Welcome to…

better scientific software

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8:30am-5:00pm, Monday 12 November 2018

Tutorial slides
http://bit.ly/sc18-bssw-tutorial

Tutorial evaluation form
http://bit.ly/sc18-eval

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License and Citation

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- Each module of this tutorial is available individually with its own citation and DOI. Details in each module. This module is DOI: 10.6084/m9.figshare.7309877
- **The requested citation the complete collection of modules representing this whole tutorial is: David E. Bernholdt, Anshu Dubey, Michael A. Heroux, and Jared O'Neal, Better Scientific Software tutorial, in SC '18: International Conference for High Performance Computing, Networking, Storage and Analysis, Dallas, Texas, 2018. DOI: 10.6084/m9.figshare.c.4293800**

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IDEAS productivity

ECP EXASCALE COMPUTING PROJECT

Tutorial Instructors

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


David


Anshu


Mike


Jared

Argonne NATIONAL LABORATORY

Sandia National Laboratories

OAK RIDGE National Laboratory

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

IDEAS productivity

ECP EXASCALE COMPUTING PROJECT

Interoperable Design of Extreme-scale Application Software (IDEAS)

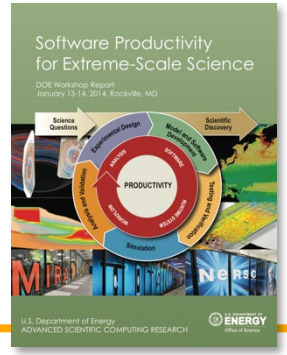
Motivation

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.

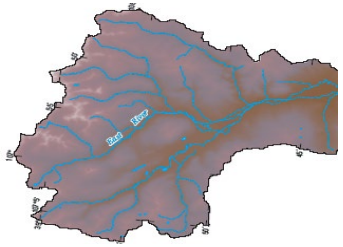


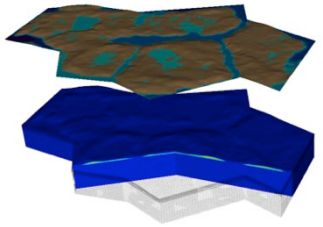
Project History

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.

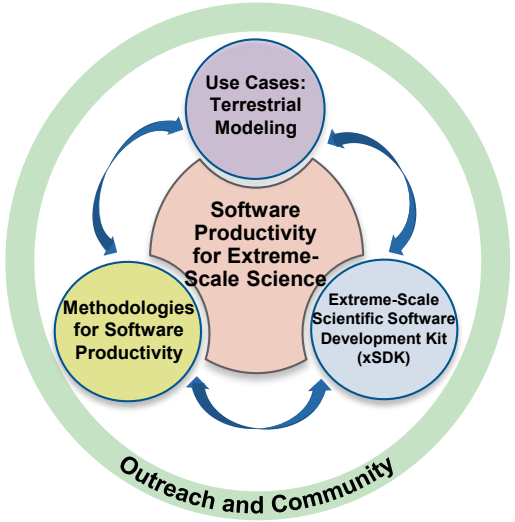
Impact on Applications & Programs

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



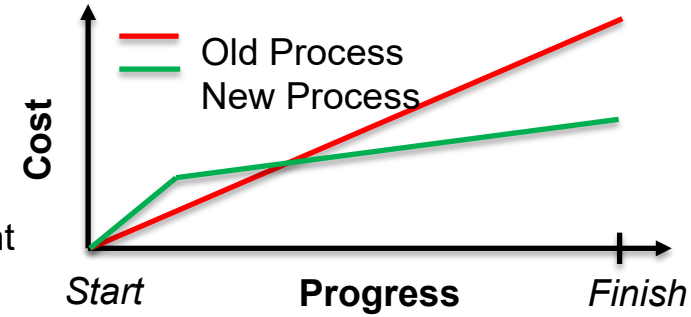
Interdisciplinary multi-institutional team (ANL, LANL, LBNL, LLNL, ORNL, PNNL, SNL, U. Oregon) with broad experience in scientific software development

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



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ideas-productivity.org

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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-9:00am	01	Overview of Best Practices in HPC Software Development	David E. Bernholdt, ORNL
9:00am-10:00am	02	Git Workflows	Jared O'Neal, ANL
10:00am-10:30am		*Break*	
10:30am-11:40am	03	Better (Small) Scientific Software Teams	Michael A. Heroux, SNL
11:40am-12:00pm	04	Improving Reproducibility through Better Software Practices	Michael A. Heroux, SNL
12:00pm-1:30pm		*Lunch (C1/2/3/4 Ballroom, 2nd floor)*	
1:30pm-2:15pm	05	An Introduction to Software Licensing	David E. Bernholdt, ORNL
2:15pm-2:55pm	06	Verification and Refactoring	Anshu Dubey, ANL
2:55pm-3:00pm	07	Code Coverage and Continuous Integration	Jared O'Neal, ANL
3:00-3:30pm		*Break*	
3:30pm-3:40pm	07	Code Coverage and Continuous Integration (continued)	Jared O'Neal, ANL
3:40pm-5:00pm	08	Hands-on Activities	Jared O'Neal, ANL, and team

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

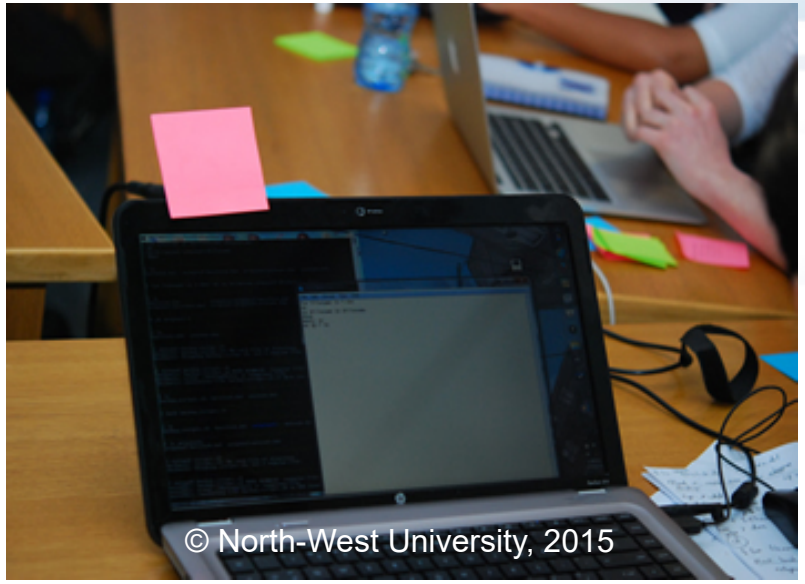
Sticky Notes

More on sticky note teaching
https://github.com/gvwilson/sticky-note-teaching

- We're passing out two colored sticky notes to each of you
- You can use these to signal us, especially during hands-on by sticking them to the top of your laptop screen like flags

Everything's cool. Ready to proceed

I could use a little help



- Remember to "reset" (take the sticky down) once you've been helped or everyone has synced

IDEAS productivity

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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 Teams
- **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/