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



See slide 2 for license details and requested citation







exascaleproject.org

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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 comprising this tutorial has been archived under a single DOI.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: <u>10.6084/m9.figshare.7581746</u>

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Tutorial Instructors

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



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



IDEAS 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.



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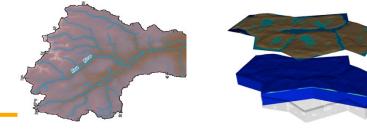
Science

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

Project History

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.



Use Cases Terrestrial Modeling Software Productivity for Extreme-Scale Science Extreme-Scale Methodologies Scientific Software for Software Development Kit (xSDK) Outreach and Commu

Productivity

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

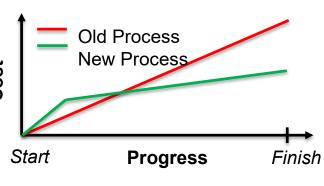
changes for exascale.

Approach

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	Торіс	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

