Software Productivity and Sustainability

David E. Bernholdt, Anshu Dubey, Todd Gamblin, Jared O’Neal, and Boyana R. Norris

Argonne Training Program for Extreme-Scale Computing summer school

Additional resources at: https://bssw-tutorial.github.io/
and click the link for today’s tutorial
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- The requested citation the overall tutorial is: Anshu Dubey and Gregory R. Watson, Better Scientific Software Tutorial, in ISC High Performance, 2022, Hamburg Germany. DOI: 10.6084/m9.figshare.19781752

- Individual modules may be cited as Speaker, Module Title, in Better Scientific Software tutorial, ISC, 2022 …

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About Us

• David E. Bernholdt, ORNL
• Anshu Dubey, ANL
• Todd Gamblin, LLNL
• Jared O’Neal, ANL
• Boyana R. Norris, U. Oregon

• Members of the IDEAS Productivity Project (present or past): http://ideas-productivity.org

• Also members of…
  • ExaStar project (ECP)
  • Spack project (ECP and other support)
  • xSDK (ECP)
The IDEAS-ECP team works with the ECP community, and beyond, 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](https://bssw.io))

For more about our work see this report: [https://doi.org/10.2172/1606662](https://doi.org/10.2172/1606662)
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
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
    • Software-focused events at major scientific meetings (e.g., SIAM, ISC, SC, etc.)
  – Typically 2-3 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
BSSw Tutorial Web Site

• [https://bssw-tutorial.github.io/](https://bssw-tutorial.github.io/) is the one URL you need to find all the resources for this tutorial
• Each tutorial event has its own page
  – We will backfill tutorials before 2021 as time permits
• Each tutorial page is considered archival
  – All of the materials used in that tutorial (or links to them)
  – Materials may be updated if we find mistakes
Explaining Slide 2

• Slide 2 in all of our presentations contains the license, citation, and acknowledgements for the tutorial

• (Software) best practice to make your license and preferred citation(s) easily findable

• Sponsor acknowledgements rarely hurt!

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License and Citation

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We Want to Interact with You!

• We find these tutorials most interesting and informative (for everyone) if you ask questions and share experiences!
  – We learn too!
  – Additional opportunities for Q&A/discussion before and after dinner
  – We’ll also be keeping an eye on the track-7-software Slack channel

• If you work on the hands-on activities, we’ll be glad to provide feedback
  – Submit a pull request and we’ll take a look

• After the tutorial email us at bssw-tutorial@lists.mcs.anl.gov
  – With questions or feedback
  – The list moderator will allow your messages to be posted

• Refer to bssw-tutorial.github.io page for all tutorial materials
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<thead>
<tr>
<th>Time (CDT)</th>
<th>Title</th>
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<tbody>
<tr>
<td>8:30 AM</td>
<td>Introduction</td>
<td>David E. Bernholdt (ORNL)</td>
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<tr>
<td>8:35 AM</td>
<td>Motivation and Overview of Best Practices in HPC Software Development</td>
<td>David E. Bernholdt (ORNL)</td>
</tr>
<tr>
<td>9:15 AM</td>
<td>Scientific Software Design</td>
<td>Anshu Dubey (ANL)</td>
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<tr>
<td>10:00 AM</td>
<td>Break</td>
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<tr>
<td>10:30 AM</td>
<td>An Introduction to Software Licensing</td>
<td>David E. Bernholdt (ORNL)</td>
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<tr>
<td>11:30 AM</td>
<td>Spack: Package Management for HPC</td>
<td>Todd Gamblin (LLNL)</td>
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<td>12:30 PM</td>
<td>Lunch</td>
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<td>1:30 PM</td>
<td>Software Testing and Verification</td>
<td>Anshu Dubey (ANL)</td>
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<tr>
<td>2:15 PM</td>
<td>Lab Notebooks for Computational Mathematics, Sciences, &amp; Engineering</td>
<td>Jared O'Neal (ANL)</td>
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<td>3:00 PM</td>
<td>Break</td>
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<tr>
<td>3:30 PM</td>
<td>Managing Computational Experiments</td>
<td>Jared O'Neal (ANL) and Anshu Dubey (ANL)</td>
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<tr>
<td>4:15 PM</td>
<td>Understanding Your Software Development</td>
<td>Boyana R. Norris (UO)</td>
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<td>5:15 PM</td>
<td><strong>Breakouts:</strong> Spack Hands-On or General Discussion</td>
<td>All</td>
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<tr>
<td>6:15 PM</td>
<td>Dinner and After-Dinner Talk</td>
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<tr>
<td>8:15 PM</td>
<td><strong>Optional Evening Discussion Session</strong></td>
<td>All</td>
</tr>
<tr>
<td>9:00 PM</td>
<td>Adjourn</td>
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