Safer Soil and Water

Computer model predicts underground substance flow

Quick read
PFLOTRAN advanced computing predicts movement of underground contaminants.

While atmospheric and aboveground environmental concerns have taken center stage, many problems affecting the world are underfoot, literally.
Soil and water, prime factors in our health, frequently encounter contaminants from toxic waste and byproducts. Researchers' next-generation computer science tracks and predicts reactive underground flows.
Los Alamos National Laboratory scientists developed a powerful massively parallel computer model called PFLOTRAN that accurately predicts multi-scale subsurface processes. The Los Alamos-led environmental modeling team includes Peter Lichtner, J. David Moulton, and Bobby Philip.
PFLOTRAN has many applications and guides safer industrial techniques; for example, it answers a computational challenge by helping geoscientists determine how carbon dioxide flows through aquifers and deep geologic formations during carbon-capture and storage (a new method to reduce greenhouse gases)—helping them prevent toxic gases from polluting our homes or drinking water.
PFLOTRAN also helps us understand radionuclide migration at nuclear facilities. At the Hanford Site, a decommissioned and highly contaminated nuclear production complex along a major river in Washington, PFLOTRAN's enhanced modeling capabilities enhance cleanup. Formerly, sub-millimeter-scale mass transfer effects thwarted remediation efforts.
How PFLOTRAN Works
PFLOTRAN accurately predicts contamination transport. Typical simulations are very computationally demanding, involving 10 or more chemical degrees of freedom on a grid of millions of nodes.
A massively parallel 3-D reservoir simulator, PFLOTRAN can model multiphase reactive flows in geologic formations based on continuum scale mass and energy conservation equations.
"Predictive modeling of reactive subsurface flows is a daunting task because of the wide range of spatial scales involved, and the wide range of time scales involved," said Lichtner, the project's principal investigator. "Currently, large-scale three-dimensional models can usually only resolve features down to the order of meters, which makes capturing phenomena at smaller scales pretty difficult. (PFLOTRAN) is designed to change that by providing multi-scale modeling capabilities at various spatial scales."
LANL's PFLOTRAN team collaborated with researchers at Argonne; Oak Ridge, and Pacific Northwest national laboratories; and the University of Illinois at Urbana-Champaign.

Computer Simulations Model Complex Contaminants

PFLOTRAN, which uses PETSc's parallel framework, will include a generic multiphase algorithm based on variable switching to incorporate phase transitions, easily customizable. Capabilities for both unstructured grids and adaptive mesh refinement on structured grids will be incorporated. Multilevel solver and upscaling capabilities and subgrid scale models will be added to the code.

To learn more about PFLOTRAN, contact Peter Lichtner at (505) 667-3420.

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"Los Alamos National Laboratory plays an indispensable role in building America as a science and technology powerhouse, and our staff are an incredible resource to the nation and the world." Michael Anastasio, Dir.

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