Welcome to…

better scientific software

David E. Bernholdt, Anshu Dubey, Jared O'Neal

2:00pm-6:00pm, Sunday 16 June 2019

U.S. DEPARTMENT OF **ENERGY** | Office of Science

NN**S**A National Nuclear Security Administration

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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**
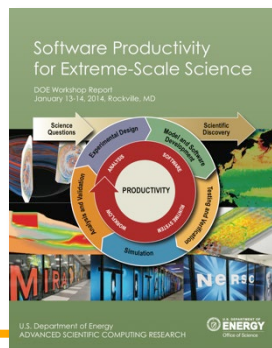
IDEAS productivity

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.
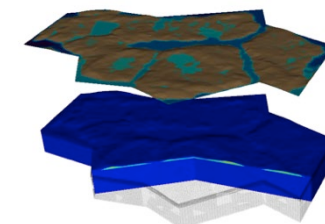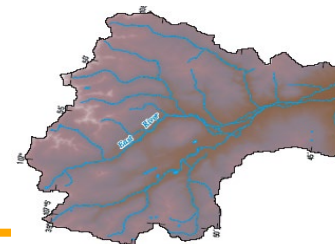
Approach

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
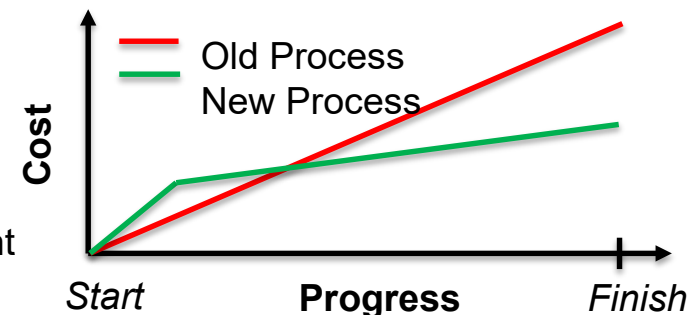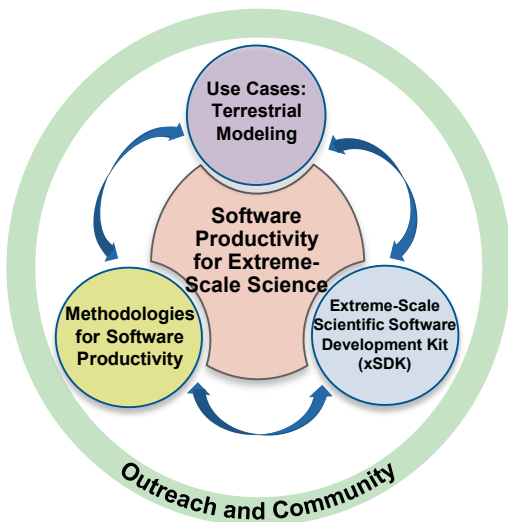
Old Process
New Process

Cost

Start   **Progress**   Finish

ideas-productivity.org

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ECP EXASCALE COMPUTING PROJECT

How does IDEAS Achieve Its Goals?

HPC/CSE Community

ECP Code Teams

Tutorials

HPC-BP Webinars

Better Scientific Software

Minisymposia, Workshops, BOFs, etc.
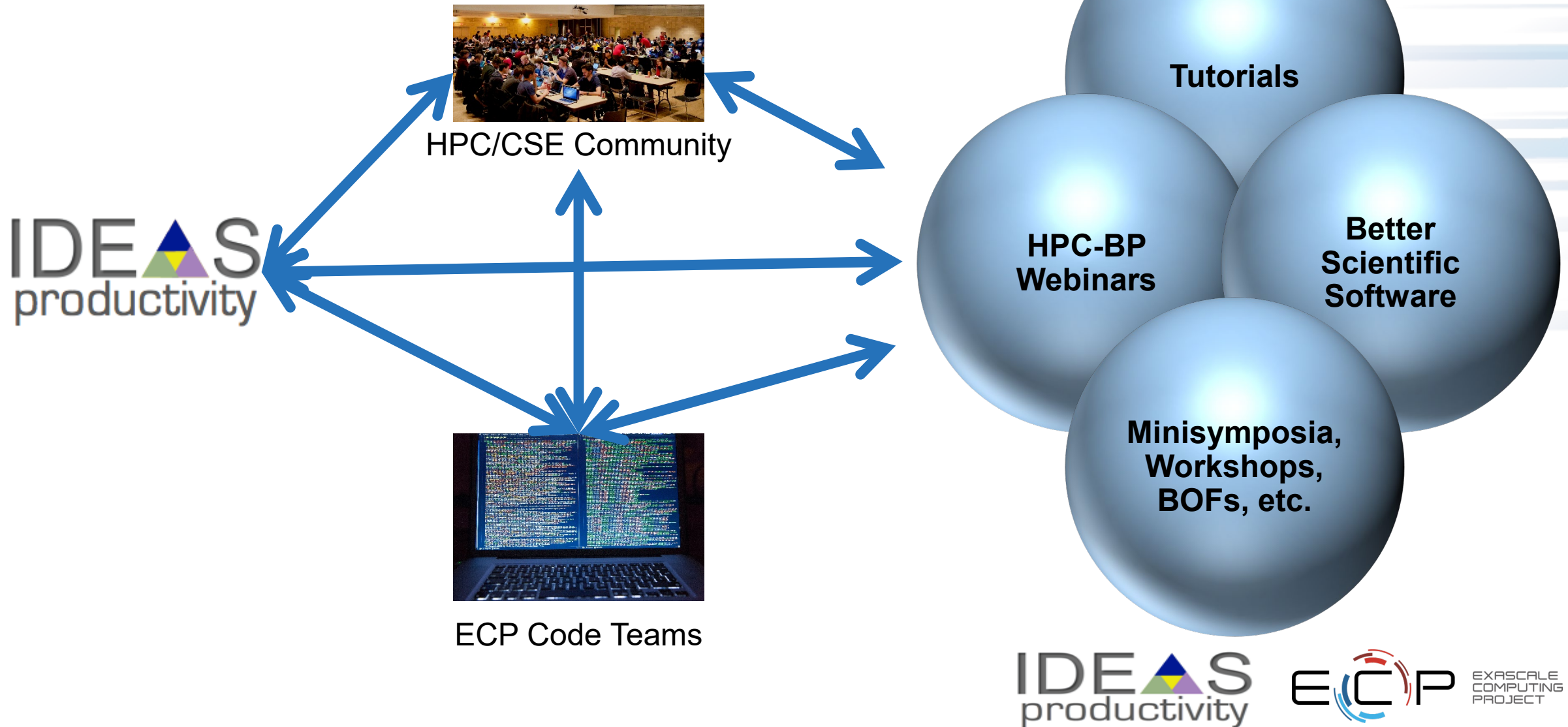
Additional Software-Related Events at ISC 2019

- **Tuesday — BOF — Spack Community BOF**

- Tuesday - Presentation - Parallel Programming - Painful or Productive?

- Tuesday - Poster - (WHPC04) Research Software Engineering enabling HPC

- Tuesday - Poster - (PP06): The International HPC Certification Program

- Tuesday - Poster - (PP09): EPEEC: Productivity at Exascale

- **Tuesday — Poster — (PP24): Helping You Improve Software Sustainability and Development Productivity: An Overview of the IDEAS Project**

- Wednesday — Focus Session — New Approaches, Algorithms Towards Exascale Computing

- **Wednesday — BOF — Software Engineering and Reuse in Computational Science and Engineering** (additional details: http://bit.ly/swe-cse-bof)

- Wednesday - BOF - Performance Portability and Productivity: Panel Discussion

Note: **Bold font** denotes events (co-)organized by the IDEAS Productivity project

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

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
2:00pm-2:40pm	01	Overview of Best Practices in HPC Software Development	Anshu Dubey, ANL
2:40pm-3:20pm	02	Better (Small) Scientific Software Teams	David E. Bernholdt, ORNL
3:20pm-4:00pm	03	Improving Reproducibility through Better Software Practices	David E. Bernholdt, ORNL
4:00pm-4:30pm		*Break*	
4:30pm-5:15pm	04	Verification & Refactoring	Anshu Dubey, ANL
5:15pm-6:00pm	05	Git Workflow & Continuous Integration	Jared O'Neal, ANL

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