Welcome to...



David E. Bernholdt, Anshu Dubey, Michael Heroux, Alicia Klinvex

8:30am-12:00pm, Monday 13 November 2017

Tutorial evaluation form: http://bit.ly/sc17-eval

Final version of tutorial slides: http://bit.ly/bssw-tutorial

Requested citation: David E. Bernholdt, Anshu Dubey, Michael Heroux, and Alicia Klinvex, Better Scientific Software, tutorial, in SC '17: International Conference for High Performance Computing, Networking, Storage and Analysis, Denver, Colorado, 2017. DOI: 10.6084/m9.figshare.c.3928039.





Tutorial Instructors

- David Bernholdt, ORNL
- Anshu Dubey, ANL
- Mike Heroux, SNL
- Alicia Klinvex, SNL









Members of the IDEAS Scientific Software Productivity Project: www.ideas-productivity.org

 Focus: Increasing CSE software productivity, quality, and sustainability





DEAS Interoperable Design of Extreme-scale productivity 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.

> **Use Cases Terrestrial**

Modeling

Software

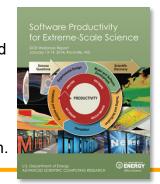
Productivity

for Extreme-Scale Science

Methodologies

for Software

Productivity



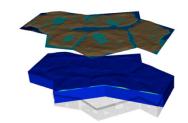
Project History

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 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

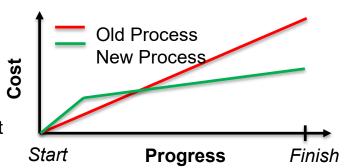
Interdisciplinary multi-institutional team (ANL, LANL, LBNL, LLNL, ORNL, PNNL, SNL, U. Oregon) with broad experience in scientific software development

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





Extreme-Scale

Scientific Software

Development Kit



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:

- Information, examples, exercises, pointers to other resources
- Not to prescribe any set of 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





Agenda

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Time	Topic	Speaker
8:30am-8:45am	Why effective software practices are essential for CSE projects	David E. Bernholdt, ORNL
8:45am-9:15am	Introduction to software licensing	David E. Bernholdt, ORNL
9:15am-9:45am	Better (small) scientific software teams	Michael A. Heroux, SNL
9:45am-10:00am	Improving Reproducibility Through Better Software Practices	Michael A. Heroux, SNL
10:00am-10:30am	Break	
10:30am-10:45am	Testing of HPC Scientific Software: Introduction	Alicia M. Klinvex, SNL
10:45am-11:15am	Verification	Anshu Dubey, ANL
11:15am-11:45am	Evaluating project testing needs	Anshu Dubey, ANL
11:45am-12:00pm	Code coverage demo and CI demo	Alicia M. Klinvex, SNL



