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

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While extreme-scale computational architectures provide unprecedented resources for scientific discovery, the community faces daunting productivity challenges for parallel application development. Difficulties include increasing complexity of algorithms and computer science techniques required in multiscale and multiphysics applications, the imperative of portable performance in the midst of dramatic and disruptive architectural changes on the path to exascale, the realities of large legacy code bases, and human factors arising in distributed multidisciplinary research teams. At the same time, software engineering and productivity approaches, processes, and tools have matured substantially in recent years and offer compelling capabilities that we need to understand, adapt, and adopt for scientific software development environments.

The project on **Interoperable Design of Extreme-scale Application Software** (IDEAS, http://www.ideas-productivity.org) has goals of qualitatively changing the culture of extreme-scale computational science and providing a foundation that enables transformative next-generation predictive science and decision support. IDEAS motivation is to increase software development productivity—a key aspect of overall scientific productivity—through an interdisciplinary and agile approach to creating extreme-scale scientific software, where modern software engineering tools, practices, and processes will improve software developer productivity, and applications will be constructed quickly and efficiently using components, libraries, and frameworks.

This poster will provide an overview of four complementary focus areas:

IDEAS Use Cases: IDEAS work is driven by two important BER use cases: climate impacts on the upper Colorado river system and hydrology and soil carbon dynamics of the Arctic tundra. These use cases will demonstrate scientific productivity gains that are possible with a software ecosystem that enables scientists to engage effectively in their areas of expertise, while readily employing cutting-edge numerical algorithms and software developed by ASCR research teams (see poster by Moulton et al. for an overview of the Use Cases).

IDEAS xSDK: The IDEAS Project involves members from five major DOE library products: Chombo, hypre, PETSc, SuperLU and Trilinos. A major deliverable of IDEAS is the Extreme-scale Scientific Software Development Kit (xSDK), which will provide an interoperability layer that will enable easy installation and usage of the IDEAS libraries.

IDEAS HowTo: In addition to xSDK development and other software efforts to address the IDEAS use cases, IDEAS will focus on methodologies ("howto" content) to cultivate best practices, processes, and tools for improved scientific software development.

IDEAS Outreach: The final piece of IDEAS is outreach and collaboration with the broader computational science community, which is also facing similar challenges and opportunities for improving productivity.

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