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IDEAS-Watersheds: Accelerating Watershed Science through a Community-Driven Software Ecosystem

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Through its Science Focus Area (SFA) projects the Subsurface and Biogeochemical Research (SBR) program is tightly integrating observations, experiments, and modeling to advance a systems-level understanding of how watersheds function, and to translate that understanding into advanced science-based models of watershed systems. To enhance and broaden the impact of the existing SFAs, the IDEAS-Watersheds project builds on the success of a synergistic family of IDEAS projects initated in 2014. Specifically, it strives to improve watershed modeling capability by increasing software development productivity - a key aspect of overall scientific productivity - through an agile approach to creating a sustainable, reliable, software ecosystem with interoperable components. In this poster we highlight the overall objectives and structure of the IDEAS-Watersheds project, which is organized around six Research Activities. There are three Partnership Activities, each undertaken jointly with one of SBR's interdisciplinary watershed focused SFA projects using concrete use cases to advance our watershed modeling capability. These projects include the Watershed Function SFA (LBNL - poster by S. Molins), the Critical Interfaces SFA (ORNL - poster by S. Painter), and the River Corridor SFA (PNNL). A Continental United States (CONUS) Activity will advance a basin-to-continental scale simulation platform (poster by L. Condon), and a Reaction Network Activity partnering with SBR's fine-scale SFAs focused on fundamental biogeochemical processes to bring those advances into geochemistry reaction modeling tools (see poster by S. Molins). These projects include the Subsurface Biogeochemistry of Actinides SFA (LLNL), the Wetland Hydrobiogeochemistry SFA (ANL), and the Groundwater Quality SFA (SLAC). Finally, a Shared Infrastructure Activity will coordinate the development of common workflow tools and software interfaces to support interoperability. We adopt a co-funding model with shared deliverables and joint funding of postdocs and SFA-IDEAS liaisons to facilitate training of early career researchers and ensure integration with the SFAs.

As an important example of emerging workflow tools we highlight plans in our partnership with the River Corridor SFA (PNNL) to work with KBase Apps and its Narrative interface. We describe our approach to develop KBase Apps that enable batch and 1D reactive tansport model simulations (e.g, with PFLOTRAN) to study the reaction networks being developed through metabolic pathway analyses. This development will establish mechanistic links between metagenomes and biogeochemical modeling, and will also support our collaboration with the Wetland Hydrobiogeochemistry SFA (ANL).