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Parallel computation of reactive transport in multiple variable density flows

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Intense land use near the shoreline has given rise to concerns relating to coastal environmental problems. Comprehensive computational tools to address such issues need to simulate the migration of contaminated dense plumes in the coastal aquifer. Up to now, most simulation models focus on salt water intrusion and contaminant transport at ambient freshwater density, thereby neglecting the coupled effect of reactive transport and density-dependent flow.

We have developed a three-dimensional model, PHWAT, which incorporates PHREEQC into SEAWAT. It can simulate multi-component reactive transport with variable density groundwater flow (Mao et al., 2005, Environmental Modelling and Software, In Press). PHWAT is a serial code and the computation time increases markedly with increasing discretisation and reaction complexity. Here we present a new, 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 then applied to model the migration of an unstable dense plume injected into fresh groundwater in a coastal aquifer, so as to investigate the grid convergence problem. The numerical results are compared favourably with existing experimental data. Following model validation, it is further applied to simulate transport of a variable density reactive acidic plume in a coastal aquifer. The results show that the geochemical reactions (dissolution and cation exchange) attenuate the migration of heavy metals, thus decreasing the risk of pollution in the coastal

area.