



Welcome to...



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for this tutorial!

**David E. Bernholdt, Anshu Dubey, Rinku Gupta,
David Rogers**

1:00-4:00pm MDT Thursday 25 March 2021

Last-minute updates, final slides, etc. at:

<https://bssw-tutorial.github.io/>



See slide 2 for
license details and
requested citation

License, Citation and Acknowledgements

License and Citation



- This work is licensed under a [Creative Commons Attribution 4.0 International License](https://creativecommons.org/licenses/by/4.0/) (CC BY 4.0).
- **The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, Rinku K. Gupta, and David M. Rogers, Better Scientific Software tutorial, in Improving Scientific Software conference, online, 2021. DOI: [10.6084/m9.figshare.14256257](https://doi.org/10.6084/m9.figshare.14256257)**
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software tutorial...

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About Us

- David Bernholdt, ORNL
- Anshu Dubey, ANL
- Rinku Gupta, ANL
- David Rogers, ORNL



David B



Anshu



Rinku



David R

- Member of the IDEAS Productivity Project: <http://ideas-productivity.org>
- **Focus: Increasing CSE software productivity, quality, and sustainability**

The IDEAS-ECP team works with the ECP community to improve developer productivity and software sustainability as key aspects of increasing overall scientific productivity

- 1 Customize and curate methodologies**
- Target scientific software productivity and sustainability
 - Use workflow for best practices content development

- 2 Incrementally and iteratively improve software practices**
- Determine high-priority topics for improvement and track progress
 - *Productivity and Sustainability Improvement Planning (PSIP)*



- 3 Establish software communities**
- Determine community policies to improve software quality and compatibility
 - Create Software Development Kits (SDKs) to facilitate the combined use of complementary libraries and tools

- 4 Engage in community outreach**
- Broad community partnerships
 - Collaboration with computing facilities
 - Webinars, tutorials, events
 - *WhatIs* and *HowTo* docs
 - Better Scientific Software site (<https://bssw.io>)

For more about our work see this report:
<https://doi.org/10.2172/1606662>

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 IDEAS and BSSw

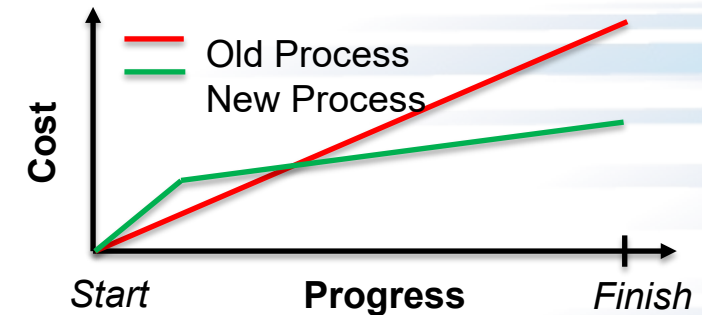
- IDEAS Productivity mailing list: <http://eepurl.com/cQCyJ5>
 - Announcements of IDEAS-organized events
 - Best Practices for HPC Software Developers webinar series
 - Strategies for Working Remotely panel series
 - Software-focused events at major scientific meetings (e.g., SIAM, ISC, SC, etc.)
 - Typically 2-3 messages per month
- 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>



Tutorial Objectives

Overview of best practices in software engineering explicitly tailored for CSE

- **Why:** Increase CSE software quality, sustainability, productivity
 - Better CSE software > better CSE research > broader CSE impact
- **Who:** Practices relevant for projects of all sizes
 - **emphasis on small teams**, e.g., a faculty member and collaborating students
- **Approach:**
 - **Useful** information, examples, exercises, pointers to other resources
 - **Not to prescribe any particular practices** as “must use”
 - Be informative about practices that have worked for some projects
 - Recommend a series of small, **incremental improvements**
 - Emphasize adoption of practices that help productivity rather than put unsustainable burden
 - **Customize as needed** for each project
- Remember: your code will live longer than you expect. *Prepare for it!*



Hands-On Activities

We have created a simple example to give you some (optional) hands-on experience with some of the concepts in this tutorial

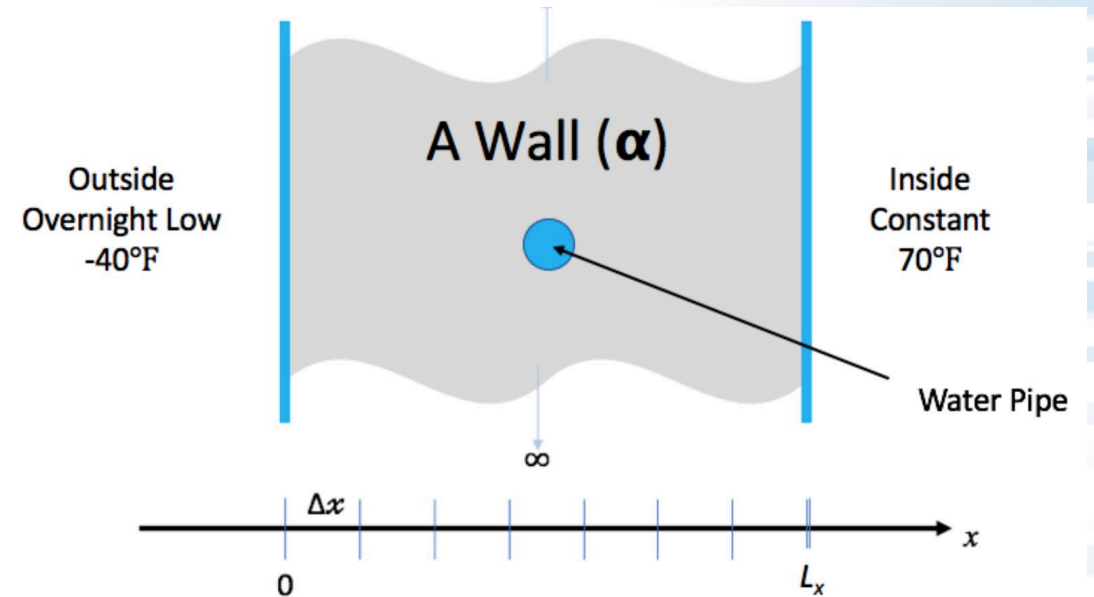
- You don't need to understand the math/physics to do the exercises, or find them useful

Because of the limited time for this tutorial, the exercises will be “*homework*”, but we'll be happy to give you feedback on your work

- We will demonstrate a few things during breaks in today's tutorial (participation optional)

Instructions on the tutorial web site:

<https://bssw-tutorial.github.io/>



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 use chat to ask questions at any time
 - We will answer in in the chat or verbally
 - We will answer as many as we can
 - If we don't get to your question, follow up with us afterwards
- If you work on the hands-on activities, we'll be glad to provide feedback
 - Submit a pull request and we'll take a look
- 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