

Interoperable software for integrated watershed scale models

Jeffrey Johnson¹, Sergi Molins¹, Ethan Coon², Reed Maxwell³

¹Lawrence Berkeley National Laboratory, Berkeley, CA

²Los Alamos National Laboratory, Los Alamos, NM

³Colorado School of Mines, Golden CO

As our models become more elaborate and move toward multiscale representations, it is more clear than ever that we need the ability to combine different computational processes and algorithms in a sensible and interoperable fashion. Proponents of modern software engineering argue that this interoperability can be achieved by wrapping existing software in modular interfaces, but the design of these interfaces must be simple enough for practitioners to use and relevant to their needs. The Interoperable Design of Extreme-scale Software Applications (IDEAS) project is exploring this challenging problem in a few different settings. We examine the interface in the Community Land Model (CLM) used by ParFlow, which is intended to be released as a reusable software component. In this context, we discuss the development of guidelines for interfaces between integrated hydrology models and land models. We also describe ongoing work on Alquimia, an interoperable interface designed to provide biogeochemical processes to flow/transport models. The Alquimia interface now supports fully implicit integration of reaction terms, augmenting its previous operator-split treatment. This new feature allows users of Alquimia to study the effects of different methods for coupling transport and reaction processes, and simplifies the process of benchmarking. Finally, we outline ongoing efforts to characterize and define extensible interfaces for other processes and process couplings commonly present in modeling across BER.