Poster #215

Interoperable Design of Extreme-scale Application Software (IDEAS): Improving Developer Productivity and Software Sustainability

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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 improve the productivity of software developers and the sustainability of software artifacts—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 adoption of more powerful source code management tools, expanded automated testing, and improvements in flexible multiphysics frameworks and interoperability of components that enable application scientists to focus on their areas of expertise while easily employing cutting-edge external software. See three IDEAS use-case posters led by C. Steefel, S. Painter, and L. Condon.

xSDK: A central 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 second release of the xSDK in February 2017 included four numerical libraries (hypre , PETSc , SuperLU , and Trilinos) and two domain packages (the Alquimia geochemistry interface and the PFLOTRAN subsurface application). Draft xSDK community package policies help to address challenges in interoperability and sustainability of software developed by diverse groups.

HowTo: To help improve developer productivity and software sustainability while ensuring continued scientific success, we are creating methodologies for *Productivity and Sustainability Improvement Plans (PSIPs)*. A PSIP is a tool for helping a software team to increase software quality while decreasing the effort, time, and cost to develop, deploy, maintain, and extend software over its intended lifetime. The PSIP workflow is intended to be lightweight and fit in with a project's standard planning and development process.

Outreach: The final piece of IDEAS is outreach and collaboration with the broader computational science and engineering (CSE) community. In spring 2017 we will launch a web-based portal as the hub of a community of interest/practice in software engineering for high-performance CSE.