Welcome to…

better scientific software

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9:00am-12:30pm, Monday 14 January 2019

U.S. DEPARTMENT OF ENERGY | Office of Science

NNSA National Nuclear Security Administration

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- Each module of this tutorial is available individually with its own citation. The complete collection of modules comprising this tutorial has been archived under a single DOI.

- **The requested citation for the complete collection of modules comprising tutorial is: David E. Bernholdt, Anshu Dubey, and Jared O'Neal, Better Scientific Software Tutorial, in Exascale Computing Project Annual Meeting, Houston, Texas, 2019. DOI: 10.6084/m9.figshare.7581746**

Tutorial Instructors

- David Bernholdt, ORNL
- Anshu Dubey, ANL
- Jared O'Neal, ANL

David   Anshu   Jared

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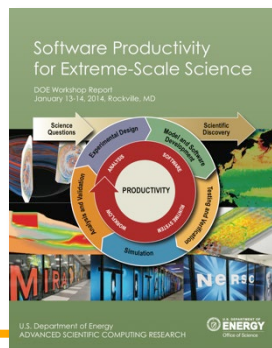
IDEAS productivity

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 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.
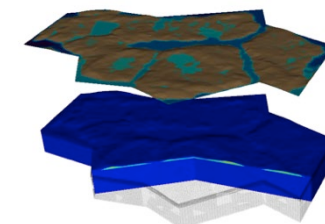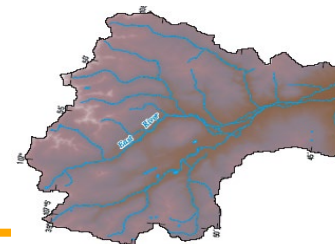

Approach

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
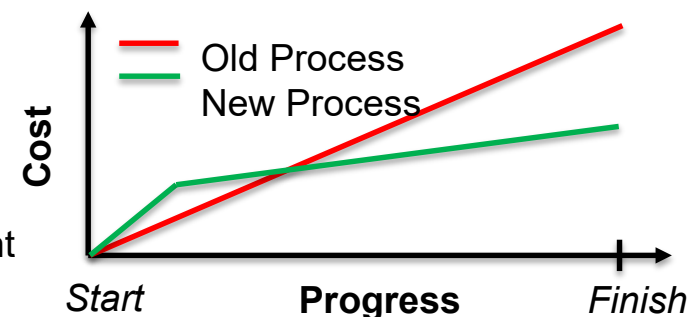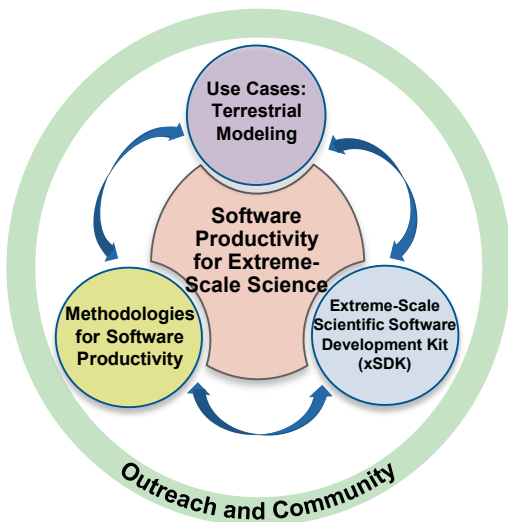
ideas-productivity.org

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
9:00am-9:30am	01	Overview of Best Practices in HPC Software Development	Anshu Dubey, ANL
9:30am-10:00am	02	Better (Small) Scientific Software Teams	David E. Bernholdt, ORNL
10:00am-10:30am	03	Improving Reproducibility through Better Software Practices	David E. Bernholdt, ORNL
10:30am-11:00am		*Break*	
11:00am-11:45am	04	Verification & Refactoring	Anshu Dubey, ANL
11:45am-12:30pm	05	Git Workflow & Continuous Integration	Jared O'Neal, ANL