Evaluating the Performance of Parallel Subsurface Simulators: An Illustrative Example with PFLOTRAN

Objective

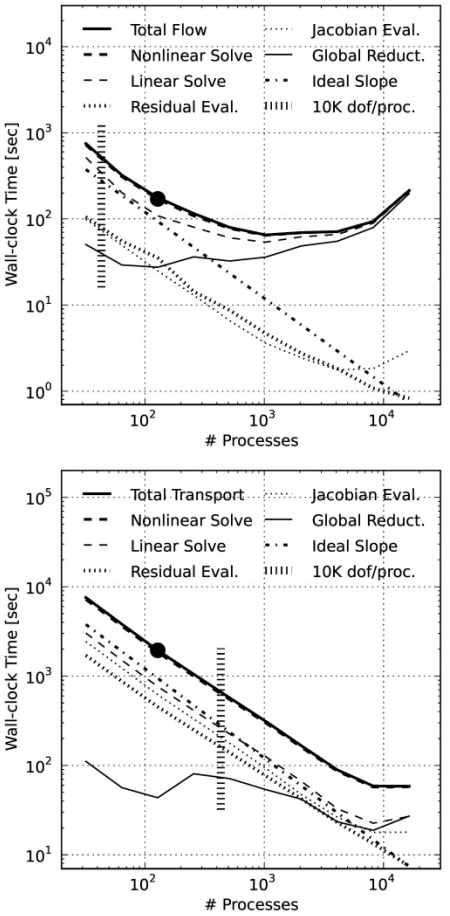
- Although high-performance computing appears to be high priority in future earth system modeling, few publications exist detailing simulator parallel performance on state of the art machines.
- The goal is to provide a reference point for efficient simulator performance based on challenging real-world simulation scenarios.

Approach/Results

- PFLOTRAN performance was evaluated on three real-world scenarios:
  - In situ copper leaching within a 5-spot flow regime
  - Regional flow and transport with injection, extraction, and undulating river stage
  - Hanford 300 Area IFRC variably-saturated flow and uranium surface complexation
- PFLOTRAN demonstrates excellent scalability for flow and transport when the number of unknowns (dofs) is above 10K/process.
- For geochemical transport, the number of unknowns may drop much lower to ~100s/process with near-linear (ideal) performance.
- As expected, weak scaling performance (where #dofs/process is constant as # processes increase) is poor due to the use of conventionally-preconditioned Krylov solvers.

Significance and Impact

- A comprehensive reference point is provided for subsurface simulator parallel performance.
- The detailed analyses presented may be applied to simulators to determine the root cause of breakdown in parallel performance.



Breakdown of parallel performance for IFRC flow and geochemical transport illustrating impact of computationally expensive global reductions.

Hammond, G.E., P.C. Lichtner and R.T. Mills (2014) Evaluating the Performance of Parallel Subsurface Simulators: An Illustrative Example with PFLOTRAN, *Water Resources Research*, 50, doi:10.1002/2012WR013483.