Unleashing Modeler Creativity: IDEAS on How Flexible Software can Further Process Understanding

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BER Program: SBR

Project: IDEAS-Watersheds. Los Alamos National Laboratory **Project Website**: https://ideas-productivity.org/ideas-watersheds/ **Project Abstract**:

Building process understanding through models requires a careful balance of process complexity and spatial scale. Too little process complexity or too coarse of a spatial scale insufficiently describes the system, while too much process complexity or too fine a spatial scale makes understanding difficult to glean from model runs. Finding this balance is central to the art of modeling and relies on the physical insights of the modeler. However, rigid software tools often make it difficult and time consuming to express these insights in models.

IDEAS-Watersheds, in building on work from IDEAS-Classic,[1] is exploring how an ecosystem of interoperable and flexible software tools can enable the fast construction of new models that are customized to a particular science question and informed by data. In partnership with the ORNL Critical Interfaces SFA, we show how mesh infrastructure, subgrid models, application programming interfaces, and flexible software design can come together to enable multiscale, multiphysics models of biogeochemical processing in stream corridors. Specifically, we represent transport in stream networks, and in each reach of the network, embed a travel-time based model of reactive transport to describe the processing of chemical components in streambeds and banks. The hierarchical structure of this model is enabled through Amanzi's infrastructure, while ATS's flow and transport processes are coupled to PFLOTRAN's geochemistry through the Alquimia interface. The resulting model allows biogeochemical processes to be represented at an appropriate spatial scale, while remaining computationally tractable compared to full 3D simulations. This type of model structural flexibility is a powerful tool for modelers, giving new insight into physical processes through investigations of model structure.

Coon, E.T., J.D. Moulton, and S.L. Painter. "Managing complexity in simulations of land surface and near-surface processes." *Environ. Modelling & Software* 78 (2016): 134-149.