better scientific software

Software Sustainability

Presented by

PESO

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ECP EXASCALE COMPUTING PROJECT

IDEAS productivity

David E. Bernholdt

Argonne Training Program on Extreme-Scale Computing summer school (2026)

Slides, late-breaking updates, etc. at:
https://bssw-tutorial.github.io/
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- **The requested citation the overall tutorial is:** David E. Bernholdt, Software Sustainability track, in Argonne Training Program on Extreme-Scale Computing, St. Charles, Illinois, 2026. DOI: 10.6084/m9.figshare.33139910.
- Individual modules may be cited as *Speaker, Module Title*, in *Tutorial Title*, …

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About Us

- David E. Bernholdt, ORNL

David
he/him

- Participant in the Consortium for the Advancement of Scientific Software (CASS) and DOE/ASCR software stewardship projects: https://cass.community/
  - Members of the PESO project
- Past involvement in
  - Exascale Computing Project
  - IDEAS Productivity family of projects: https://ideas-productivity.org/
  - And more!

Building an Online Community

https://bssw.io

- **New community-based resource for scientific software improvement**
- A central hub for sharing information on practices, techniques, experiences, and tools to improve developer productivity and software sustainability for computational science & 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
- Help CSE researchers **increase effectiveness** as well as leverage and impact
- **Facilitate CSE collaboration via software** in order to advance scientific discoveries

Site users can…

- **Find information** on scientific software topics
- **Contribute new resources** based on your experiences
- Create content tailored to the unique needs and perspectives of a focused scientific domain

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- BSSw Digest: https://bssw.io/pages/receive-our-email-digest
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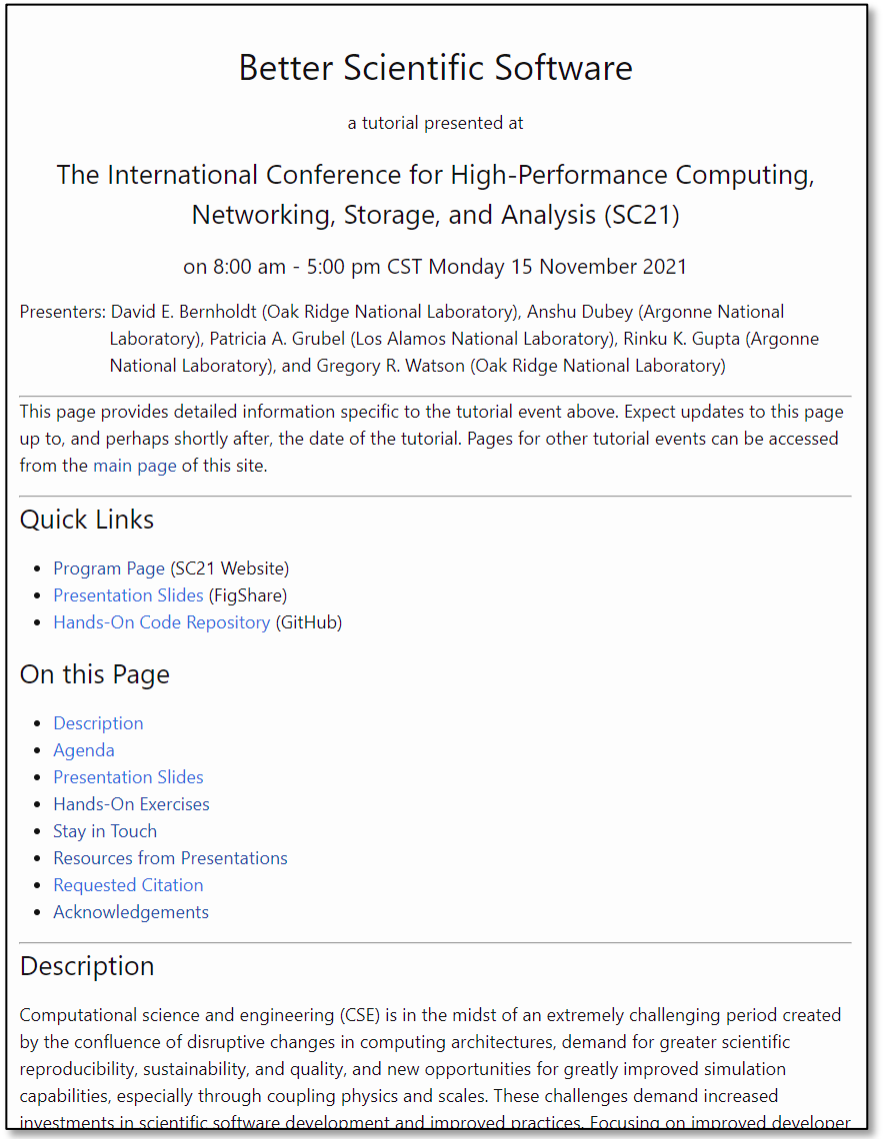
BSSw Tutorial Web Site

- https://bssw-tutorial.github.io/ is the one URL you need to find all the resources for this tutorial
- Each tutorial event has its own page
- Each tutorial page is considered archival
  - All of the materials used in that tutorial (or links to them)
  - Materials may be updated if we find mistakes



Better Scientific Software

a tutorial presented at

The International Conference for High-Performance Computing, Networking, Storage, and Analysis (SC21)

on 8:00 am - 5:00 pm CST Monday 15 November 2021

Presenters: David E. Bernholdt (Oak Ridge National Laboratory), Anshu Dubey (Argonne National Laboratory), Patricia A. Grubel (Los Alamos National Laboratory), Rinku K. Gupta (Argonne National Laboratory), and Gregory R. Watson (Oak Ridge National Laboratory)

This page provides detailed information specific to the tutorial event above. Expect updates to this page up to, and perhaps shortly after, the date of the tutorial. Pages for other tutorial events can be accessed from the main page of this site.

Quick Links

- Program Page (SC21 Website)
- Presentation Slides (FigShare)
- Hands-On Code Repository (GitHub)

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Description

Computational science and engineering (CSE) is in the midst of an extremely challenging period created by the confluence of disruptive changes in computing architectures, demand for greater scientific reproducibility, sustainability, and quality, and new opportunities for greatly improved simulation capabilities, especially through coupling physics and scales. These challenges demand increased investments in scientific software development and improved practices. Focusing on improved developer

Explaining Slide 2

- Slide 2 in all of our presentations contains the license, citation, and acknowledgements for the tutorial
- (Software) best practice to make your license and preferred citation(s) easily findable
- Sponsor acknowledgements rarely hurt!

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- **The requested citation the overall tutorial is:** Anshu Dubey, David E. Bernholdt, Better Scientific Software tutorial, in ISC High Performance, Hamburg, Germany and online, 2024

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  - With questions or feedback
  - The list moderator will allow your messages to be posted
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Agenda

The agenda is also available on the tutorial web page. Visit https://bssw-tutorial.github.io and click on the link for today's tutorial

Time	Title	Presenter
3:00 PM	Introduction	David E. Bernholdt (ORNL)
3:05 PM	Motivation and Overview of Best Practices in HPC Software Development	David E. Bernholdt (ORNL)
3:30 PM	Scientific Software Design	David E. Bernholdt (ORNL)
4:00 PM	*Break*	
4:30 PM	Software Testing and Verification	David E. Bernholdt (ORNL)
5:00 PM	Refactoring Scientific Software	David E. Bernholdt (ORNL)
5:30 PM	Improving Reproducibility Through Better Software Practices	David E. Bernholdt (ORNL)
6:00 PM	AI for Software Development and Maintenance	David E. Bernholdt (ORNL)
6:30 PM	*Adjourn*	