Environmental Systems Science Use Cases Drive Requirements for Community-Based Software Development

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The need to understand and predict climate impacts and feedbacks in terrestrial systems is driving a trend toward more mechanistic representations of coupled aboveground and belowground processes, thus creating challenges in multiscale and multiphysics modeling. The ***Interoperable Design of Extreme-Scale Application Software*** (IDEAS) project is exploring new community-based approaches to software development that will lead to application codes that are more accessible to developers and users, enhancing their productivity (see IDEAS overview poster by McInnes et al.). To guide this work in IDEAS, two Use Cases have been selected that address scientific questions for existing Environmental Systems Science application projects, as well as exercise components of established and new codes.

Use Case 1 focuses on the East River Watershed within the Upper Colorado River Basin, a snowmelt dominated, 750 km^2 high elevation headwaters catchment that is under study as part of LBNL's Genomes to Watershed Scientific Focus Area (SFA). The LBNL SFA will investigate how climate change impacts biogeochemical cycling in a watershed mediated by hydrology and the distribution and function of dynamic microbial communities. This Use Case considers a portion of the lower East River dominated by a broad flood plain in which stream meanders and associated hyporheic zone flow contribute to carbon cycling. Resolving redox and other geochemical gradients at scales < 1 meter, while upscaling these results to the larger (5km) scale river system, is the computational challenge that will drive advances in interoperability and performance in the Amanzi/ATS, ParFlow-Crunch and PFLOTRAN codes. Also, IDEAS will explore a multiscale model coupling framework in a similar setting under the PNNL SFA (see poster by Scheibe et al.).

Use Case 2 links to the NGEE Arctic program, focusing on software interoperability and productivity enhancements to enable more realistic simulations of permafrost thaw and active layer dynamics in polygonal patterned ground at the Barrow Environmental Observatory. The IDEAS project will combine fine-scale simulations of permafrost thermal hydrology using the Arctic Terrestrial Simulator (ATS) with PFLOTRAN's geochemistry engine through the chemistry interface library, Alquimia. To demonstrate reuse of physics components in new applications, IDEAS is extending ATS's fine-scale modeling capabilities to the intermediate scale through the use of mesh and model domain abstractions. Here, thermal hydrology will be simulated on a set of independent 1D columns, where each column represents an ice-wedge polygon. Those columns will be coupled to each other laterally through 2D simulations of overland flow including dynamic topography.

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