Poster #21-11

Interoperable Design of Extreme-scale Application Software (IDEAS): A Family of Synergistic Projects Focused on Improving 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 initial phase of the IDEAS Scientific Software Productivity Project, recently dubbed IDEAS-Classic, (https://ideas-productivity.org/ideas-classic) was jointly funded by the Offices of Advanced Scientific Computing Research (ASCR) and Biological and Environmental Research (BER). IDEAS-Classic worked to enhance scientific productivity by improving the productivity of software developers and the sustainability of software artifacts — through an interdisciplinary and agile approach centered on adapting modern software engineering tools, practices, and processes to build a flexible scientific software ecosystem.

IDEAS-Classic has leveraged three BER use cases to motivate and test agile software methodologies, and to improve compatibility among complementary packages through creation of the Extreme-scale Scientific Software Development Kit (xSDK). IDEAS-Classic has also spearheaded outreach, featuring the new Better Scientific Software (BSSw) community portal (https://bssw.io) and the webinar series (https://ideas-productivity.org/events/hpc-best-practices-webinars/). Building on this success, IDEAS has grown into a family of synergistic projects to improve scientific productivity by qualitatively improving software productivity and sustainability. This poster highlights three current projects.

IDEAS-ECP: In support of the Exascale Computing Project (ECP), we continue development, customization, and curation of agile methodologies; work with individual ECP teams through Productivity and Sustainability Improvement Planning; and expand content for the BSSw site.

xSDK4ECP: To help support the seamless combined use of diverse, independently developed software packages in ECP, the xSDK continues to grow. The third release of the xSDK in December 2017 included a total of seven numerical libraries and two domain packages (the Alquimia geochemistry interface and the PFLOTRAN subsurface application).

IDEAS-Watersheds: The three BER use cases (climate impacts on the upper Colorado river system; hydrology and soil carbon dynamics of the Arctic; and hydrologic, land surface, and atmospheric process coupling over the contiguous U.S.) continue to evolve, providing motivation, testing, and evaluation of agile methodologies. Recent advances include improvements in multiscale frameworks and leveraging interoperable components to provide new scientific capabilities. In addition, we explore the critical role and benefits of a dedicated software engineer to

oversee development processes, code reviews, testing and code releases. See three IDEAS-Watersheds posters led by D. Dwivedi, S. Painter, and L. Condon.