



Welcome to...



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Assisted by Patricia Grubel, Rinku Gupta

8:30am-5:00pm, Monday 18 November 2019



Tutorial slides

<http://bit.ly/sc19-bssw-tutorial>



See slide 2 for
license details and
requested citation

Tutorial evaluation

<http://bit.ly/sc19-bssw-eval>



License, Citation and Acknowledgements



License and Citation

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- **The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, Michael A. Heroux, and Jared O'Neal, Better Scientific Software tutorial, in SC '19: International Conference for High Performance Computing, Networking, Storage and Analysis, Denver, Colorado, 2019. DOI: [10.6084/m9.figshare.10114880](https://doi.org/10.6084/m9.figshare.10114880)**
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software Tutorial...

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David



Anshu



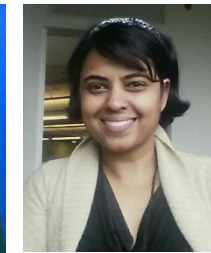
Mike



Jared



Pat



Rinku



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



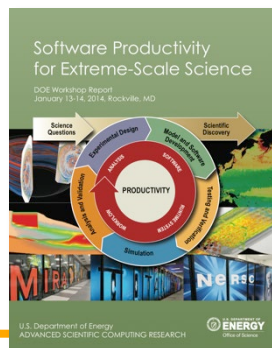
Interoperable Design of Extreme-scale Application Software (IDEAS)

Motivation

Enable **increased scientific productivity**, realizing the potential of extreme- scale computing, through **a new interdisciplinary and agile approach to the scientific software ecosystem**.

Objectives

Address confluence of trends in hardware and increasing demands for predictive multiscale, multiphysics simulations.
Respond to trend of continuous refactoring with efficient agile software engineering methodologies & improved software design.

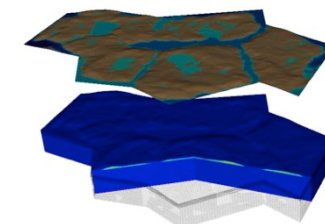
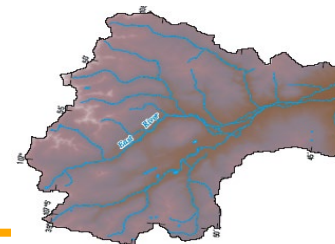


Project History

IDEAS began in 2014 as a DOE ASRC/BER partnership to improve application software productivity, quality, and sustainability. In 2017, the DOE Exascale Computing Project (ECP) began supporting IDEAS to help application teams improve developer productivity and software sustainability while making major changes for exascale.

Impact on Applications & Programs

Terrestrial ecosystem use cases tied initial IDEAS activities to programs in DOE Biological and Environmental Research (BER). The Exascale Computing Project (ECP) supports a broad portfolio of applications furthering science, energy, national security, and economic competitiveness.



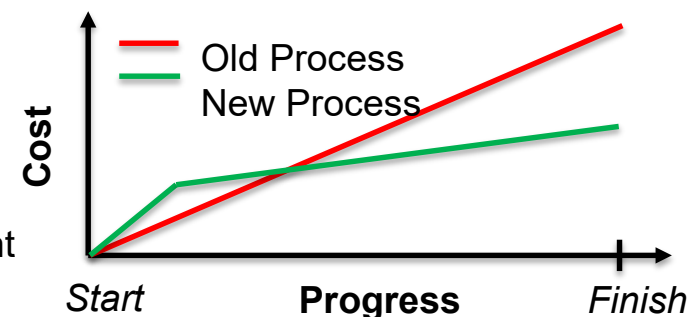
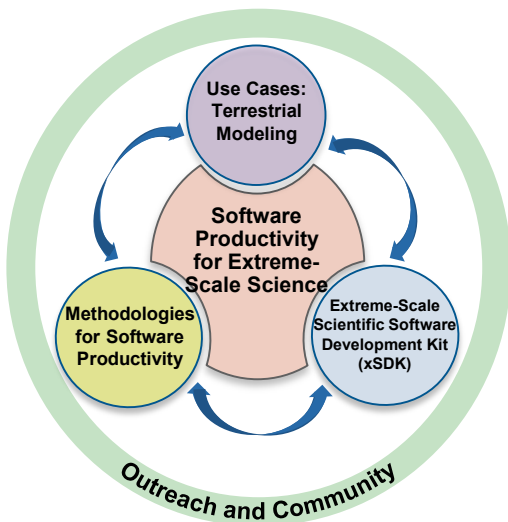
Approach

Interdisciplinary multi-institutional team (ANL, LANL, LBNL, LLNL, ORNL, PNNL, SNL, U. Oregon) with broad experience in scientific software development

Close partnerships with applications teams ensures impact on science Identification, documentation and dissemination of **best practices** for BER and ECP software teams and the broader community

Catalyzing **software process improvements** through tailored engagement with individual projects

Working to bend the curve of software development costs downwards



U.S. DEPARTMENT OF
ENERGY

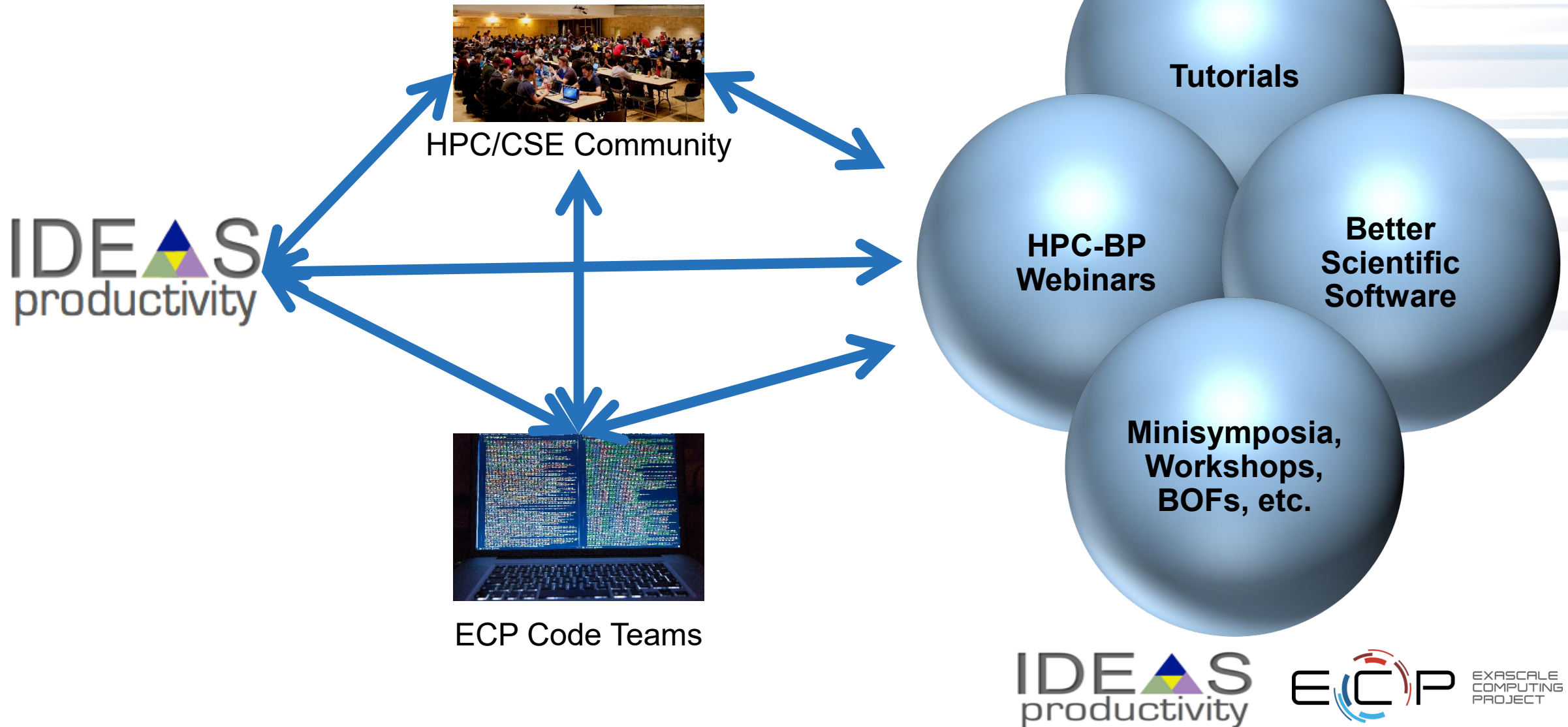
Office of
Science

ideas-productivity.org



EXASCALE
COMPUTING
PROJECT

How does IDEAS Achieve Its Goals?



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



Additional Software-Related Events at SC19

Bold events (co-)organized by IDEAS

Day/Time	Event Type	Event Title
Sunday	Tutorial	<u>Floating-Point Analysis and Reproducibility Tools for Scientific Software</u>
Sunday	Workshop	<u>The 2019 International Workshop on Software Engineering for HPC-Enabled Research (SE-HER 2019)</u>
Monday	Tutorial	<u>Better Scientific Software</u>
Monday	Tutorial	<u>Managing HPC Software Complexity with Spack</u>
Monday	Workshop	<u>3rd International Workshop on Software Correctness for HPC Applications (Correctness 2019)</u>
Monday	Students@SC	<u>Students@SC: Modern Software Design, Tools, and Practices</u>
Tuesday	BoF	<u>Extreme-Scale Scientific Software Stack (E4S)</u>
Tuesday	BoF	<u>Exchanging Best Practices in Supporting Computational and Data-Intensive Research</u>
Tuesday	Panel	<u>Developing and Managing Research Software in Universities and National Labs</u>
Wednesday	BoF	<u>Software Engineering and Reuse in Modeling, Simulation, and Data Analytics for Science and Engineering</u>
Thursday	BoF	<u>Quality Assurance and Coding Standards for Parallel Software</u>
Thursday	Panel	<u>Sustainability of HPC Research Computing: Fostering Career Paths for Facilitators, Research Software Engineers, and Gateway Creators</u>
Friday	Panel	<u>The Road to Exascale and Beyond is Paved by Software: How Algorithms, Libraries and Tools Will Make Exascale Performance Real</u>

Who Are You?

- Undergrad students
 - Graduate students
 - Postdocs
 - Faculty/staff
 - Manager
 - Other
- Academia
 - National Laboratories
 - Government
 - Industry
 - Other
- Domain scientist
 - Computer scientist
 - Applied mathematician
 - Other

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
8:30am-8:40am	00	Introduction and Setup	David E. Bernholdt, ORNL
8:40am-9:15am	01	Overview of Best Practices in HPC Software Development	David E. Bernholdt, ORNL
9:15am-10:00am	02	An Introduction to Software Licensing	David E. Bernholdt, ORNL
<i>10:00am-10:30am</i>		<i>Break</i>	
10:30am-11:30am	03	Agile Methodologies and Useful GitHub Tools	Michael A. Heroux, SNL
11:30am-12:00pm	04	Improving Reproducibility through Better Software Practices	Michael A. Heroux, SNL
<i>12:00pm-1:30pm</i>		<i>Lunch</i>	
1:30pm-2:15pm	05	Software Design and Testing	Anshu Dubey, ANL
2:15pm-2:45pm	06	Git Workflows	Jared O'Neal, ANL
2:45pm-3:00pm	07	Code Coverage and Continuous Integration	Jared O'Neal, ANL
<i>3:00-3:30pm</i>		<i>Break</i>	
3:30pm-3:50pm	07	Code Coverage and Continuous Integration (continued)	Jared O'Neal, ANL
3:50pm-5:00pm	08	Hands-on Activities and Additional Q&A	All

Setup for Hands-On Activities

A few things that you can multi-task on while the tutorial proceeds

- **GitHub account**
 - First used in module 03 Agile Methodologies
- **Travis CI account** linked to your GitHub account if you would like to use hands-on time to create your own repository linked with Travis CI
 - First used in module 07 Coverage/CI or module 08 Hands-On
- **Optional:** access to **additional tools** for a deeper dive in the Hands-On Activities
 - First used in module 08 Hands-On

Sign Up for a GitHub Account

1. Go to <https://github.com/>
2. Enter a username, your email address, and a password
3. Verify that you're a real person
4. Select the free plan
5. Complete or skip the interests survey
6. Check your email and complete the verification
7. *You're ready to go!*

Connect your GitHub Account to Travis CI

1. Go to <https://travis-ci.com/>
2. Click Sign Up with GitHub
3. Authorize Travis CI to access your GitHub account

Taking the Hands-On Elbows-Deep (Optional)

Depending on your interests, you will need access to a system with some or all of the following tools:

- Could be local or remote
- Git
- Python and perl
- A compiler suite (examples will be available in C++ and Fortran)
- Gcov code coverage tool (part of GCC compiler suite)

Additional tools of possible interest, but not strictly necessary

- Doxygen
- Ruby, rake & FRUIT Fortran Unit Test Framework (talk to Jared if interested)
 - <https://sourceforge.net/p/fortranxunit/wiki/Home/>