Welcome to…

better scientific software

Please follow the link or use the QR code to get the latest updates for this tutorial!

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Assisted by Deborah Stevens

2:30pm-6:30pm ET Tuesday 10 November 2020

Last-minute updates, final slides, etc. at:
https://betterscientificsoftware.github.io/bssw-tutorial-sc20/

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, Better Scientific Software tutorial, in SC '20: International Conference for High Performance Computing, Networking, Storage and Analysis, online, 2020. DOI: 10.6084/m9.figshare.12994376**
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software tutorial…

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About Us

- David Bernholdt, ORNL
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David


Anshu


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Deborah

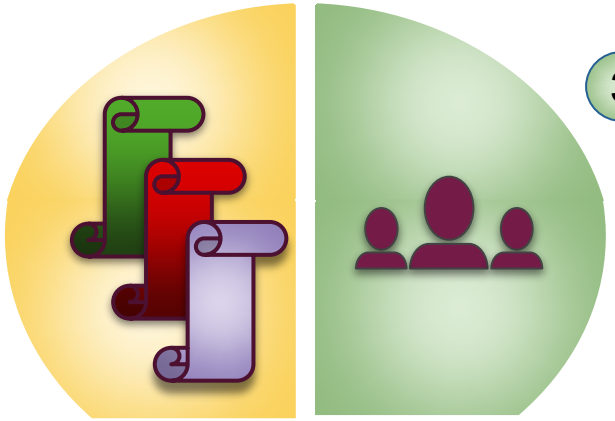
- With help from: Deborah Stevens, ANL

- 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



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

2 Incrementally and iteratively improve software practices

- Determine high-priority topics for improvement and track progress
- *Productivity and Sustainability Improvement Planning (PSIP)*

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)

IDEAS productivity

ECP EXASCALE COMPUTING PROJECT

Advancing Scientific Productivity through Better Scientific Software: Developer Productivity and Software Sustainability Report

Disruptive changes in computer architectures and the complexities of tackling new frontiers in extreme-scale modeling, simulation, and analysis present daunting challenges to software productivity and sustainability.

This newly released report explains the IDEAS approach, outcomes, and impact of work (in partnership with the ECP and broader computational science community).

Target readers are all those who care about the quality and integrity of scientific discoveries based on simulation and analysis. While the difficulties of extreme-scale computing intensify software challenges, issues are relevant across all computing scales, given universal increases in complexity and the need to ensure the trustworthiness of computational results.

January 2020

https://exascaleproject.org/better-scientific-productivity-through-better-scientific-software-the-ideas-report

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
    - 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

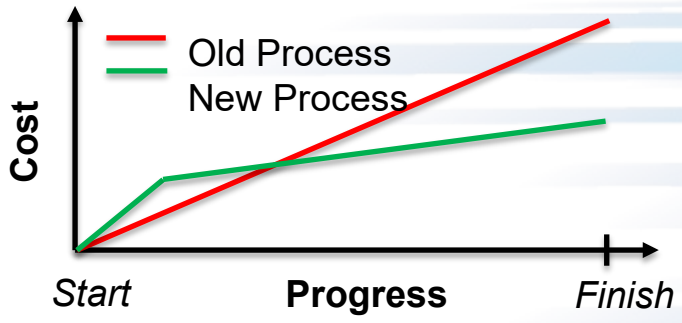
Additional Software-Related Events at SC20

Day/Time	Event Type	Event Title (and Link for Details)
Monday, Nov. 9 10:00am-2:00pm ET	Tutorial	Managing HPC Software Complexity with Spack: Part 1
Tuesday, Nov. 10 10:00am-2:00pm ET	Tutorial	Managing HPC Software Complexity with Spack: Part 2
Wednesday, Nov. 11 10:00am-6:30pm ET	Workshop	Seventh SC Workshop on Best Practices for HPC Training and Education
Wednesday, Nov. 11 2:30pm-6:30pm ET	Workshop	Correctness 2020: 4th International Workshop on Software Correctness for HPC Applications
Thursday, Nov. 12 10:00am-1:00pm ET	Workshop	RSE-HPC-2020: Research Software Engineers in HPC
Friday, Nov. 13 10:00am-6:10pm ET	Workshop	EduHPC20: Workshop on Education for High-Performance Computing
Friday, Nov. 13 10:00am-6:10pm ET	Workshop	P3HPC: 3rd International Workshop on Performance Portability and Productivity
Tuesday, Nov. 17 3:30pm-4:30pm ET	State of the Practice	Responding to Pandemic Driven Change
Wed., Nov. 18 11:30am-12:45pm ET	BOF	Spack Community BOF (TP or XO registration required; XO available for free)
Thursday, Nov. 19 2:30pm-3:45pm ET	BOF	Software Engineering and Reuse in Modeling, Simulation, and Data Analytics for Science and Engineering (TP or XO registration required; XO available for free)

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

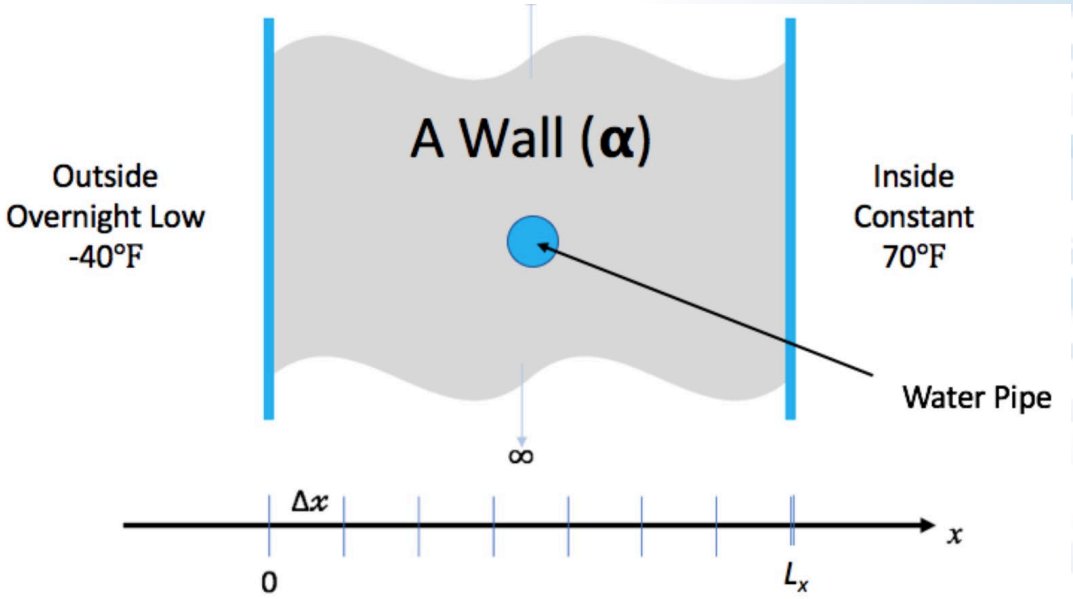
We have created a simple example to give you some (optional) hands-on experience with some of the concepts in this tutorial

- 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://betterscientificsoftware.github.io/bssw-tutorial-sc20/**



Handling Questions and Discussion

- The main presentations have been pre-recorded
  - Please use the **question channel** to ask questions during the presentations and the live segments. The speaker and the rest of the tutorial team will be monitoring and will respond
  - We will also keep an eye on the **chat channel**, but that's more for extended follow-on discussions
- During the **breaks**, we will be available for **live Q&A** (also via questions/chat) and will provide some **live demos** of concepts in the hands-on exercises
  - *Participation is optional* – we know you need breaks too
- **Please complete an evaluation of this tutorial**
  - **Evaluation link is in the tutorial info page on the EventScribe web site**
- After the tutorial, you'll continue to have access to the recording…
- …and we'll be around too – **email us at bssw-tutorial@lists.mcs.anl.gov**
  - The list moderator will allow your messages to be posted

IDEAS productivity

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