Richard T. Mills

Progress and challenges in simulating subsurface reactive flows at the petascale and beyond.

To provide true predictive utility, subsurface simulations often must accurately resolve--in three dimensions--complicated, multi-phase flow fields in highly heterogeneous geology with numerous chemical species and complex chemistry. This task is especially daunting because of the wide range of spatial scales involved--from the pore scale to the field scale--ranging over six orders of magnitude, and the wide range of time scales ranging from seconds or less to millions of years. This represents a true "Grand Challenge" computational problem, requiring not only the largest-scale ("ultrascale") supercomputers, but accompanying advances in algorithms for the efficient numerical solution of systems of PDEs using these machines, and in mathematical modeling techniques that can adequately capture the truly multi-scale nature of these problems.

In this talk, I will describe some of the current and anticipated challenges involved in simulating subsurface reactive flows at the petascale and beyond, and discuss how they are being addressed in the development of the computer code PFLOTRAN and the underlying PETSc solver framework. Additionally, I will touch on what I perceive to be major challenges at the computing ultrascale for implicit time-stepping codes in general.

Speaker bio:

Richard Tran Mills is a research scientist at Oak Ridge National Laboratory, where he is a member of the Computational Earth Sciences Group within the Computer Science and Mathematics Division. His research interests include parallel and high performance computing, computational science and scientific computing, execution context-aware scientific software, subsurface flow and reactive transport, and geospatiotemporal data mining. Richard earned his Ph.D. in Computer Science in 2004 at the College of William and Mary, where he was a Department of Energy Computational Science Graduate Fellow. Prior to that, he studied geology and geophysics (in addition to Volunteers Football, of course) at the University of Tennessee, Knoxville as a Chancellor's Scholar.