Interoperable Design of Extreme-scale Application Software (IDEAS): Software development methodologies that enhance scientific productivity

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While emerging extreme-scale computers provide unprecedented resources for scientific discovery, the community faces daunting productivity challenges due to the complexities of multiphysics, multiscale applications and evolving computer architectures. The IDEAS Scientific Software Productivity Project (https://ideas-productivity.org) is working to increase software development productivity—a key aspect of overall scientific productivity—through an interdisciplinary and agile approach that centers on adapting modern software engineering tools, practices, and processes to build a flexible scientific software ecosystem. This poster highlights work in four focus areas.

Use Cases: Three important BER use cases drive our work: climate impacts on the upper Colorado river system; hydrology and soil carbon dynamics of the Arctic tundra; and hydrologic, land surface, and atmospheric process coupling over the contiguous U.S. Recent use-case advances include expanded testing and numerical library usage—critical as we build a software ecosystem that enables application scientists to focus on their areas of expertise while easily employing cutting-edge external software. See four IDEAS use-case posters led by J. Johnson, C. Steefel, S. Painter, and L. Condon.

xSDK: A central IDEAS activity is development of an Extreme-scale Scientific Software Development Kit (xSDK) — a collection of related and complementary software elements that provide the building blocks, tools, models, processes, and related artifacts for rapid and efficient development of high-quality applications. The first release of the xSDK in early 2016 will include four numerical libraries (hypre, PETSc, SuperLU, and Trilinos) and the Alquimia geochemistry interface. Draft xSDK package compliance standards and xSDK standard configure and CMake options help to address challenges in interoperability and sustainability of software developed by diverse groups.

HowTo: To help cultivate best practices and processes for improved scientific software development, we have written concise *WhatIs* and *HowTo* documents that characterize important software topics in ``bite-sized'' levels of detail that enable software teams to consider improvements at a small but impactful scale. Topics include software configuration, testing, documentation, performance portability, and interoperability.

Outreach: The final piece of IDEAS is outreach and collaboration with the broader computational science and engineering (CSE) community, which is also facing similar productivity challenges. We are developing training materials in collaboration with ALCF, NERSC, and OLCF. We also have established the CSE Software Forum (https://cse-software.org) as an umbrella for a community of interest/practice in software engineering for CSE on high-performance computers.

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