



DR. TIM SCHEIBE, PACIFIC NORTHWEST NATIONAL LABORATORY



Dr. Scheibe develops a scientific vision for multiscale and computational science within EMSL, provides a national perspective on the future scientific and technological needs, and sets a strategy to integrate EMSL capabilities to address key scientific issues in environmental molecular science relevant to BER missions. He came to this position after 22 years at PNNL building a reputation as an internationally recognized expert in environmental hydrogeology. Primary research focus is on characterization and modeling of multiscale heterogeneity and its impacts on reactive transport in groundwater systems. Projects include both computational and field experimental elements.

A HYBRID MULTISCALE FRAMEWORK FOR SUBSURFACE FLOW AND REACTIVE TRANSPORT SIMULATIONS

Extensive research efforts have been invested in reducing model errors to improve the predictive ability of biogeochemical earth and environmental system simulators, with applications ranging from contaminant transport and remediation to impacts of biogeochemical elemental cycling (e.g., carbon and nitrogen) on local ecosystems and regional to global climate. While improved process understanding can be achieved through scientific study, such understanding is usually developed at small scales. Process-based numerical models are typically designed for a particular characteristic length and time scale. For application-relevant scales, it is generally necessary to introduce approximations and empirical parameterizations to describe complex systems or processes. This single-scale approach has been the best available to date because of limited understanding of process coupling combined with practical limitations on system characterization and computation. The application of advanced computational resources, new scientific process descriptions, and state-of-the-art characterization methods to advance predictive understanding of the larger system behavior requires the development of multiscale simulators. Accordingly there has been much recent interest in novel multiscale methods in which microscale and macroscale models are explicitly coupled in a single hybrid multiscale simulation. A limited number of hybrid multiscale simulations have been developed for biogeochemical earth systems, but they mostly utilize application-specific and sometimes ad-hoc approaches for model coupling. We are developing a generalized approach to hierarchical model coupling designed for high-performance computational systems. In this presentation I will describe the generalized approach and provide two example implementations.

Date: Monday, October 12, 2015

Place: Sloan 175

Time: 4:10 p.m.—5:00 p.m.