Poster #21-13

Modeling Across Scales while Maintaining Links to Laboratory and Fine-scale Field Investigations: Cases Studies using the Advanced Terrestrial Simulator

Scott L. Painter[1*], Ethan T. Coon[1], and Ahmad Jan[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;

Contact: paintersl@ornl.gov

BER Program: SBR
Project: IDEAS
Project Website: https://ideas-productivity.org/ideas-classic/

Representing the emergent effects of fine-scale processes and heterogeneities on system-scale behavior, a critical challenge for system-scale environmental simulations in general, is particularly difficult for process-rich simulations that attempt to maintain clear links to field and laboratory investigations. Three examples illustrate how system insights can guide the design of efficient multiscale strategies for addressing that challenge and how highly configurable software facilitates implementation of those strategies. We previously showed that the thermal hydrology of polygonal tundra could be efficiently simulated at scale using a novel spatial structure based on insights gained from fine-scale simulations (Jan et al. 2018). We describe an extension of that approach that recovers the large-scale effects of subgrid microtopography through use of subgrid models informed by fine-scale simulations. Significantly, this multiscale computational strategy enables decadal, catchment-scale simulations without simplifying the three-phase physics of freezing soil, thus maintaining a clear link to laboratory and site-scale investigations of those processes. The software advances required to implement the polygonal tundra use case were also leveraged in a second use case focused on reactive transport in stream corridors. In that application, a subgrid model is used at each channel location in a stream network to represent transport and multicomponent biogeochemical reactions in the hyporheic zone. By writing the subgrid model in Lagrangian travel time form, computationally demanding three-dimensional reactive transport simulations are replaced with the one-dimensional reactive transport simulations, where each represents an ensemble of trajectories in the hyporheic zone. That multiscale approach allows multicomponent biogeochemical reactions such as redox processes to be modeled at their native small scales while embedded in reach-to-watershed scale simulations. Well-established geochemical modeling tools can be used to represent the reaction system using the Alquimia interface (https://github.com/LBL-EESA/alquimia-dev) for coupling. We apply the approach to a hypothetical reactive tracer test and demonstrate that formation of anaerobic zones within the hyporheic zone can affect the scaling of reactive tracer breakthrough from the laboratory to the field. In the final example, we demonstrate how related ideas and software tools can accelerate computationally demanding integrated surface/subsurface hydrology simulations at watershed scales. Specifically, we describe a multi-scale domain decomposition strategy that exploits the weak coupling that naturally exists between subwatersheds to improve numerical performance.

Publications: Jan, A., E.T. Coon, S.L. Painter, R. Garimella, and J.D. Moulton. Comput Geosci (2018) 22: 163. https://doi.org/10.1007/s10596-017-9679-3.