Analysis of hydrogeologic modeling shows effectiveness of multiscale hybrid methods

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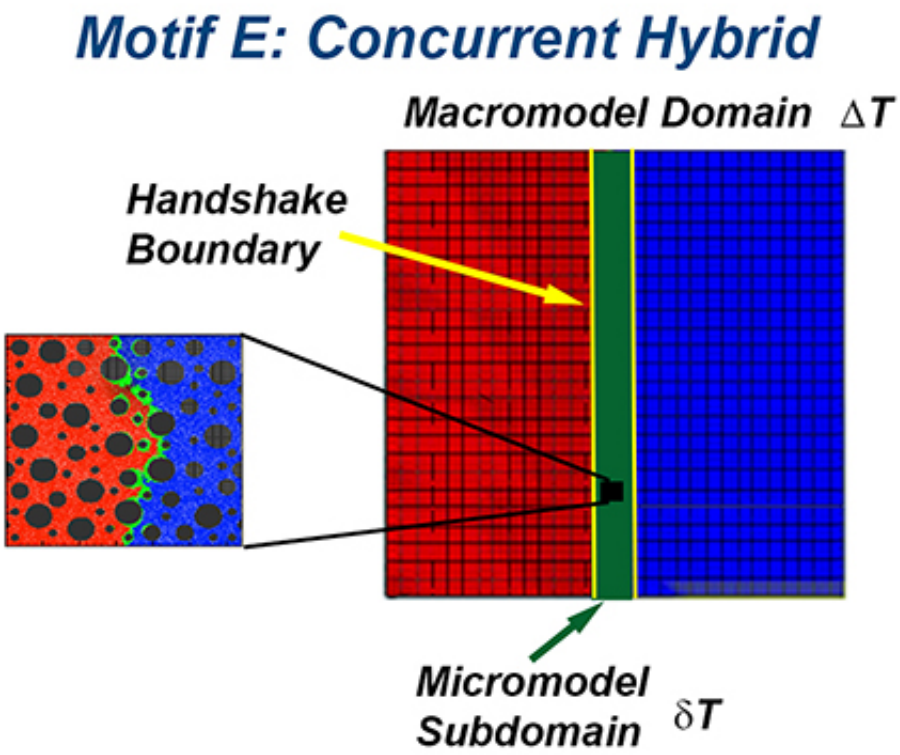

This diagram of the concurrent multiscale hybrid approach illustrates one of seven motifs examined in this work. The micromodel is defined only on some subset of the overall model domain, while the micro and macro models run independently on differing time steps. They are synchronized through the "handshake" boundary condition at selected time intervals, shown here as a sharp divide.

Accurately modeling how groundwater and its constituents move and react in the subsurface poses significant challenges for hydrogeologists. Researchers from PNNL and four universities collaborated to review multiscale modeling methods and approaches across a wide range of disciplines, focusing on hybrid methods that combine multiple models defined at different scales in a single simulation. Applying these methods to subsurface flow and reactive transport problems is a recent and promising undertaking—highly relevant to many U.S. Department of Energy (DOE) mission areas. With this effort, scientists have provided a general framework for application that can guide users toward methods that are most appropriate for particular problems.

There is a huge disparity between the scales at which scientists can observe and quantify fundamental processes and scales they need to predict system behavior for environmental management. Improving the tools that provide the ability to predict requires better representation of fundamental (small-scale) mechanisms in large-scale simulations. The researchers point out novel approaches based on using high-performance computation to couple different environmental systems models across scales, offering a pathway to improve their predictive capability.

In their work, the scientists analyzed a range of both conventional and emerging multiscale modeling approaches, grouping them into seven individualized "motifs." Each motif includes a number of associated specific methods that can be applied to problems with diverse sets of individual attributes. The resulting paper provides a series of questions; discusses which particular application problems can be assigned to one or more motifs; includes references to associated methods within each motif; and offers examples of applications for each motif, including recent ones from hydrogeology.

The authors hope to stimulate awareness of emerging multiscale hybrid methods within the groundwater modeling community and eventual

widespread use of a new class of subsurface flow and transport simulators that link pore- and continuum-scale models explicitly. Several major projects funded by DOE, including PNNL's Subsurface Biogeochemical Research Scientific Focus Area and the Interoperable Design of Extreme-scale Application Software (IDEAS) projects, have major elements focused on multiscale modeling as applied to pressing environmental scientific problems and will draw on the approaches initiated by this work.

More information: Scheibe TD, EM Murphy, X Chen, AK Rice, KC Carroll, BJ Palmer, AM Tartakovsky, I Battiato, and BD Wood. 2015. "An Analysis Platform for Multiscale Hydrogeologic Modeling with Emphasis on Hybrid Multiscale Methods." *Groundwater* 53(1):38-56. DOI: 10.1111/gwat.12179.

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