Welcome to…

David E. Bernholdt

RF SciDAC 2020 Workshop

Tutorial slides
https://doi.org/10.6084/m9.figshare.11918397

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License and Citation

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- **The requested citation the overall tutorial is: David E. Bernholdt, Better Scientific Software tutorial, in RF SciDAC 2020 Workshop, Knoxville, Tennessee. DOI: 10.6084/m9.figshare.11918397**
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software Tutorial…

Acknowledgements

Tutorial Instructors

David

- David Bernholdt, ORNL

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

- Member of the RAPIDS SciDAC Institute for Computer Science and Data: https://rapids.lbl.gov/
- **Focus: assist Office of Science (SC) application teams in overcoming computer science and data challenges in the use of DOE supercomputing resources to achieve science breakthroughs**

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)

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

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-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

...uting Project (ECP) provides a unique opportunity to advance computational science ...e-scale computing. However, disruptive changes in computer architectures and the ...e-scale modeling, simulation, and analysis present daunting challenges to the ...ainability of software artifacts.

...IDEAS project within ECP (called IDEAS-ECP) to foster and advance software ...computational science, as a key aspect of improving overall scientific productivity. ...es, and impact of work (in partnership with the ECP and broader computational

...quality and integrity of scientific discoveries based on simulation and analysis. While ...sify software challenges, issues are relevant across all computing scales, given ...o ensure the trustworthiness of computational results.

...te.

January 2020

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

The RAPIDS Institute

Solving computer science and data challenges for Office of Science application teams to achieve science breakthroughs on DOE platforms.

- **Technology Focus Areas**
  - **Data Understanding** – scalable methods, robust infrastructure, machine learning
  - **Scientific Data Management** – I/O libraries, coupling, knowledge management
  - **Platform Readiness** – hybrid programming, deep memory hierarchy, autotuning, correctness
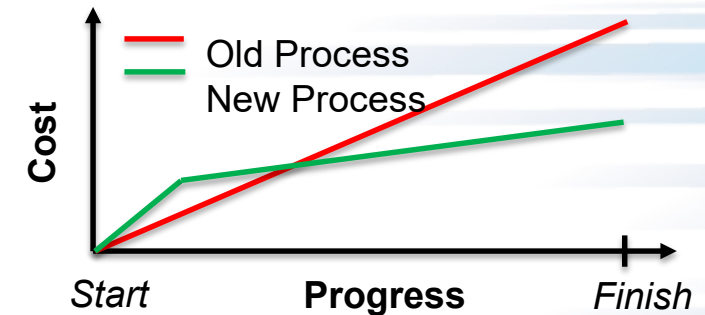- **Application Engagement**
  - *Tiger Teams* engage experts in multiple areas
  - Software productivity: verification and validation, etc.
  - Outreach activities connect with broader community
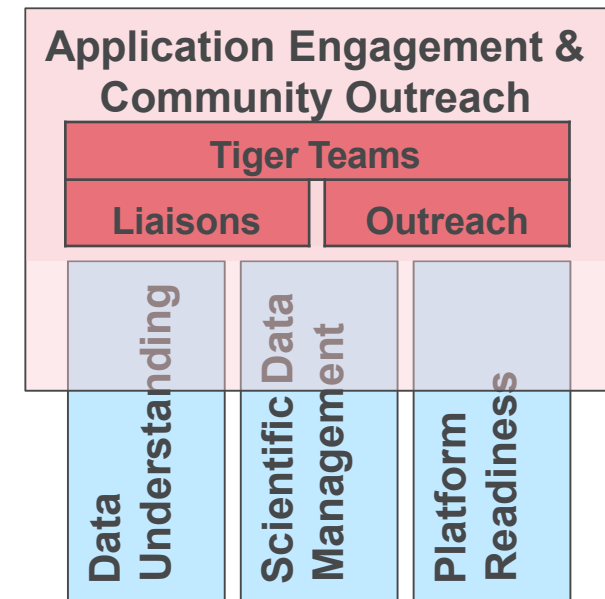
Tutorial Objectives

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!

Agenda

Time	Module	Topic	Speaker
1:00pm-1:05pm	00	Introduction	David E. Bernholdt, ORNL
1:05pm-1:30pm	01	Overview of Best Practices in HPC Software Development	David E. Bernholdt, ORNL
1:30pm-2:00pm	02	Agile Methodologies and Useful GitHub Tools	David E. Bernholdt, ORNL
2:00pm-2:30pm	03	Improving Reproducibility through Better Software Practices	David E. Bernholdt, ORNL
2:30pm-2:45pm		Q&A	All
2:45pm-3:30pm		*Break*	
3:30pm-4:15pm	04	Software Design and Testing	David E. Bernholdt, ORNL
4:14pm-4:45pm	05	Continuous Integration	David E. Bernholdt, ORNL
4:45pm-5:00pm		Q&A	All

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