Multiscale Science and Modeling: Task 4

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Task 4 of the FY15-17 PNNL SBR SFA Plan will develop an integrative multiscale modeling framework to establish quantitative connections among the suite of models and experiments being developed by Tasks 1-3 across physical and temporal scales. We will develop fundamental understanding of multiscale interactions among scale-specific processes and phenomena, then design the multiscale computational methods and algorithms based on that foundation. We will apply a multiscale modeling framework called the “Multiscale Analysis Platform” (MAP), previously developed by our project team. The MAP embodies a series of questions that guides the user to one of several multiscale modeling motifs, depending on system characteristics. The motifs span a wide range of multiscale modeling approaches from formal upscaling with closure to a number of different hybrid multiscale methods. The MAP approach integrates bottom-up rigorous model development and top-down optimal model deployment into a framework for application-scale modeling in which predictive accuracy and computational burden are balanced. Physics-based model development follows a bottom-up approach that, through rigorous upscaling techniques, allows construction of effective medium (upscaled) representations of fine-scale processes with different degrees of coupling and complexity. A unique element of our approach is the formulation of diagnosis criteria that define applicability ranges of the resulting upscaled representations formulated in terms of macroscale variables. These criteria guide the adaptive top-down use of multiscale hybrid methods where needed (direct linkage to microscale models) together with simpler upscaled models, where applicable, in an optimal (in terms of simplicity and predictive capabilities) deployment of physics-based models for science-informed application-scale predictions. The multiscale framework will employ the Subsurface Interaction Zone (SIZ) multiscale facies concept identified as an integrating element of this research. At each scale of interest, facies will be defined based on available data and the ability to resolve detailed features at that scale. At the fine scale, for example, facies models may differentiate fine-grained domains dominated by diffusive mass transfer (seasonally anoxic) from surrounding advective coarse-textured regions. At the local scale, SIZ facies may reflect stratigraphic structures within the Hanford and Ringold formations that control flow paths of advective groundwater-river water exchange feeding the fine-scale domains. At the reach scale, SIZ facies may reflect the geometry of the Hanford-Ringold interface and paleochannels and their control on bulk river-groundwater exchange rates.