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Modelling 3D reactive transport in variable density flow using parallel computation

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Worldwide, intense land use near shorelines engenders coastal environmental problems. A challenging problem is simulation of the migration of contaminated dense plumes in from a coastal aquifer to the sea. Most simulation models focus on density-dependent salt-water intrusion, but with contaminant transport at ambient freshwater density, thereby neglecting the possible coupled effect of reactive transport and density-dependent flow. PHWAT is a 3D finite-difference model, which combines PHREEQC and SEAWAT. It is suitable for simulating multi-component reactive transport with variable density groundwater flow (Mao et al., 2005, Environmental Modelling and Software). PHWAT is a serial code and the computation time increases markedly with increasing grid size and reaction complexity. Here we present a parallel version of PHWAT. Comparison of the serial and parallel versions shows that the latter can dramatically reduce simulation clock time, with the speed-up increasing with the problem complexity. The parallel version of PHWAT is applied to model the migration of an unstable dense plume injected into fresh groundwater in a coastal aquifer. We examine numerical issues of grid convergence and the development of instabilities at the saltwater/freshwater interface. The converged numerical results were compared favourably with existing experimental data. This validated numerical model was adopted to assess the extent of the contamination in a coastal aquifer due to organic pollutants, and to evaluate possible remediation strategies.