Welcome to…

better scientific software

David E. Bernholdt, Anshu Dubey, James M. Willenbring

2:30pm-6:00pm, Tuesday 4 February 2020

Tutorial slides
http://bit.ly/ecp4pm-bssw-tutorial

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License and Citation

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- **The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, James M. Willenbring, Better Scientific Software tutorial, in Exascale Computing Project Fourth Annual Meeting, Houston, Texas. DOI: 10.6084/m9.figshare.11786868**
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software Tutorial…

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IDEAS productivity

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Tutorial Instructors

- David Bernholdt, ORNL
- Anshu Dubey, ANL
- James Willenbring, SNL

David

Anshu

Jim

- Members of the IDEAS Productivity Project: http://ideas-productivity.org
- **Focus: Increasing CSE software productivity, quality, and sustainability**

Argonne NATIONAL LABORATORY

OAK RIDGE National Laboratory

Sandia National Laboratories

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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)

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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

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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

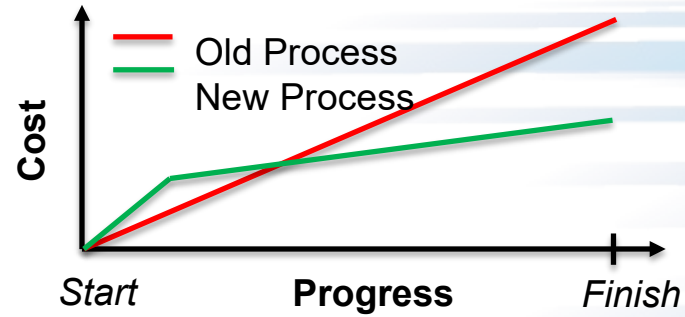
Follow IDEAS and BSSw

- IDEAS Productivity mailing list: http://eepurl.com/cQCyJ5
  - Announcements of IDEAS-organized events
    - Best Practices for HPC Software Developers webinar series
    - 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!

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Agenda

Time	Module	Topic	Speaker
2:30pm-2:35pm	00	Introduction	David E. Bernholdt, ORNL
2:35pm-3:00pm	01	Overview of Best Practices in HPC Software Development	David E. Bernholdt, ORNL
3:00pm-3:30pm	02	Agile Methodologies and Useful GitHub Tools	Jim Willenbring, SNL
3:30pm-4:00pm		*Break*	
4:00pm-4:30pm	03	Improving Reproducibility through Better Software Practices	David E. Bernholdt, ORNL
4:30pm-5:15pm	04	Software Design and Testing	Anshu Dubey, ANL
5:15pm-5:45pm	05	Git Workflows	Jim Willenbring, SNL
5:45pm-6:00pm	06	Continuous Integration	David E. Bernholdt, ORNL

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Additional IDEAS Activities at the ECP 4AM

Day	Time	Room	Event Title
Tuesday	10:30am-12:00pm	Founders II	Breakout: Collaboration Opportunities with the BSSw Fellows
Tuesday	10:30am-12:00pm	Founders III	BOF: Cultivating Software Sustainability and Productivity through BSSw.io
Tuesday	2:30pm-3:30pm	Founders I	Breakout: The Scope and Role of DevOps in HPC
Wednesday	2:30pm-4:00pm	Founders I	Breakout: Hands-on with Progress Tracking Cards: A Lightweight Method for Improving Your Software Practices
Thursday	1:30pm-4:30pm	Champions I	Breakout: Developing Engaged and Productive Virtual Teams
Tuesday-Thursday		Discovery B	Poster #77: Rate Your Project's Software Practices!
Tuesday-Thursday		Discovery B	Poster #78: Lightweight Software Quality Practice — PSIP: Productivity and Sustainability Improvement Planning
Tuesday-Thursday		Discovery B	Poster #114: Better Scientific Software: So Your Code Will See the Future
Tuesday-Thursday		Discovery B	Poster #115: IDEAS-ECP: Advancing Software Productivity for Exascale Applications
Tuesday-Thursday		Meeting Lobby	IDEAS Desk: Let's talk about software *(available during all breaks and selected poster and breakout slots)*

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Who Are You?

- Undergrad students
- Graduate students
- Postdocs
- Faculty/staff
- Manager
- Other

- Academia
- National Laboratories
- Government
- Industry
- Other

- Domain scientist
- Computer scientist
- Applied mathematician
- Other

- AD
- HI
- ST
- None of the above

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