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Benchmark modeling with parallelized three-dimensional numerical code for water flow and solute transport in a porous medium

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For complex three-dimensional geometries and spatially detailed heterogeneous soil structures, excessive number of nodes in the computational domain often requires a parallelized numerical model. In this study, the parallel version of three-dimensional model (S3D) is introduced. Water flow in a variably saturated porous system is described by Richards' equation, solute transport by advection-dispersion equation. Conjugate gradient method and PETSC libraries are used to solve the finite element method matrices on an array of computer processors connected in parallel. First, we present a set of benchmarking scenarios, in which the results obtained by the S3D model are compared with analytical solutions and/or predictions based on one- and two-dimensional numerical models. The proposed scenarios cover a wide range of simulated processes and boundary conditions to test and verify the three-dimensional code properly. In the next step, water flow and tracer transport is simulated through heterogeneous soil sample. The heterogeneous flow pattern is triggered using the X-ray computed tomography images of undisturbed soil sample and simple scaling concept to describe spatially variable soil properties. The simulated soil sample contains more than 1.5 million of nodes. Results suggest that the parallel version of S3D model is consistent with one- and two-dimensional model predictions, numerically robust and efficient in respect to computing time.