Software Productivity and Sustainability

David E. Bernholdt, Anshu Dubey, Todd Gamblin, and Jared O'Neal

Argonne Training Program on Extreme-Scale Computing summer school (2024)

Presented by

COLABS: Collaboration for Better Software for Science

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Slides, late-breaking updates, etc. at:
https://bssw-tutorial.github.io/
and click the link for today's tutorial

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Acknowledgements

About Us

- David E. Bernholdt, ORNL
- Anshu Dubey, ANL
- Todd Gamblin, LLNL
- Jared O'Neal, ANL

David
he/him

Anshu
she/her

Todd
he/him

Jared
he/him

- Participants in the Consortium for the Advancement of Scientific Software (CASS) and DOE/ASCR software stewardship projects: https://cass.community/
- Members of the IDEAS Productivity family of projects: https://ideas-productivity.org/
- Lead for the Spack project: https://spack.io/ (Todd)
- Also…
  - SciDAC: RAPIDS Institute, fusion energy sciences, nuclear physics
  - NSF Cyberinfrastructure for Sustained Scientific Innovation (CSSI) program
  - Past: Exascale Computing Project
  - 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

Follow BSSw

- BSSw Digest: https://bssw.io/pages/receive-our-email-digest
  - Updates on BSSw content
    - New blog posts, events, and resources
    - BSSw Fellowship
  - Typically 1-2 messages per month
  - Also: RSS feed: https://bssw.io/items.rss

The Importance of Naming

- Computing is rife with terminology that many consider harmful and exclusionary
  - Examples include: whitelist/blacklist, master/slave, and master (standalone)

- We support efforts to replace such language with more inclusive language

- In this tutorial, we strive to use inclusive language
  - Example: we use "main" for the default git branch, even where outside sources we reference may use "master"

- We welcome suggestions for further improvements in our tutorial

- Additional information:
  - The Inclusive Naming Initiative
  - The BSSw.io resource on inclusive naming provides some additional context and links

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!

License, Citation and Acknowledgements

License and Citation

- This work is licensed under a Creative Commons Attribution 4.0 International License (CC BY 4.0).
- **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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We Want to Interact with You!

- We find these tutorials most interesting and informative (for everyone) if you ask questions and share experiences!
  - We learn too!
- Please raise your hand at any time to ask a question
- After the tutorial email us at bssw-tutorial@lists.mcs.anl.gov
  - With questions or feedback
  - The list moderator will allow your messages to be posted
- Refer to bssw-tutorial.github.io page for all tutorial materials

Agenda (1/2)

Time (CDT)	Title	Presenter
8:30 AM	Introduction	David E. Bernholdt (ORNL)
8:35 AM	Motivation and Overview of Best Practices in HPC Software Development	David E. Bernholdt (ORNL)
9:15 AM	Scientific Software Design	Anshu Dubey (ANL)
10:00 AM	*Break*	
10:30 AM	Spack: Package Management for HPC	Todd Gamblin (LLNL)
11:30 AM	Spack Hands-On	Todd Gamblin (LLNL)
12:30 PM	*Lunch*	

Agenda (2/2)

Time (CDT)	Title	Presenter
12:30 PM	*Lunch*	
1:30 PM	Software Testing and Verification	Anshu Dubey (ANL)
2:30 PM	Refactoring Scientific Software	Anshu Dubey (ANL)
3:00 PM	*Break*	
3:30 PM	Software Licensing	David E. Bernholdt (ORNL)
4:30 PM	Improving Reproducibility Through Better Software Practices	David E. Bernholdt (ORNL)
5:30 PM	Lab Notebooks for Computational Mathematics, Sciences, & Engineering	Jared O'Neal (ANL)
6:30 PM	*Adjourn*	