

David E. Bernholdt (ORNL), Anshu Dubey (ANL), Michael A. Heroux (SNL),
Jared O'Neal (ANL), and the rest of the IDEAS Productivity Team

Introduction and Call to Action

- IDEAS = Interoperable Design of Extreme-Scale Application Software
- **IDEAS-ECP (2017-present)**
 - Funded by Exascale Computing Project (ECP)
 - Work with the ECP community to improve developer productivity and software sustainability as key aspects of increasing overall scientific productivity
- IDEAS-Classic (2014-2017)
 - Funded by DOE / ASCR + BER Terrestrial Ecosystem Modeling
 - Improving interoperability of key DOE numerical libraries
- **Fundamental goals**
 - Increase the awareness of, and attention to, software development, productivity, and sustainability throughout the HPC/computational science and engineering (CSE) software community
 - Engage with...
 - Research sponsors and other stakeholders
 - Specific software development teams
 - Broader HPC/CSE community

We're not a Community without You

- Be part of the community **talking about and acting on** software development, productivity, and sustainability!
- Join us for software-related events at PASC, ISC and other conferences
 - PASC: Poster CSM09 (Thursday)
 - PASC: Minisymposium MS55 -- Towards Sustainable Scientific Software through Better Engineering, Development, Documentation, Publication and Curation (Friday)
 - ISC: Tutorial on Better Scientific Software (Sunday)
 - ISC: Tutorial and BOF on Spack (Sunday and Tuesday)
 - ISC: Poster PP24 (Tuesday)
 - ISC: BOF on Software Engineering for Computational Science and Engineering (Wednesday)
 - ISC: Focus Session on New Approaches, Algorithms Towards Exascale Computing (Wednesday)
- Organize software-focused events – on your own, or join with us!
- Follow the IDEAS Productivity Project: <https://ideas-productivity.org/>
 - Join us for events, including: HPC Best Practices Webinar Series, tutorials, minisymposia, posters, birds of a feathers, etc.
 - Tell us what topics you'd like hear (or present) in a webinar or a tutorial
 - Co-organize a workshop or minisymposium with us
 - Announcement mailing list: <http://eepurl.com/cQCyJ5> (~1-2/month)
 - Email Us: IDEASProductivity@gmail.com
- Use and contribute to Better Scientific Software: <https://bssw.io/>
 - Contributing: <https://bssw.io/contributes/new>
 - Mailing list: <https://bssw.io/pages/receive-our-email-digest> (~1/month)
 - Contact Us: <https://bssw.io/contact>

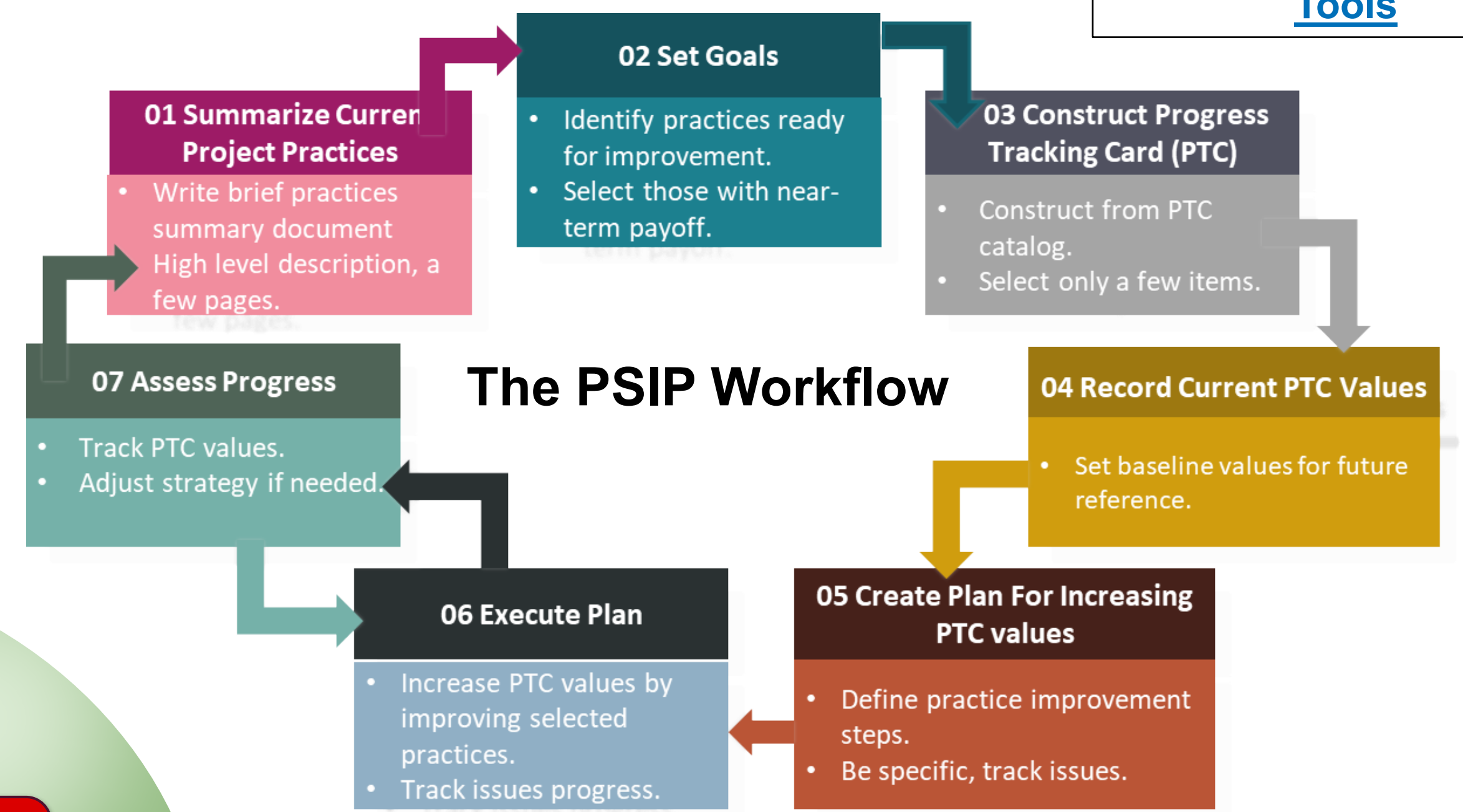
Improving the Development Experience

Productivity and Sustainability Improvement Planning (PSIP)

- A simple methodology to help improve software development practices
- Focus on small, measurable improvements over a short time frame (months)
- Numerous incremental improvements add up over time
- IDEAS Productivity project members assist ECP software teams
 - Interview to document current practices and challenges
 - Assistance selecting target for improvement and tracking progress
- Can be implemented without outside help
- Leverage available resources to learn new techniques (see Outreach and Better Scientific Software sections below)



The **PSIP Tools** GitHub repo is a collection of documents that enable the adoption and use of PSIP for a software team:
<https://github.com/better-scientificsoftware/PSIP-Tools>



Common Challenges

- Implementing or expanding testing
- Onboarding and offboarding of team members
- Making better use of modern language features
- Improving and maintaining documentation
- Understanding performance and opportunities for improvement
- Ensuring citation and credit for software
- Bringing best practices to long-lived codes
- Version control workflows
- Effective, but lightweight management of development

Outreach

Tutorials

- Full-day and half-day variants
 - Hands-on in full-day
- Recent venues
 - ATPESC (2016-2018)
 - ECP Annual Meeting (2017-2018)
 - ISC (2018-2019)
 - SIAM CSE17
 - Supercomputing (2016-2018)
- Current tutorial modules
 - Overview of Best Practices for HPC Software Developers
 - Git Workflows
 - Better (Small) Scientific Software Teams
 - Improving Reproducibility through Better Software Practices
 - An Introduction to Software Licensing
 - Verification and Refactoring
 - Code Coverage and Continuous Integration



Best Practices for HPC Software Developers Webinar Series (HPC-BP)

- Monthly series, since May 2016
 - Traditional time slot is 1-2pm ET on a Wednesday
 - Which Wednesday varies
- Offered live and archived
- Presented by the community to the community
 - Not just IDEAS
- 29 webinars to date
 - 77 attendees per webinar on average
 - 1702 attendees total, to date
- Series info, archives, and mailing list for announcements
 - <https://ideas-productivity.org/events/hpc-best-practices-webinars/>



Webinar Site

Technical Meetings and Birds of a Feather Sessions

- We help create opportunities to talk about software development, productivity, and sustainability in more “academic” environments
 - <https://ideas-productivity.org/events/>
- Birds of a Feather sessions
 - Software Engineering and Reuse for Computational Science and Engineering
 - SC15, SC16, SC17, SC18, ISC 2019
 - See <http://bit.ly/swe-cse-bof>
- Minisymposia
 - SIAM Computational Science and Engineering (2015, 2017, 2019)
 - PASC (2018, 2019)
- Thematic poster sessions
 - SIAM CSE (2017, 2019)



BOF Site

SIAM CSE19
Minisymposium
posters, archived
on FigShare



Better Scientific Software

Building an Online Community

- A **community-based resource** for scientific software improvement information exchange
- 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

Types of content on BSSw

- **Blog articles:** success stories, perspectives, opportunities, and more
- **Curated content:** short pointers to useful material already hosted elsewhere
- **Original content:** content primarily hosted on BSSw
- **Events:** increase awareness of events related to better scientific software
- **Community Landing Pages:** provide an perspective on BSSw resources tailored to a particular technical community



BSSw Monthly Email Digest

