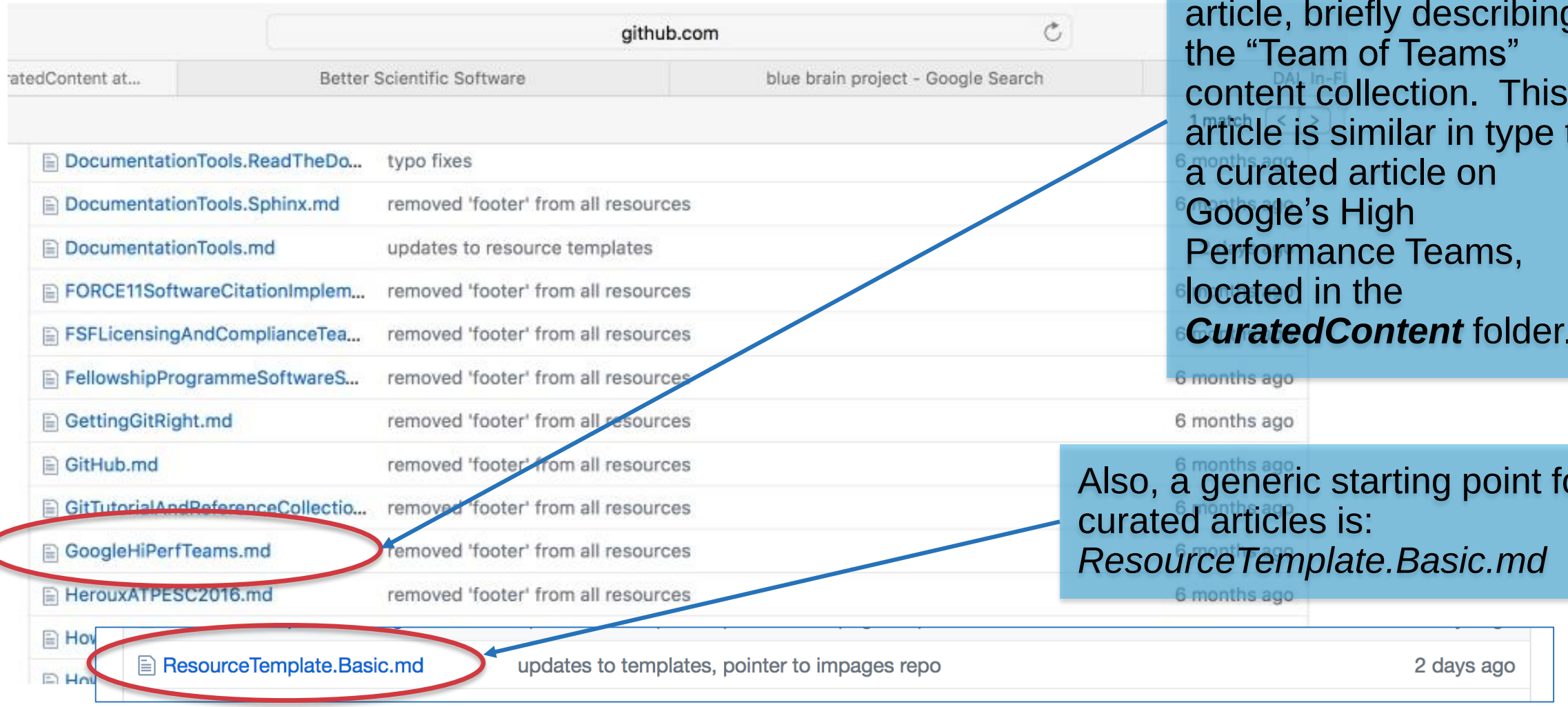


BSSw content creation is possible with any standard Git/GitHub workflow. Most content is in markdown (.md files). The GitHub web portal is very useful for this kind of writing.

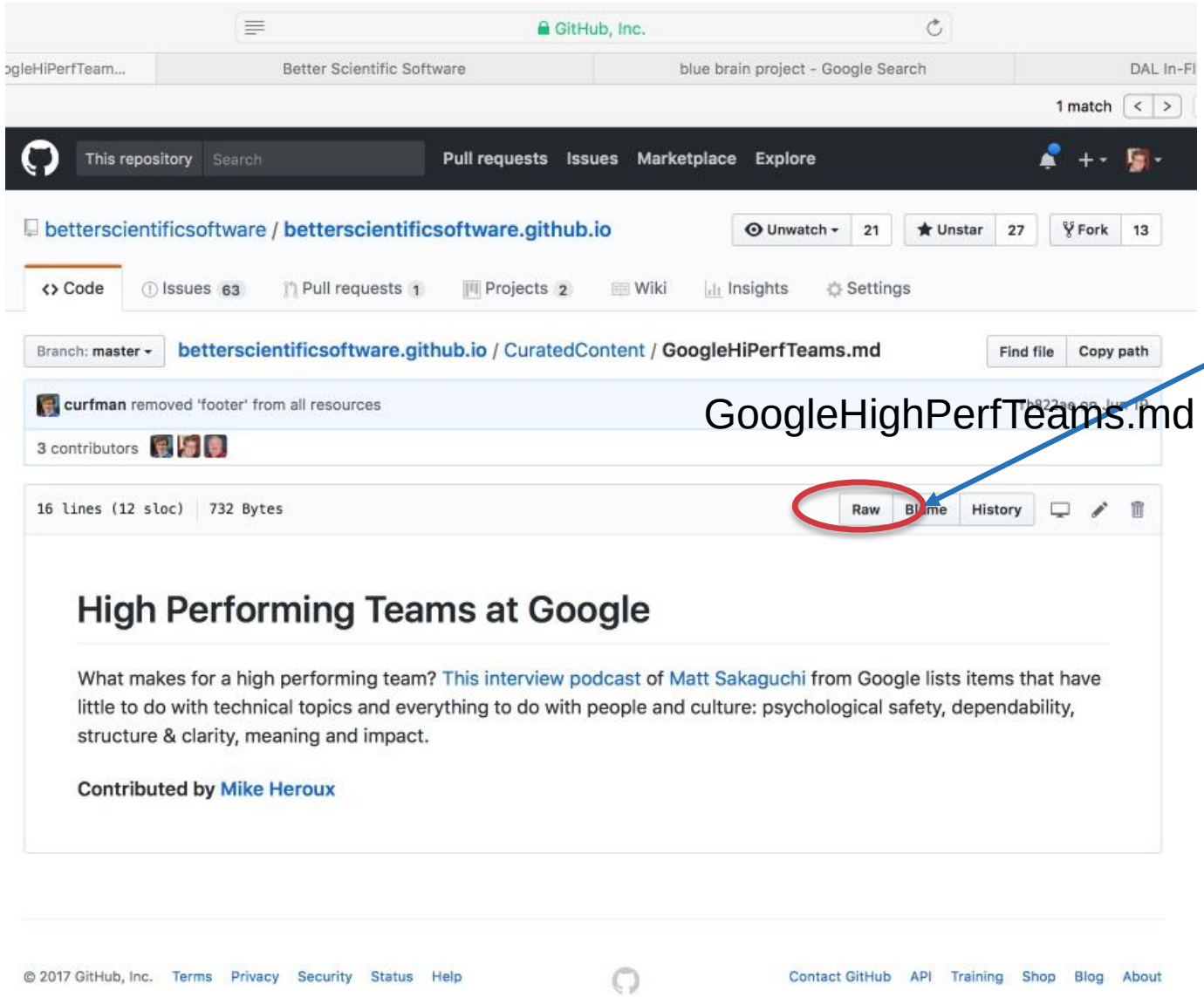
Example: Contribute “Team of Teams”: Find a similar article

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*



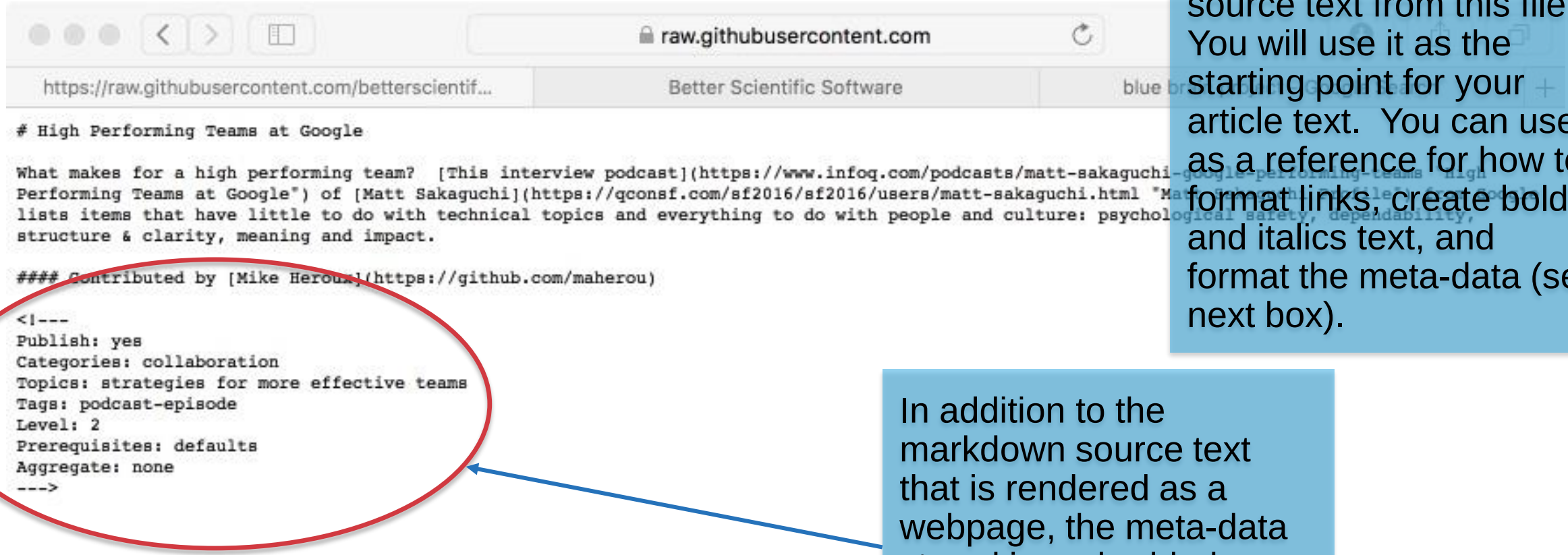
Markdown file: GoogleHighPerfTeams.md



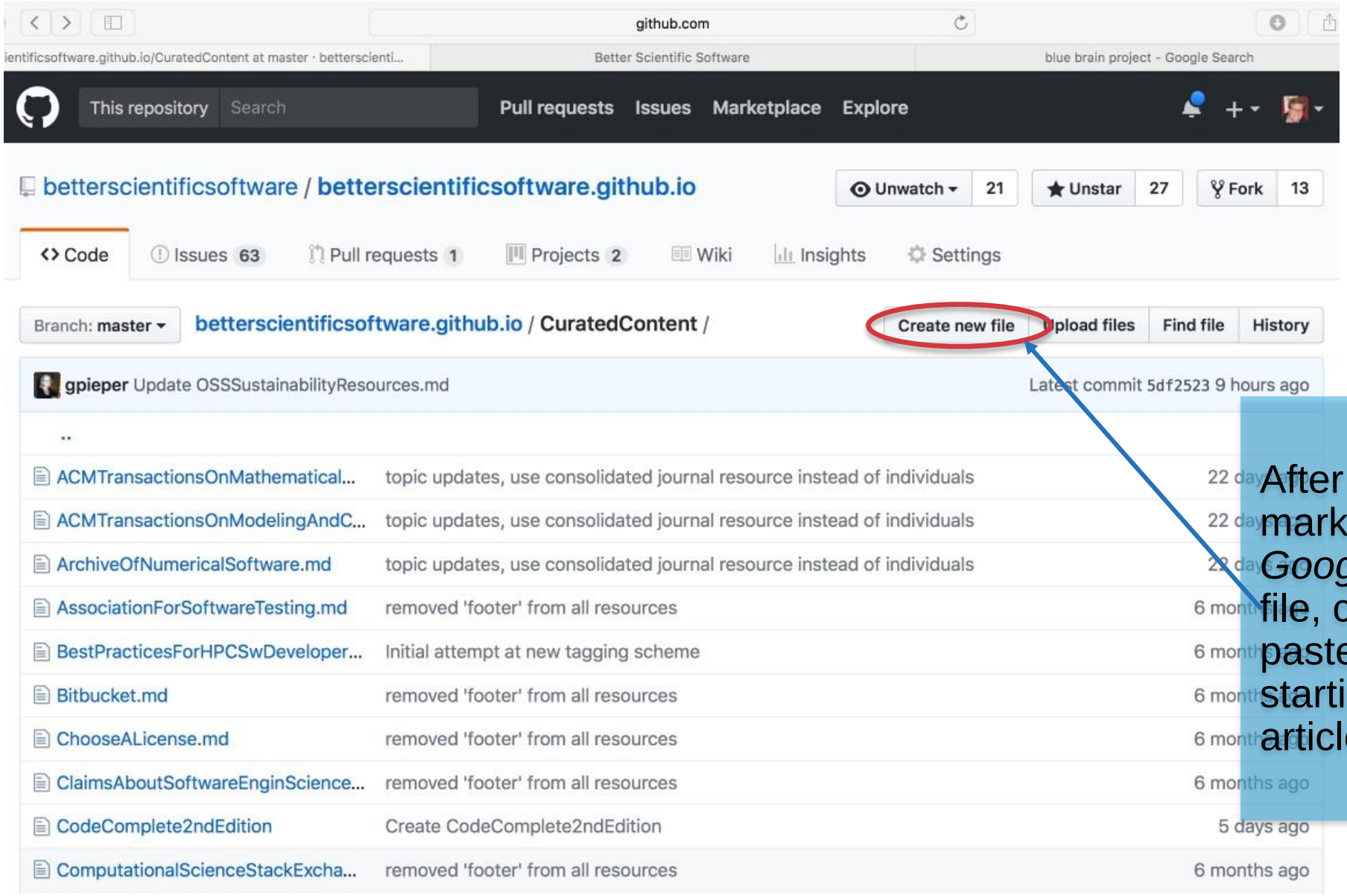
GoogleHighPerfTeams.md

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

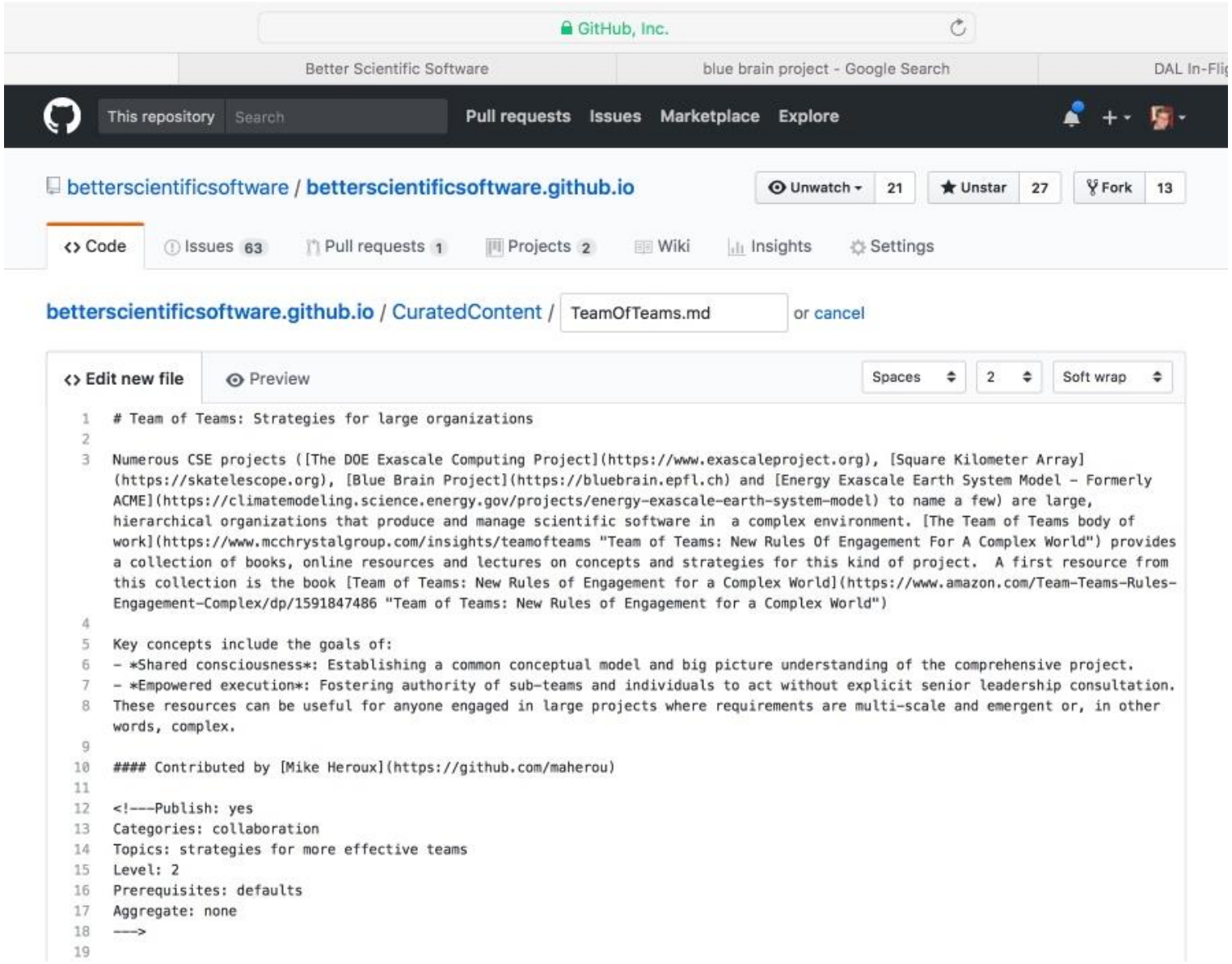


Create new file



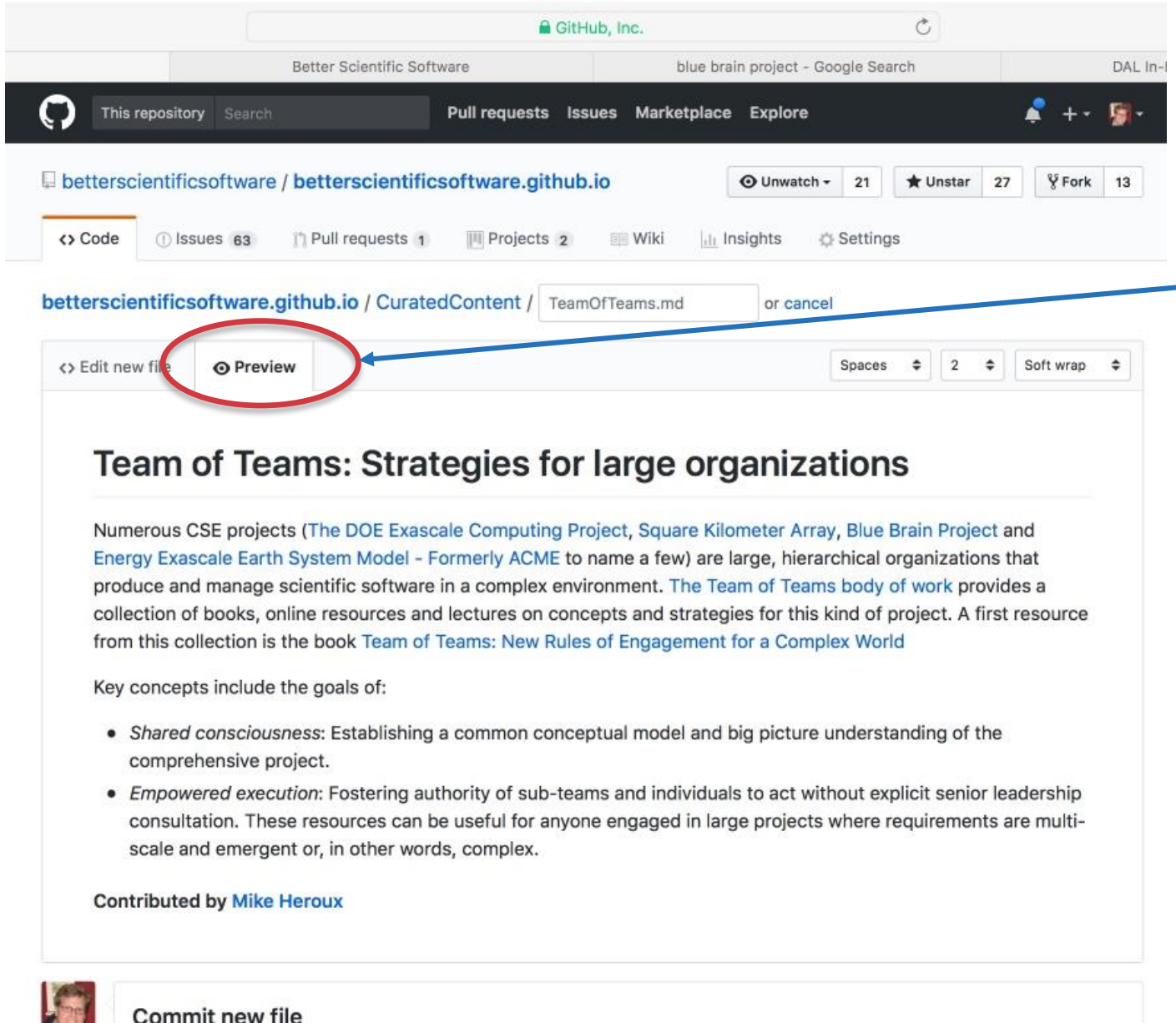
After copying the markdown source from *GoogleHiPerfTeams.md* file, create a new file and paste the source as a starting point for your article.

Create markdown file: TeamOfTeams.md



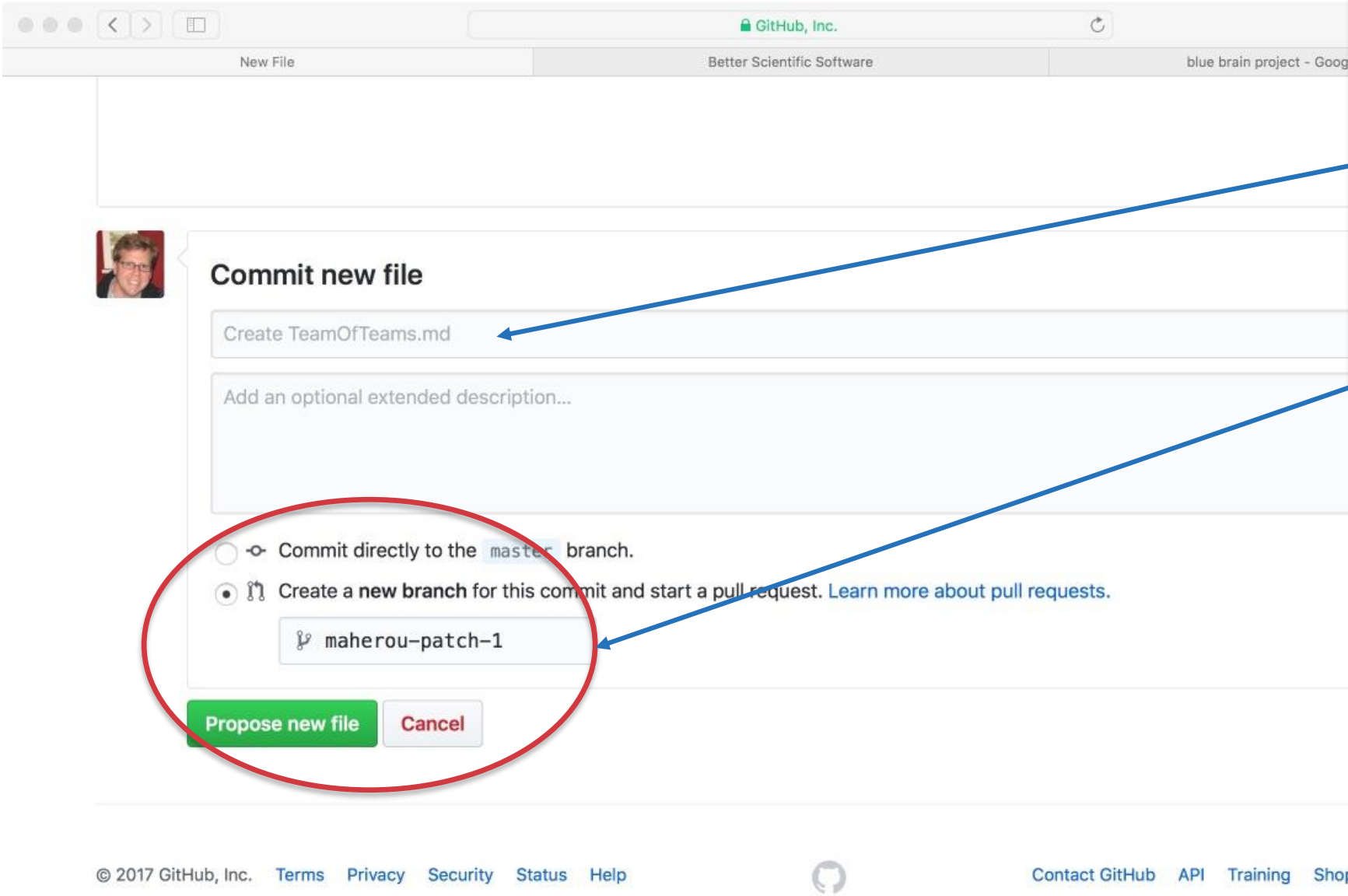
Create the content for your article. Review the *StyleGuide.md* in the main directory (remember from earlier slide) to make sure you put in the correct meta-data information.

TeamOfTeams preview



Preview your content by selecting the preview tab.

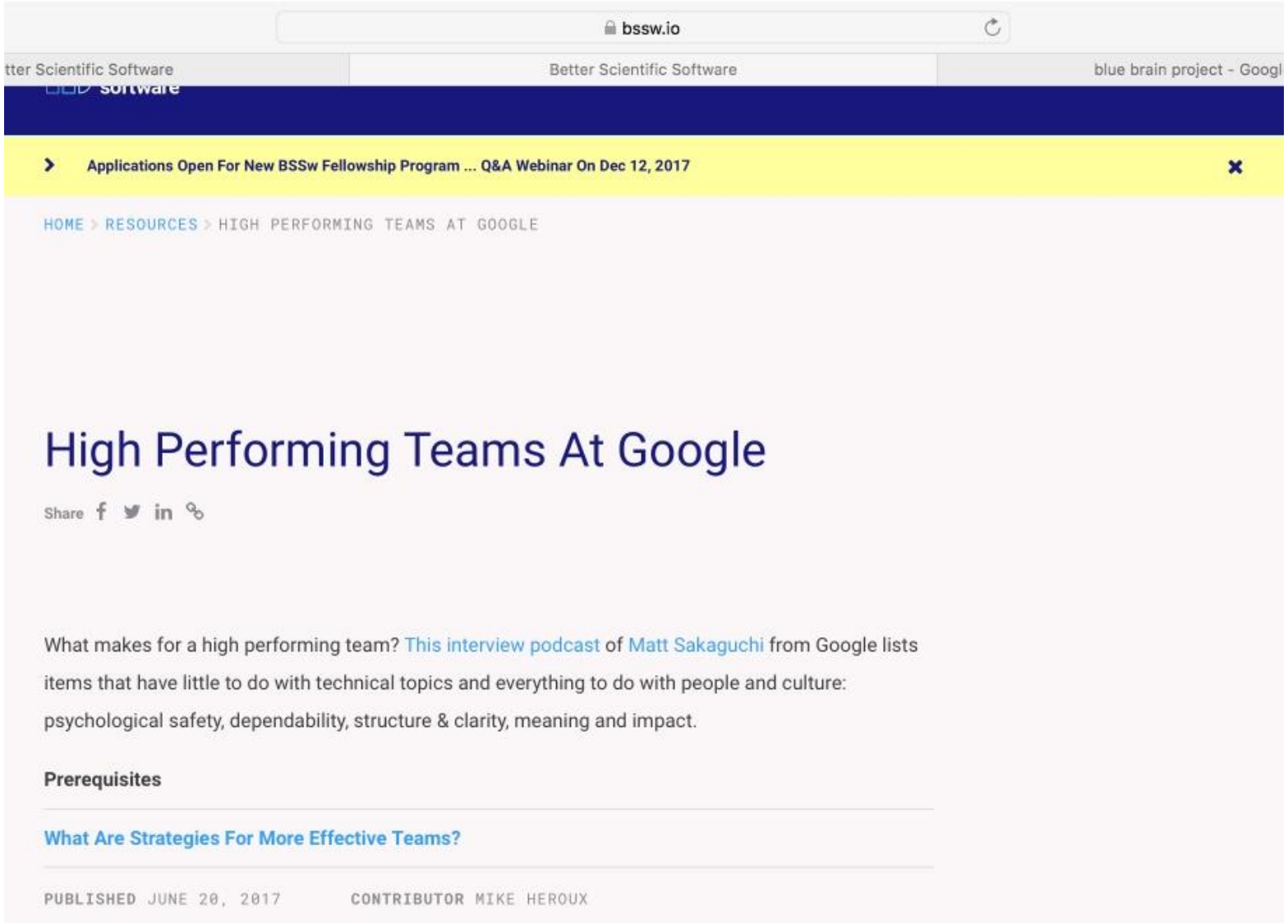
Propose new file



Create a brief one-line summary of your contribution, then an extended description. Select the option to submit a pull request. Then select “Propose new file.”

If the contribution is accepted (typically with some formatting changes handled through the pull request dialogs in GitHub), it will be pushed to bssw.io. Please remember to close your GitHub issue!

https://bssw.io/resources/high-performing-teams-at-google



GoogleHighPerfTeams.md automatically migrated and translated to this page on bssw.io web portal.

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

We *need* your input! Contribute to BSSw!

Tech tattoo

… for your laptop
actual size 2”x4”