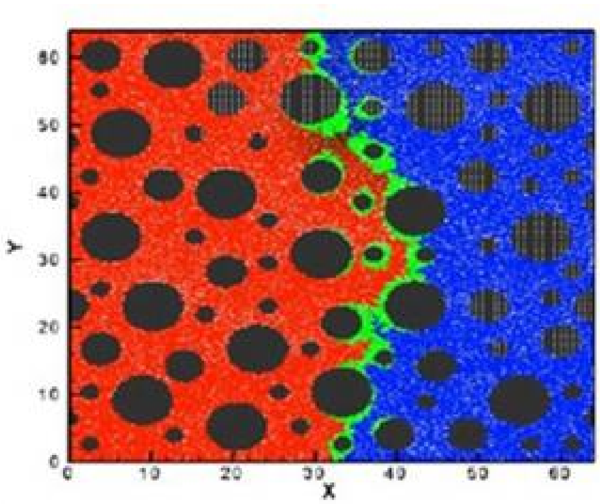
New computer model concept could solve big, real-world problems on a small, porous scale

September 7 2006



A computer simulation of various minerals and chemicals meeting and reacting. The black circles represent grains of the porous medium, such as sand, and the red and blue represent the fluid phase, with red being dissolved calcium and blue being dissolved carbonate. The green part represents areas where the mineral calcium carbonate has formed by reaction of the red and green dissolved chemicals. Pore-scale modeling such as this, when coupled with other simulation scales, helps researchers make more accurate predictions of the movement and fate of contaminants in groundwater. Pacific Northwest National Laboratory and its collaborators will work to develop a robust computer model that will join different models at multiple scales into a single hybrid model for enhanced predictability.

The Department of Energy's Pacific Northwest National Laboratory today was awarded a Scientific Discovery through Advanced Computing, or SciDAC, grant to develop a computer model that can simulate biogeochemical processes on multiple scales. This computational advancement would enable researchers to make more accurate predictions of the movement and fate of contaminants in groundwater so that appropriate cleanup and human safety measures can be applied to the problem.

DOE today announced $60 million in grants for 30 SciDAC projects over the next three to five years.

Specific to the PNNL-led project, the SciDAC program provides the framework within which computational and earth scientists will work together to bring the most powerful computers and latest software developments to bear on the challenging groundwater problem.

Organizations collaborating with PNNL on the modeling project will be the University of California, San Diego; Idaho National Laboratory; and Oak Ridge National Laboratory.

Subsurface transport processes play a central role in issues that are of concern globally, as in DOE missions, such as cleanup of Cold War legacy contamination, development of energy resources, reduction of global climate impacts through subsurface sequestration of carbon dioxide, and safe storage of subsurface waste for the long-term.

Computer models that simulate groundwater's behavior already exist, but with limited ability to share information between models at different scales. Researchers hope that a new, sophisticated model will be able to combine individual, small-scale simulations and this will create a larger picture where real-world problems can be analyzed and, hopefully, solved with a single model instead of developing them on a case-by-case basis.

Big problems, such as cleaning up contaminated groundwater at old plutonium production sites, are often complex on the surface, and even more complicated below the surface – that is, at the “pore” scale.

Consider a five-foot pathway of water that’s flowing underground. It isn’t a “clean” tunnel; rather, it’s a mixture of water, minerals, contaminants, and dirt, making it a stew that researchers must examine closely in order to determine how and where the water will flow.

If researchers simply examined the stew on the large scale, they might neglect small-scale (e.g., microscopic- or pore-scale) processes that ultimately control the large-scale behavior. But with a sophisticated computer model that marries various simulations representing different processes on a variety of scales, ranging from microbial growth in pores to migration of contaminants to rivers or wells, researchers get a clearer picture of what’s happening underground now and what’s likely to happen in the future.

A similar project that received a SciDAC grant will seek to enhance groundwater monitoring so that researchers can better understand the migration of radionuclides. The knowledge gained from detailed modeling could help with remediation efforts in locations where cleaning up the groundwater is necessary to avoid contamination of areas it contacts, such as rivers. PNNL will collaborate with Los Alamos National Laboratory on the project.

Source: Pacific Northwest National Laboratory