Introduction to the IDEAS Software Productivity Project

Mike Heroux (SNL), Lois Curfman McInnes (ANL), J. David Moulton (LANL), David Bernholdt (ORNL), Hans Johansen (LBNL)

And all IDEAS project members

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Confluence of trends

- **Fundamental trends:**
  - Disruptive HW changes: Requires thorough algorithm/code refactoring
  - Demands for coupling: Multiphysics, multiscale
- **Challenges:**
  - Need refactorings: Really, continuous change
  - Modest app development funding: No monolithic apps
  - Requirements are unfolding, evolving, not fully known *a priori*
- **Opportunities:**
  - Better design and SW practices & tools are available
  - Better SW architectures: Toolkits, libraries, frameworks
- **Basic strategy: Focus on <u>productivity</u>**

Interoperable Design of Extreme-scale Application Software (IDEAS)

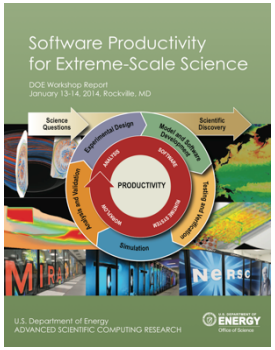
Motivation

Enable ***increased scientific productivity,*** realizing the potential of extreme-scale computing, through ***a new interdisciplinary and agile approach to the scientific software ecosystem.***

Objectives

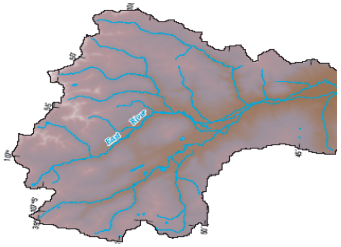
Address confluence of trends in hardware and increasing demands for predictive multiscale, multiphysics simulations.

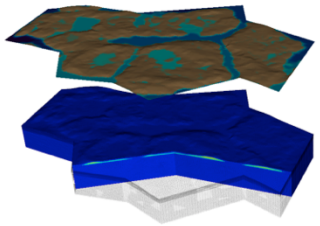
Respond to trend of continuous refactoring with efficient agile software engineering methodologies and improved software design.

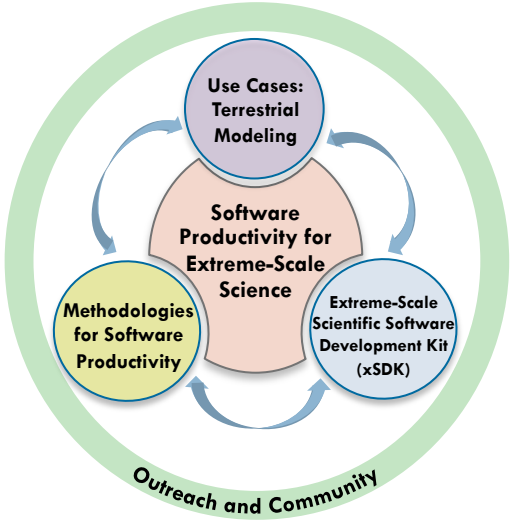


Impact on Applications & Programs

Terrestrial ecosystem ***use cases tie IDEAS to modeling and simulation goals*** in two Science Focus Area (SFA) programs and both Next Generation Ecosystem Experiment (NGEE) programs in DOE Biologic and Environmental Research (BER).







Approach

ASCR/BER partnership ensures delivery of both crosscutting methodologies and metrics with impact on real application and programs.

Interdisciplinary multi-lab team (ANL, LANL, LBNL, LLNL, ORNL, PNNL, SNL)

ASCR Co-Leads: Mike Heroux (SNL) and Lois Curfman McInnes (ANL)

BER Lead: David Moulton (LANL)

Topic Leads: David Bernholdt (ORNL) and Hans Johansen (LBNL)

Integration and synergistic advances in three communities deliver scientific productivity; outreach establishes a new holistic perspective for the broader scientific community.

www.ideas-productivity.org

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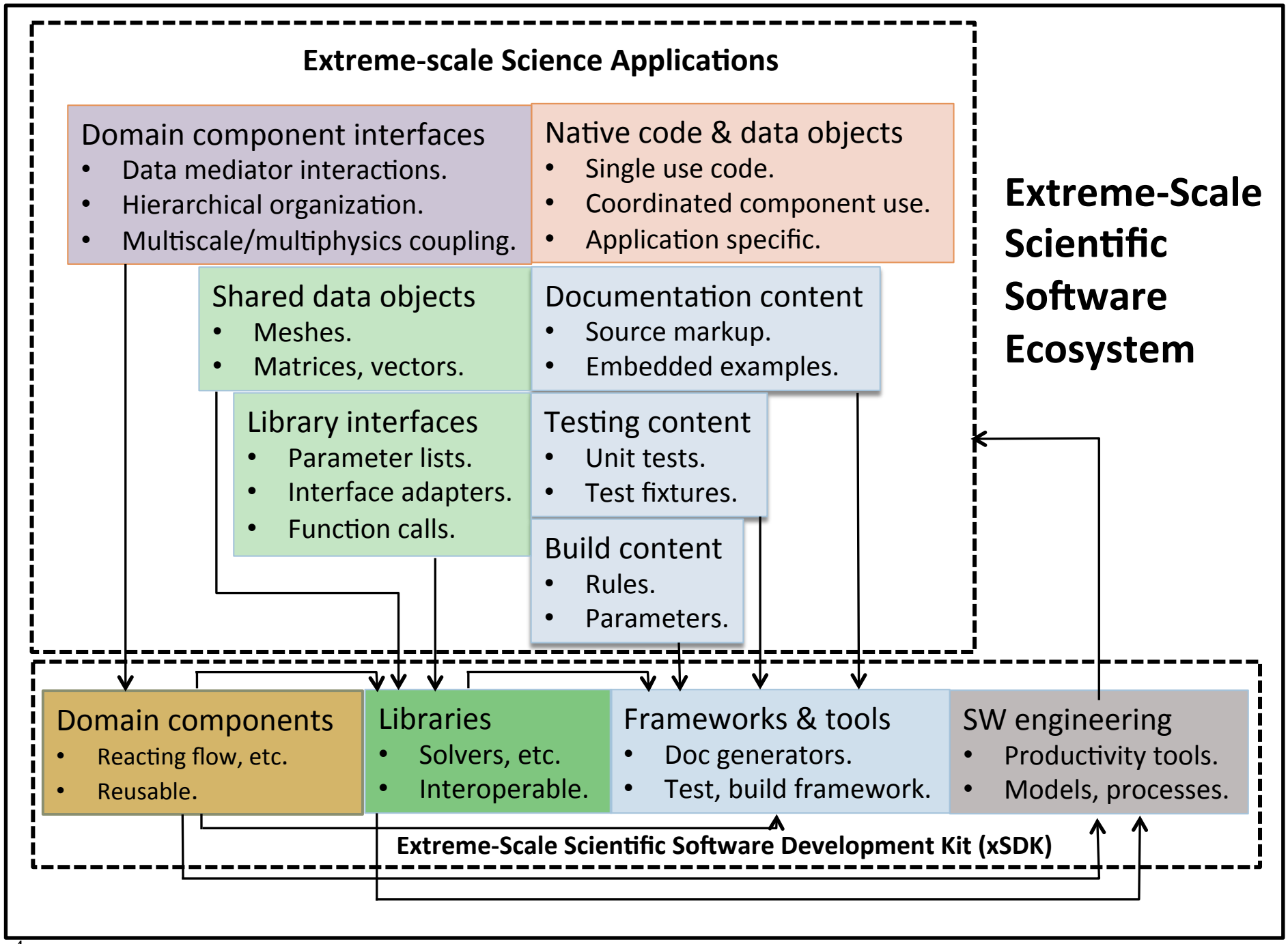
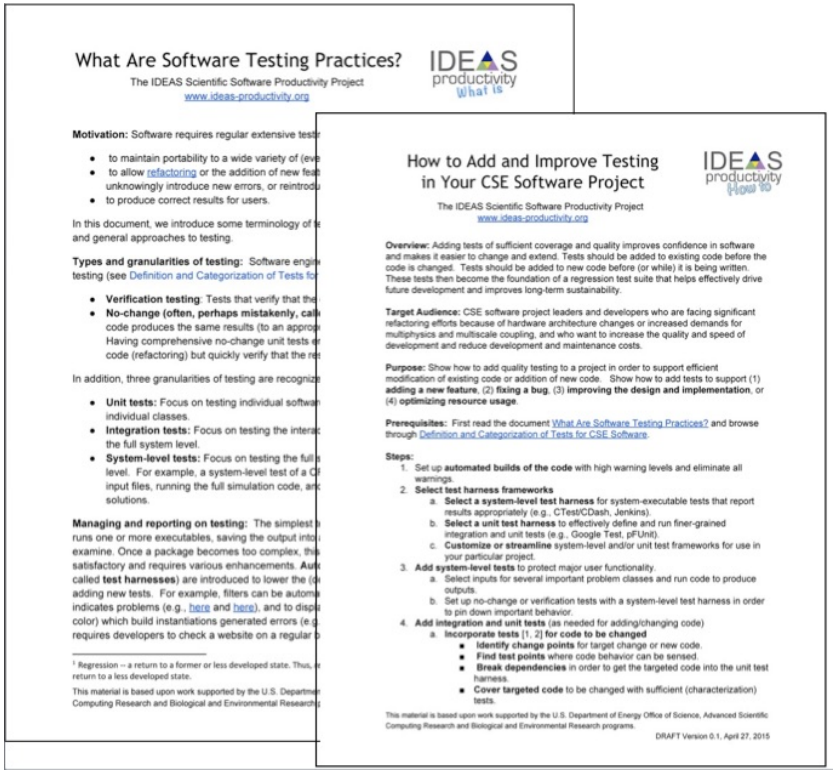

Extreme-scale Science Applications
Domain component interfaces
• Data mediator interactions.
• Hierarchical organization.
• Multiscale/multiphysics coupling.
Native code & data objects
• Single use code.
• Coordinated component use.
• Application specific.
Shared data objects
• Meshes.
• Matrices, vectors.
Documentation content
• Source markup.
• Embedded examples.
Library interfaces
• Parameter lists.
• Interface adapters.
• Function calls.
Testing content
• Unit tests.
• Test fixtures.
Build content
• Rules.
• Parameters.
Extreme-Scale Scientific Software Ecosystem
Domain components
• Reacting flow, etc.
• Reusable.
Libraries
• Solvers, etc.
• Interoperable.
Frameworks & tools
• Doc generators.
• Test, build framework.
SW engineering
• Productivity tools.
• Models, processes.
Extreme-Scale Scientific Software Development Kit (xSDK)

IDEAS 'What is' and 'How to' docs

- **Motivation:** Scientific software teams have a wide range of levels of maturity in software engineering practices
  - Baseline survey of *xSDK* and *BER Use Case* teams
- **Approach:**
  - **'What Is' docs:** 2-page characterizations of important software project topics
  - **'How To' docs:** brief sketch of best practices
    - Emphasis on ``bite-sized'' topics enables CSE software teams to consider improvements at a small but impactful scale
- **Initial emphasis:**
  - *What is CSE Software Productivity?*
  - *What are Software Testing Practices?*
  - *How to Add and Improve Testing in Your CSE Software Project*
- **Topics in progress:**
  - Refactoring tools and approaches
  - Best practices for using interoperable libraries
  - Designing for performance portability
  - Etc.

https://ideas-productivity.org/resources/howtos

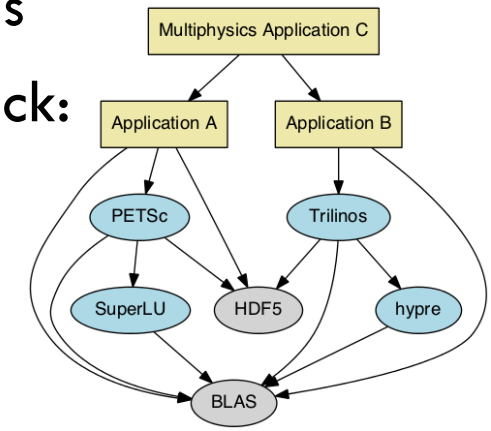


Impact: Provide baseline nomenclature and foundation for next steps in SW productivity and SW engineering for CSE teams.

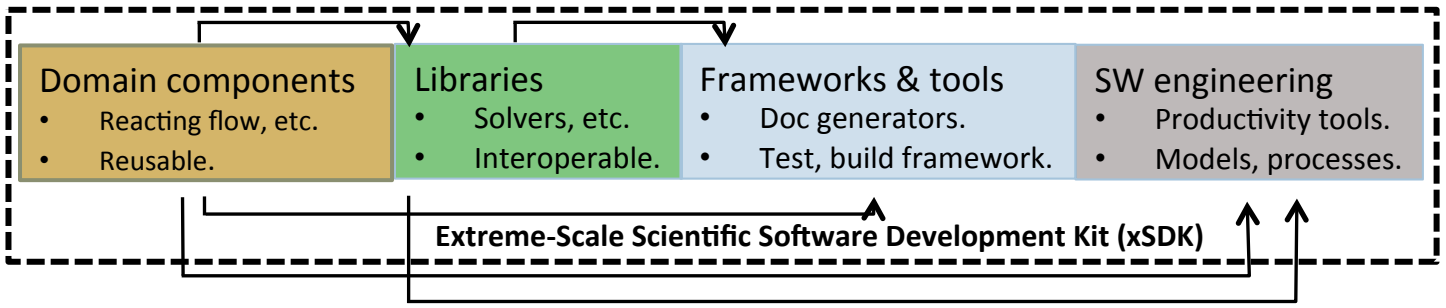
xSDK: Working toward the development of a highly effective extreme-scale scientific software ecosystem

Focus: Increasing the functionality, quality, and interoperability of important scientific libraries and development tools

- **xSDK foundations:** Seeking community feedback: https://ideas-productivity.org/resources/xsdk-docs/
  - xSDK package compliance standards
  - xSDK standard configure and CMake options
- Library interoperability
- Designing for performance portability



Standard xSDK package installation interface facilitates combined use of xSDK libraries (initially hypre, PETSc, SuperLU, Trilinos), as needed by BER use cases and other multiphysics apps.



IDEAS productivity

Better software productivity is essential for extreme-scale CSE

- **Better SW productivity can give us better, faster *and* cheaper**
  - **Better:** Science, portability, robustness, composability
  - **Faster:** Execution, development, dissemination
  - **Cheaper:** Fewer staff hours and lines of code

Essential mechanism for progress
- In time of disruptive change
- In presence of multiple design tradeoffs

- **IDEAS project**
  - **Enabling production of high-quality science results, rapidly and efficiently**
    - Multiscale terrestrial ecosystem science
    - Broadly: DOE extreme-scale scientific apps
  - **Delivering first-of-a-kind extreme-scale scientific software ecosystem**
    - xSDK
    - SWP methodologies ("HowTo")
    - Outreach and community