

Better Scientific Software

Presented by

**COLABS: Collaboration
for Better Software for
Science**

Anshu Dubey

Better Scientific Software tutorial @ ISC24

In collaboration with



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- Individual modules may be cited as *Speaker, Module Title*, in *Tutorial Title*, ...



Acknowledgements

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About Us

- Anshu Dubey, ANL



Anshu
she/her

- Lead PI for COLABS: Collaboration for Better Software for Science
- Application Engagement Lead for the RAPIDS SciDAC Institute
- Member of the IDEAS Productivity Project: <http://ideas-productivity.org>

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>
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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!

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License and Citation



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 - We learn too!
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 - 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

You may also be interested in other software-related events at ISC24!

Visit <https://bssw.io/events/isc24-software-related-events>

(link is also on tutorial webpage)

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 (CEST)	Title
2:00 PM	Introduction
2:05 PM	Motivation and Overview of Best Practices in HPC Software Development
2:20 PM	Scientific Software Design
2:50 PM	Software Testing and Verification
3:30 PM	Refactoring Scientific Software
4:00 PM	<i>Break</i>
4:30 PM	Lab Notebooks
5:15 PM	Documentation
6:00 PM	Adjourn