



Supporting Science the IDEAS Way

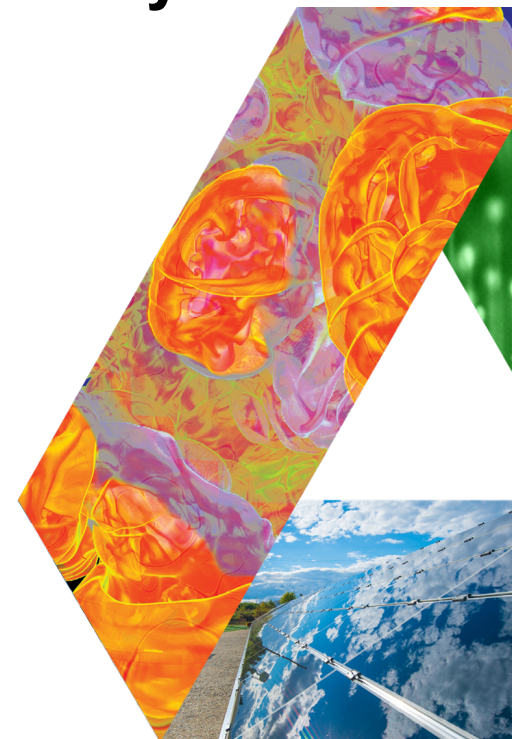


Anshu Dubey
Argonne National Laboratory

Xpert Network Webinar

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exascaleproject.org



U.S. DEPARTMENT OF
ENERGY

Office of
Science



Acknowledgements

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- This work was performed in part at the Argonne National Laboratory, which is managed by UChicago Argonne, LLC for the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.

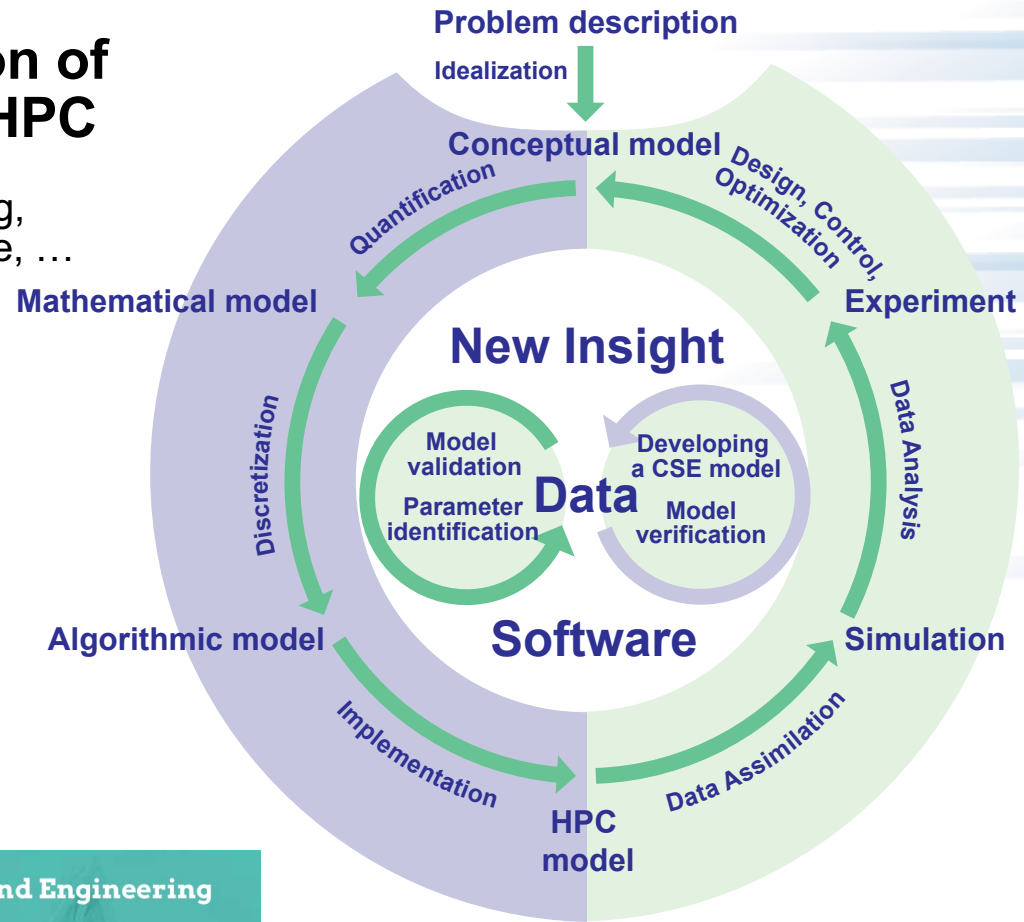
Software is the foundation of sustained collaboration in HPC

- computational science and engineering, data science, learning/AI, infrastructure, ...

Software quality is critical for science quality

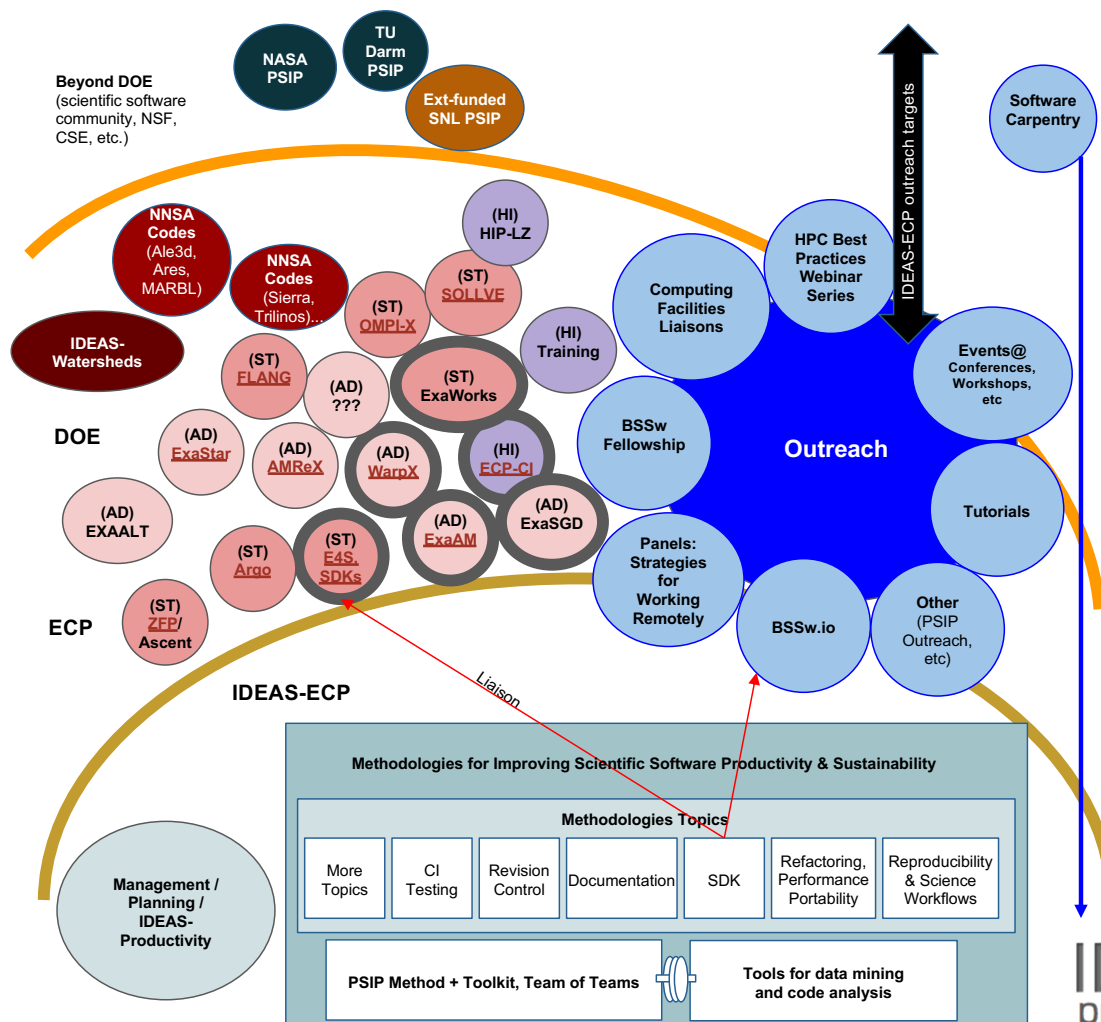
Ref: [Research and Education in Computational Science and Engineering](#),
U. Rude, K. Willcox, L.C. McInnes,
H. De Sterck, **SIAM Review**, 2018

SIAM Activity Group on Computational Science and Engineering



IDEAS
productivity

ECIP
EXASCALE
COMPUTING
PROJECT



IDEAS-ECP

<https://ideas-productivity.org/ideas-ecp>

Focus: Help ensure that DOE investment in the exascale software ecosystem is as productive and sustainable as possible.

A map of teams, activities, connections between them, and connections to the outside world.

Figure by Hai Ah Nam

IDEAS
productivity

ECP

EXASCALE
COMPUTING
PROJECT

Deeper Dive into a Few Activities

Better Scientific Software: 2021 Highlights

SHARE in f t



2021 HIGHLIGHTS

**Community portal
for engaging in
better scientific
software**

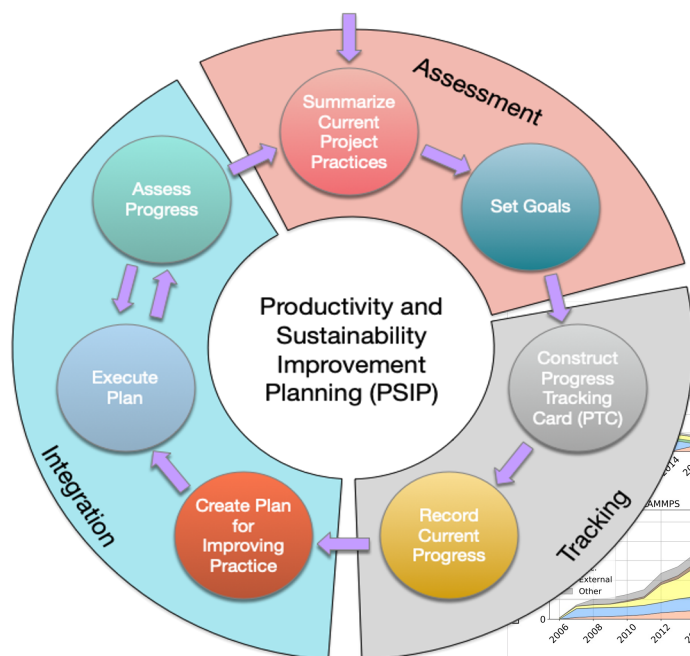
Resources for

- ☐ Better Planning
- ☐ Better Development
- ☐ Better Performance
- ☐ Better Reliability
- ☐ Better Collaboration
- ☐ Better Skills

Artifacts

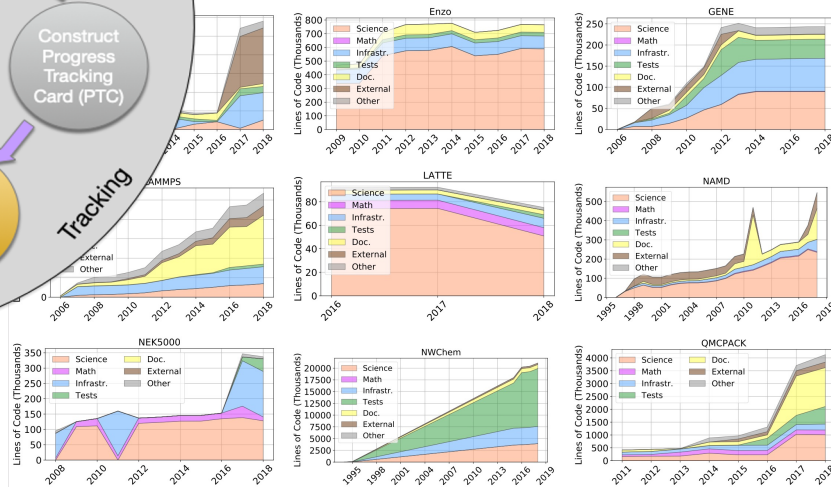
- ☐ Curated content
- ☐ Original articles
- ☐ Blogs
- ☐ Events

Tools and Methodologies



Reference:

Grannan A, Sood K, Norris B, Dubey A. Understanding the landscape of scientific software used on high-performance computing platforms. *The International Journal of High Performance Computing Applications*. 2020;34(4):465-477. doi:[10.1177/1094342019899451](https://doi.org/10.1177/1094342019899451)



Reference:

Elaine M. Raybourn, Greg Watson, Elsa Gonsiorowski, Reed Milewicz, David M. Rogers, Benjamin H. Sims, Jim Willenbring. (in press) Automating Software Productivity Planning: Lightweight Tools for Upgrading Team Practices. The International Conference on Software Engineering Research and Practice (SERP'21), July 26-29, 2021.

Tools

Repository Analysis

- ☐ Contribution & activity
- ☐ Issues
- ☐ Turnarounds
- ☐ Categorization

Documentation

- ☐ Automate syncing with code

Methodologies

- ☐ PSIP
- ☐ Howtos
- ☐ Capture knowledge and document it

BSSw Tutorials

Screenshot from SC21

BSSw Tutorial Web Site

- <https://bssw-tutorial.github.io/> is the one URL you need to find all of 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

Better Scientific Software
A tutorial presented at:
The International Conference for High-Performance Computing, Networking, Storage, and Analysis (SC21)
on 8/9 Nov - 1:00 pm CST Monday 15 November 2021
Presenters: David S. Bernholdt (Oak Ridge National Laboratory, Oak Ridge, Tennessee), Rinku Gupta (Oak Ridge National Laboratory, Oak Ridge, Tennessee), Johannes Gebert (Oak Ridge National Laboratory), and Gregory K. Watson (Oak Ridge National Laboratory)

Quick Links:

- Program Page (SC21 Website)
- Presentation Slides (Right)
- Download Code Repository (GitHub)

On this Page:

- Description
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- Presentation Slides
- Download Code Repository
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Description:

Computational science and engineering (CSE) is in the midst of an extremely challenging period caused by the confluence of disruptive change in computing architecture, demand for greater security, reproducibility, sustainability, and quality, and new opportunities for greatly improved simulation capabilities, especially through emerging hardware and software. These challenges demand increased investment in research, education, and workforce development to ensure the future success of the CSE community.

IDEAS productivity ECP EXASCALE COMPUTING PROJECT

Greg Watson Rinku Gupta Johannes Gebert...
David Rogers David Bernholdt Sian Jin
Daniel Magorian Charles Cheung Patricia Grube...
John LaGrone (SMU) Video feed Joanna Leng
Ben Cronheim Carol Warren Powers
Perrefort, Daniel Jose... Brian Wylie Olli Lupton
08088 Ryan M Kasoar, Elliott...
08088 Ryan M Kasoar, Elliott (STFC,...)

Unmute Start Video Security Participants 25 Chat Share Screen Pause/Stop Recording Live Transcript Breakout Rooms Reactions Leave

Topics

Existing Modules

- ☐ Design
- ☐ Agile methodologies
- ☐ Git workflows
- ☐ Reproducibility
- ☐ Testing and CI
- ☐ Refactoring

Under Development

- ☐ Packaging
- ☐ Documentation

Venues

- ☐ SC
- ☐ ISC
- ☐ ECP annual meetings
- ☐ SEA
- ☐ SIAM-CSE

Other Outreach Activities

BSSw Fellowships

- ❑ Collaboration with NSF and Krell Institute
- ❑ Selected annually based on project proposals
- ❑ Growing a community

Panel Series

- ❑ Strategies for working remotely
- ❑ Performance portability in the Exascale Computing Project

Birds of Feather Sessions at Conferences

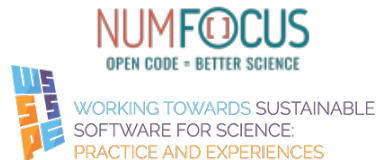
- ❑ SC
- ❑ ISC

Webinar series: Best Practices for HPC Software Developers

- ❑ Longest ongoing outreach activity

52	Wed 12 May 2021 1:00 pm EDT	<i>Automated Fortran-C++ Bindings for Large-Scale Scientific Applications,</i>
53	Wed 9 Jun 2021 1:00 pm EDT	<i>Using the PSIP Toolkit to Achieve Your Goals – A Case Study at The HDF Group,</i>
54	Wed 7 Jul 2021 1:00 pm EDT	<i>Mining Development Data to Understand and Improve Software Engineering Processes in HPC Projects,</i>
55	Wed 4 Aug 2021 1:00 pm EDT	<i>Software Engineering Challenges and Best Practices for Multi-Institutional Scientific Software Development,</i>
56	Wed 15 Sep 2021 2:00 pm EDT	<i>What I Learned from 20 Years of Leading Open Source Projects,</i>
57	Wed 13 Oct 2021 1:00 pm EDT	<i>Migrating to Heterogeneous Computing: Lessons Learned in the Sierra and El Capitan Centers of Excellence,</i>
58	Wed 10 Nov 2021 1:00 pm EST	<i>55+ years in High-Performance Computing: One Woman's Experiences and Perspectives,</i>
59	Wed 8 Dec 2021 1:00 pm EST	<i>Scientific software ecosystems and communities: Why we need them and how each of us can help them thrive,</i>

Impact



Together we are promoting communication regarding software productivity and sustainability

Changes are already visible in the culture of scientific computing

- Research Software Alliance: <https://www.researchsoft.org>
- Software Sustainability Institute: <https://www.software.ac.uk>
- US Research Software Sustainability Institute: <https://urssi.us/>
- NumFOCUS: <https://www.numfocus.org>
- WSSSPE: <http://wssspe.researchcomputing.org.uk/>
- Software Carpentry: <https://software-carpentry.org>
- Research Software Engineering (RSE) movement: <https://society-rse.org> <https://us-rse.org>
- IDEAS Productivity: <https://ideas-productivity.org>
- Better Scientific Software: <https://bssw.io>
- And more ...

Ref: [Community Organizations: Changing the Culture in Which Research Software Is Developed and Sustained](#), D.S. Katz, L.C. McInnes, et al, **IEEE CISE**, 2019

