Coupling PEST/PEST++ And COMSOL Multiphysics® For Hydrogeophysical Model Calibration Using Pilot Points

Andres Gonzalez Quiros[1], Jean-Christophe Comte[1]

[1]University of Aberdeen, Aberdeen, Scotland, UK

Abstract

The calibration of groundwater models is usually limited by the scarcity of direct hydraulic data. The estimation of heterogeneous distribution of hydraulic properties can be improved through a joint or coupled inversion in which the calibration dataset is complemented with geophysical information. The procedure requires a coupled multiphysical forward model and the implementation of an inversion methodology capable to produce a geologically realistic distribution of subsurface materials. In this work we show how the open source and model-independent calibration software PEST/PEST++ can be coupled with COMSOL Multiphysics® for the calibration of heterogeneous groundwater models using a multiphysical calibration dataset. The estimation of hydraulic properties is performed in scatter locations, known as pilot points, that are interpolated into the domain of investigation using a geostatistical model. To illustrate the approach, we implement the methodology in a coupled hydrogeophysical model solved in COMSOL Multiphysics® in which electrical resistivity data is jointly used with borehole data for the calibration of saltwater intrusion in a heterogeneous coastal aquifer. To solve the groundwater flow-transport problem we use Darcy's Law and Transport of Diluted Species from the Porous Media Flow Module. The electrical resistivity problem is solved using the AC/DC Module. Both problems are linked by a petrophysical model and solved simultaneously. Pre-processing and post-processing steps are performed in MATLAB®, which is connected to COMSOL Multiphysics® using the LiveLink™ for MATLAB®. The coupled inversion is run using a batch file that includes additional applications for the implementation of the pilot points as required by PEST. In calibration mode, PEST/PEST++ searches a unique parameter field of minimum error variance by minimising an objective function using the Gauss-Levenberg-Marquardt (GLM) algorithm. To avoid non-uniqueness, PEST uses Tikhonov regularisation and singular value decomposition. Using PEST++, the capabilities of PEST can be extended for implementation of global optimisation through differential evolution, global sensitivity analysis, with the methods of Morris and Sobol, and posterior uncertainty analysis using an iterative Ensemble Smoother. In this work we show an example of implementation of the iterative Ensemble Smoother to the same hydrogeophysical scenario. To increase computational efficiency we use run parallelisation connecting the COMSOL Server™ with either BEOPEST or PANTHER, for PEST or PEST++, respectively. The methodology can be applied to real field datasets and adapted or extended for application in other multiphysical environmental models developed with COMSOL Multiphysics®.