



# Welcome to...



Check this web site  
for the latest updates  
for this tutorial!

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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...

## Acknowledgements

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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>

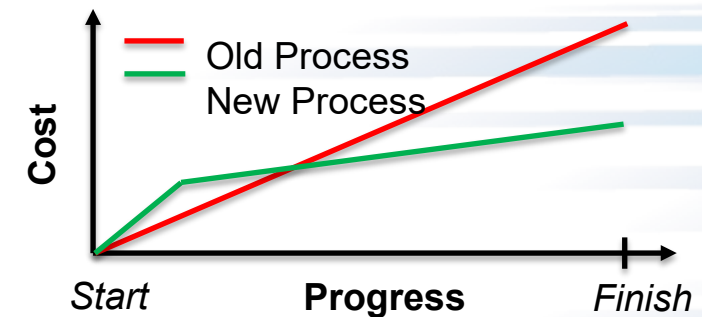




# Tutorial Objectives

## 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

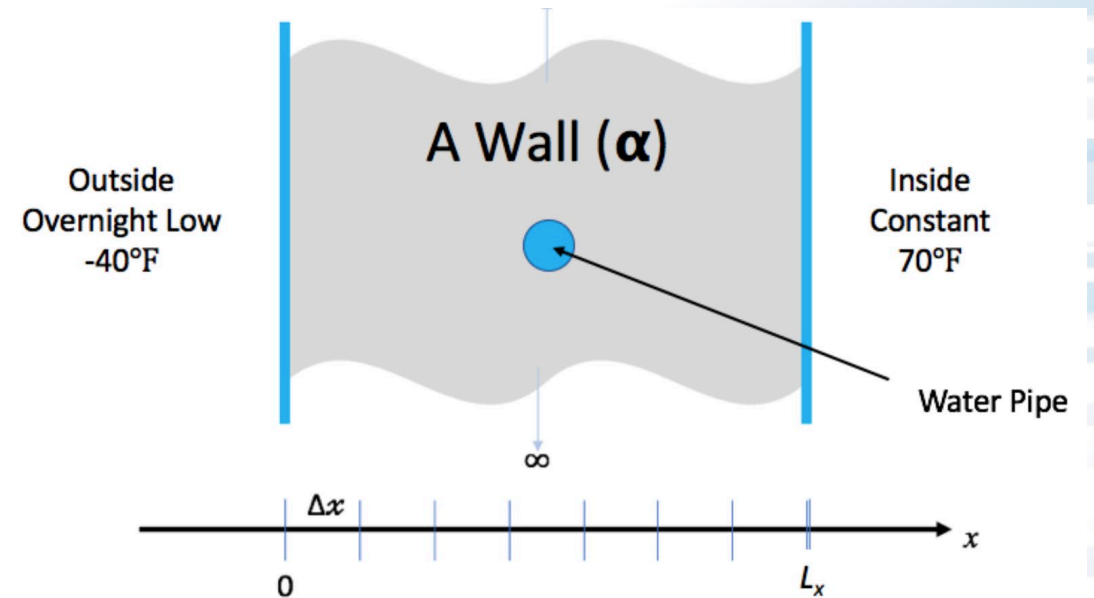
We have created a simple example to give you some (optional) hands-on experience with some of the concepts in this tutorial

- 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

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](mailto:bssw-tutorial@lists.mcs.anl.gov)
  - With questions or feedback
  - The list moderator will allow your messages to be posted