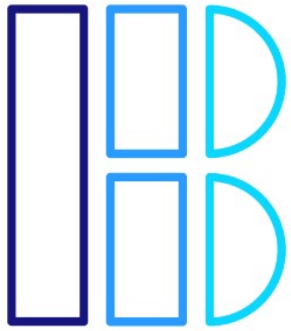
Welcome to…



better scientific software

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

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- **The requested citation 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**
- Individual modules may be cited as *Speaker, Module Title*, in Software Productivity Track…

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IDEAS productivity

ECP EXASCALE COMPUTING PROJECT

Tutorial Instructors

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- With help from: Pat Grubel, LANL; Rinku Gupta, ANL; David Rogers, ORNL

- 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

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

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

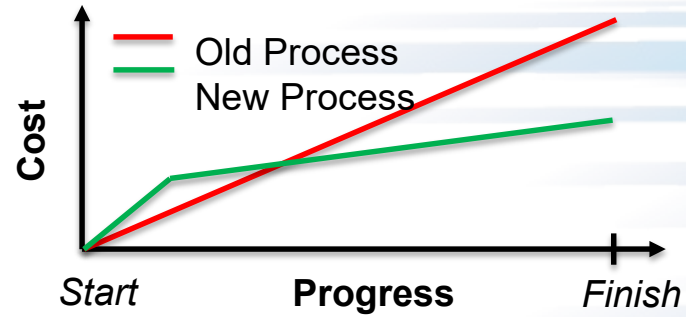
Follow IDEAS and BSSw

- 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