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Better Scientific Software tutorial

@ Improving Scientific Software conference (2023)

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- The requested citation the overall tutorial is: David E. Bernholdt, Patricia A. Grubel, and David M. Rogers, Better Scientific Software tutorial, in Improving Scientific Software, Boulder, Colorado and online, 2023. DOI: 10.6084/m9.figshare.22179748.
- Individual modules may be cited as Speaker, Module Title, in Tutorial Title, ...

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Science through computing is, at best, as credible as the software that produces it!





Today, We Covered Many Topics...

- Designing software for flexibility and extensibility
- Refactoring software
- Collaborative software development
- Packaging
- Testing strategies for complex software systems
- Reproducibility





And there are Many More We Didn't Have Time For

- Documentation
- Licensing
- Continuous integration testing
- Distribution
- Issue tracking
- Configuration and building
- Debugging strategies
- Building and sustaining communities around software
- Software publication and citation
- Requirements gathering
- Understanding and debugging floating-point math
- Performance and performance portability

- Also important topics, but...
- Less distinction between research software and other software
- More informational resources available
- Next-level concerns for starting researchers
- There's only so much time in the day!





But you're a researcher. You can't afford to spend "all" of your time on software engineering.

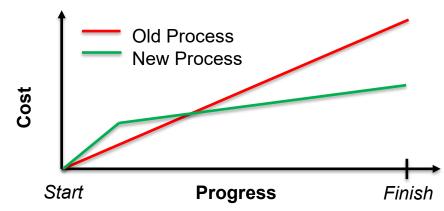




A Final Recommendation: Continual, Incremental Software Process Improvement

Target: your project should include "just enough" software engineering so that you can meet your short-term and longer-term scientific goals effectively

- Identify your team's "pain points" in your software development processes
 - Help: RateYourProject assessment tool: <u>https://rateyourproject.org/</u>
- 2. Set a goal for something to improve
 - Target processes and behaviors, not just tasks
 - Pick something that you can address in a few months that will give you a noticeable benefit
- 3. Agree on a plan to address it, identify markers of progress and what is "done"
 - Write them down
 - Help: Progress tracking card examples: https://bssw-psip.github.io/ptc-catalog/catalog
- 4. Work your plan, track your progress
- 5. When you are done, celebrate...
- ...then pick a new pain point to address



The new process costs something to implement, but it pays off over time

Productivity and Sustainability Improvement Planning https://bssw.io/psip



A goal of <u>BSSw.io</u> is to provide resources for improving your software processes. If you find useful resources that aren't on BSSw.io, consider contributing. Its easy and quick.





Thanks, and Keep in Touch!

- Email comments and questions to <u>bssw-tutorial@lists.mcs.anl.gov</u>
- See the tutorial web site for an archive of all the materials from this tutorial
 - <u>https://bssw-tutorial.github.io/</u>
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