Better Scientific Software tutorial

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2:00pm-6:00pm CEST 24 June and 25 June 2021

(8:00am-12:00pm EDT)

Final slides, hands-on activities, last-minute updates, etc. at:
https://bssw-tutorial.github.io/
and click the link for today's tutorial

License, Citation and Acknowledgements

License and Citation

- **The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, Patricia A. Grubel, Rinku K. Gupta, and David M. Rogers, Better Scientific Software tutorial, in ISC High Performance, online, 2021. DOI: 10.6084/m9.figshare.14642520**
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software tutorial…

Acknowledgements

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IDEAS productivity

ECP EXASCALE COMPUTING PROJECT

About Us

- David Bernholdt, ORNL
- Anshu Dubey, ANL
- Patricia Grubel, LANL
- Rinku Gupta, ANL
- David Rogers, ORNL


David B
he/him


Anshu
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- 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

IDEAS productivity

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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

IDEAS productivity

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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

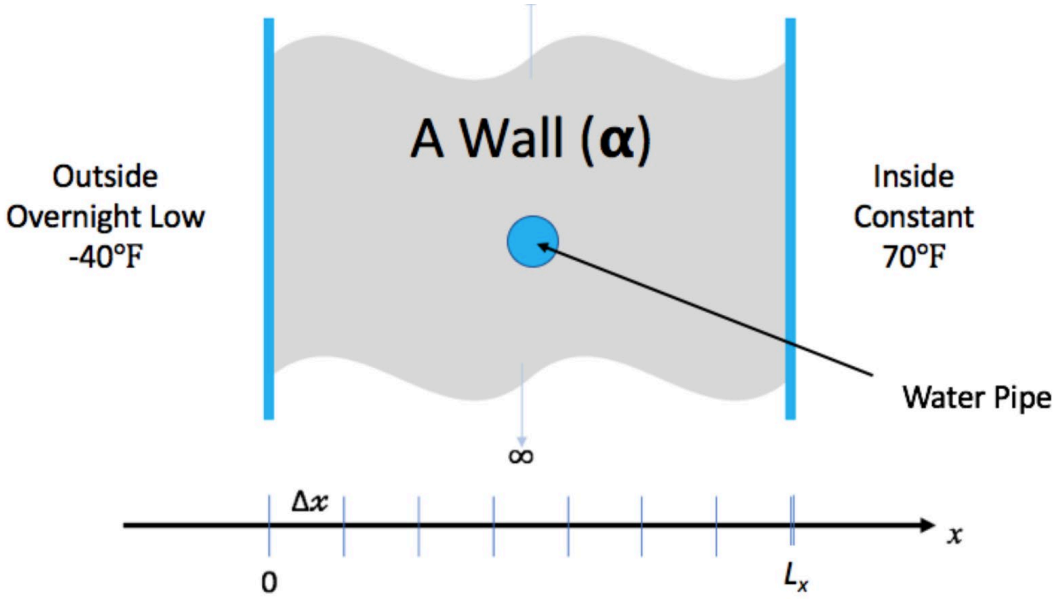
Hands-On Activities

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

We have time in the agenda for the hands-on activities, but feel free to continue working on them outside of the tutorial. We'll give feedback on pull requests and issues filed (or email us, see next slide).

Instructions on the tutorial web site:
https://bssw-tutorial.github.io/
and click the link for today's tutorial



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