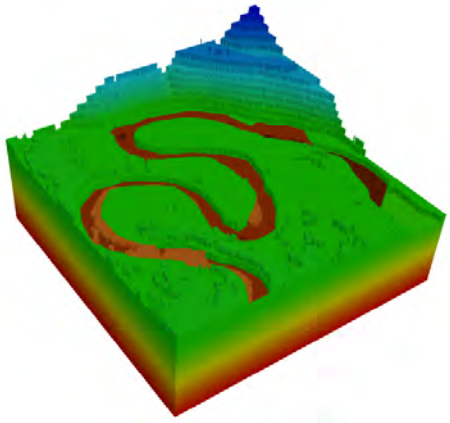
Testing Code Interoperability and Productivity on Modeling Integrated Surface-Subsurface Water Flow and Biogeochemical Cycling in the Hyporheic Zone – IDEAS Use Case 1

Dipankar Dwivedi[1], Carl Steefel[1], Erica Woodburn[1], David Moulton[2], Ethan Coon[2], Lauren Foster[3], Reed Maxwell[3]

[1]Lawrence Berkeley National Laboratory, [2]Los Alamos National Laboratory, [3]Colorado School of Mines

The overarching goal of **I**nteroperable **D**esign of **E**xtreme-scale **A**pplication **S**oftware (IDEAS) is to leverage enhancements in software library interoperability and design to enable a new level of spatial and time resolution as well as process fidelity in the modeling of multi-scale terrestrial ecosystems. To demonstrate the approach, the Use Case 1 of IDEAS effort focuses on the development of a set of benchmark problems that leverage interoperable software components to investigate the roles of integrated surface-subsurface water flow, transport, and biogeochemical cycling in the East River Watershed, Colorado. The shorter-term objective is to understand the effects of hyporheic zone exchange in tight meanders of the lower East River floodplain on nutrient (especially nitrogen), carbon, and metal riverine fluxes from the greater watershed. The longer term objective is to develop an approach for upscaling results to larger domain sizes (e.g., 10 km by 10 km). The initial benchmarks will make use of high resolution LIDAR and bathymetric data to investigate productivity issues on an approximately 175 meter by 175 meter horizontal by 25 meter vertical modeling domain with the lateral grid resolution of 0.5 meters. The benchmark simulations are being developed using the codes ParFlow, Amanzi-ATS, and PFLOTRAN, which provide slightly contrasting modeling approaches for quantifying integrated hydrological and biogeochemical response. ParFlow relies on tightly coupled surface and subsurface water simulations and terrain stepping treatment of topography on a fixed grid, Amanzi-ATS uses variable resolution unstructured grids to capture important interfaces and gradients, while PFLOTRAN will soon have the capability for integrated surface and subsurface water flow. These codes take advantage of improvements in interoperability by accessing biogeochemistry through the Alquimia interface.



3-D modeling domain for lower East River meanders. Domain size is approximately 175m by 175m by 25m with a lateral grid resolution of 0.5 m.

We are also beginning the development of an East River watershed scale simulation based on an approximately 10 km by 10 km modeling domain using the same 0.5 meter resolution LIDAR data that will require exascale computing platforms. This will test the ability of the codes to make use of the high resolution topography on a larger watershed-scale domain. These will also be compared with the results of 10 meter resolution simulations over the same domain.