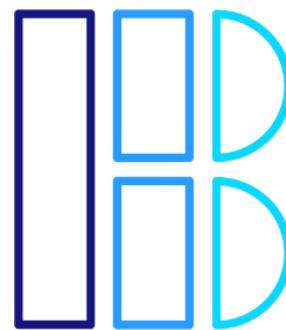




Welcome to...



**David E. Bernholdt, Anshu Dubey, Mark C. Miller,
Katherine M. Riley, and James M. Willenbring**

Software Productivity Track, ATPESC 2020



Tutorial slides: <https://app.box.com/folder/118663987937>
or <https://doi.org/10.6084/m9.figshare.12719834>



See slide 2 for
license details and
requested citation

License, Citation and Acknowledgements



License and Citation

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- The requested citation for the overall tutorial is: David E. Bernholdt, Anshu Dubey, Mark C. Miller, Katherine M. Riley, and James M. Willenbring, Software Productivity Track, in Argonne Training Program for Extreme Scale Computing (ATPESC), August 2020, online. DOI: [10.6084/m9.figshare.12719834](https://doi.org/10.6084/m9.figshare.12719834)
- Individual modules may be cited as *Speaker, Module Title*, in Software Productivity Track...

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Tutorial Instructors

- David Bernholdt, ORNL
- Anshu Dubey, ANL
- Mark Miller, LLNL
- Katherine Riley, ANL
- James Willenbring, SNL
- With help from: Pat Grubel, LANL; Rinku Gupta, ANL; David Rogers, ORNL; Deborah Stevens, ANL
- Member of the IDEAS Productivity Project: <http://ideas-productivity.org>
- **Focus: Increasing CSE software productivity, quality, and sustainability**



David



Katherine



Anshu



Jim



Mark

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>)

Building an Online Community

<https://bssw.io>

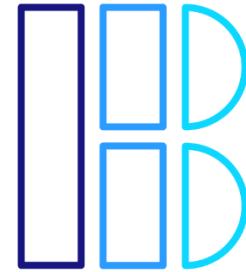
- **New community-based resource for scientific software improvement**
- A central hub for sharing information on practices, techniques, experiences, and tools to improve developer productivity and software sustainability for computational science & engineering (CSE)

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



better
scientific
software

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.

BETTER SCIENTIFIC PRODUCTIVITY THROUGH BETTER SCIENTIFIC SOFTWARE: THE IDEAS REPORT
01/30/20

ECP EXASCALE COMPUTING PROJECT

ECP-U-RPT-2020-0001

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

IDEAS-ECP Team and Collaborators

January 28, 2020

U.S. DEPARTMENT OF ENERGY | Office of Science

NNSA National Nuclear Security Administration

January 2020

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

Follow IDEAS and BSSw

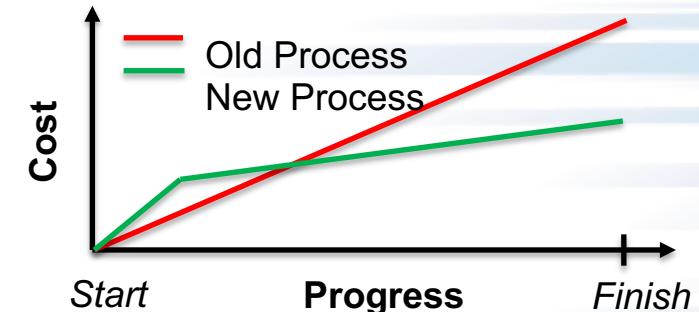
- IDEAS Productivity mailing list: <http://eepurl.com/cQCyJ5>
 - Announcements of IDEAS-organized events
 - Best Practices for HPC Software Developers webinar series
 - Strategies for Working Remotely panel series
 - Major scientific meetings (e.g., SIAM, ISC, SC, etc.)
 - Typically 1-2 messages per 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
 - Emphasis on 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 a repository, based on the Heat Equation example used on Tuesday that we will use to demonstrate some concepts, and there will be some exercises you can do as “*homework*”, if desired.

You will need...

- **GitHub account**
- **Fork of the tutorial GitHub repository**
 - <https://github.com/betterscientificsoftware/hello-numerical-world-atpesc-2020>
 - You can submit your work for feedback by making pull requests to the upstream repo
 - We will provide feedback as quickly as we can, but please be patient
- **Access to a working development environment for C++ and/or Fortran**
 - Typical Linux or Mac systems should be fine (git, editor, compilers, make, etc.)
 - Using a remote system is fine

Handling Questions and Discussion

- We'll try to stop for questions from time to time
- Members of the IDEAS team will be monitoring the chat
- If the presenter asks for questions, you can unmute and ask
- Otherwise, please use chat
- We can also be available during breaks, lunch, and after the session for additional conversations
 - Please use the chat to let us know who you'd like to talk to just before the break
 - And remember that we may need a break too
- Also, feel free to email us at bssw-tutorial@lists.mcs.anl.gov
 - The list moderator will allow your messages to be posted

Agenda

Time (Central TZ)	Module	Topic	Speaker
9:30am-9:45am	00	Introduction	David E. Bernholdt, ORNL
9:45am-10:15am	01	Overview of Best Practices in HPC Software Development	Katherine M. Riley, ANL
10:15am-10:45am	02	Agile Methodologies	James M. Willenbring, SNL
10:45am-11:00am	03	Git Workflows	James M. Willenbring, SNL
<i>11:00am-11:15am</i>		<i>Break (and Q&A with speakers)</i>	
11:15am-12:00pm	04	Software Design	Anshu Dubey, ANL
12:00pm-12:45pm	05	Software Testing	Anshu Dubey, ANL
<i>12:45pm-1:45pm</i>		<i>Lunch (and Q&A with speakers)</i>	
1:45pm-2:00pm	06	Agile Methodologies Redux	James M. Willenbring, SNL
2:00pm-3:00pm	07	Refactoring	Anshu Dubey, ANL
<i>3:00pm-3:15pm</i>		<i>Break (and Q&A with speakers)</i>	
3:15pm-3:45pm	08	Continuous Integration	Mark C. Miller, LLNL
3:45pm-4:30pm	09	Reproducibility	David E. Bernholdt, ORNL
4:30pm-4:45pm	10	Summary	David E. Bernholdt, ORNL

