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Efficient calibration of a distributed *pde*-based hydrological model using grid coarsening

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SUMMARY

Partial-differential-equation based integrated hydrological models are now regularly used at catchment scale. They rely on the shallow water equations for surface flow and on the Richards' equations for subsurface flow, allowing a spatially explicit representation of properties and states. However, these models usually come at high computational costs, which limit their accessibility to state-of-the-art methods of parameter estimation and uncertainty quantification, because these methods require a large number of model evaluations. In this study, we present an efficient model calibration strategy, based on a hierarchy of grid resolutions, each of them resolving the same zonation of subsurface and land-surface units. We first analyze which model outputs show the highest similarities between the original model and two differently coarsened grids. Then we calibrate the coarser models by comparing these similar outputs to the measurements. We finish the calibration using the fully resolved model, taking the result of the preliminary calibration as starting point. We apply the proposed approach to the well monitored Lerma catchment in North-East Spain, using the model HydroGeoSphere. The original model grid with 80,000 finite elements was complemented with two other model variants with approximately 16,000 and 10,000 elements, respectively. Comparing the model results for these different grids, we observe differences in peak discharge, evapotranspiration, and near-surface saturation. Hydraulic heads and low flow, however, are very similar for all tested parameter sets, which allows the use of these variables to calibrate our model. The calibration results are satisfactory and the duration of the calibration has been greatly decreased by using different model grid resolutions.

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1. Introduction

Recently, partial-differential-equation (*pde*) based hydrological models, that couple the shallow-water equations for surface flow and the Richards' equations for subsurface flow, have been successfully applied in various settings, from catchment scale (e.g., Condon et al., 2013; Goderniaux et al., 2011; Li et al., 2008; Shao et al., 2013) to continental scale (Lemieux et al., 2008). They are regarded as useful tools to represent hydrological processes, especially when studying spatially distributed surface–subsurface interactions or catchments driven by climatic or irrigation changes (Pérez et al., 2011), two problems difficult to analyze with simpler "bucket"-type models. However, *pde*-based models are usually computationally very demanding (Blasone et al., 2008) and sometimes require days of CPU time for a single forward run (Goderniaux et al., 2009) on a current desktop computer.

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As a result, calibration of these models, which typically requires a large number of model evaluations, can be a slow, tedious, and subjective process. To reduce the number of simulations needed, model calibration of pde-based models is often limited to a trialand-error process (e.g., Bonton et al., 2012; Calderhead et al., 2011; Goderniaux et al., 2009; Li et al., 2008; Pérez et al., 2011; Xevi et al., 1997), even though Blasone et al. (2008) and McMichael et al. (2006) have also proposed ensemble-based approaches. In the latter approaches, multiple parameters sets are generated by Monte-Carlo methods and weighted or modified depending on the likelihood of model outcomes in comparison to measurement (Beven and Binley, 1992). However, the large number of simulations needed renders approaches involving Monte-Carlo methods almost impossible for large *pde*-based models because of their long simulation times. The importance of sensitivity analysis to decrease the number of calibration parameters, and thus the required number of simulation runs, has also been recognized (e.g., Muleta and Nicklow, 2005; Christiaens and Feyen,







2002). Nevertheless, even for the most efficient calibration methods available today, the number of simulations needed would still be too large to apply these methods to integrated *pde*-based models. Therefore, model reduction is currently the only feasible option to calibrate such models.

Simulation time is known to greatly depend on spatial discretization (e.g., Vazquez et al., 2002). Typically, finer grids cause a non-linear increase of computational costs compared to coarser ones due to the larger number of unknowns. However, a sufficiently fine mesh is needed to realistically represent the topography of the catchment, which is important to properly simulate run-off, infiltration, and surface-subsurface exchange fluxes, or to characterize zones with large changeability in state variables. Therefore, to trade off model accuracy and simulation time, the spatial discretization should be chosen carefully in distributed models. Various studies have been conducted to find the minimum spatial discretization needed to adequately represent the catchment under consideration (e.g., Bruneau et al., 1995; Carrera-Hernandez et al., 2012; Chaplot, 2014; Chaubey et al., 2005; Cotter et al., 2003; Dutta and Nakayama, 2009; Kuo et al., 1999; Moglen and Hartman, 2001; Molnár and Julien, 2000). In general, the grid cell size must be smaller for catchments with highly uneven relief than for those with smooth topography (Chaplot, 2014). In addition, problems as the modeling of erosion (Hessel, 2005), spatially varying evapotranspiration (Sciuto and Diekkrüger, 2010), or reactive transport (Chaplot, 2005) are more sensitive to grid size than the simulation of hydraulic heads or discharge, especially low flow. The choice of spatial discretization therefore depends also on the simulation objectives (Cotter et al., 2003).

The importance of the resolution of spatial discretization has been recognized before, particularly in studies on reactive transport (Mehl and Hill, 2002). In this field, grid telescoping, i.e., the modeling of a reactive transport problem using two grids, namely a coarse grid representing the whole catchment and a fine one representing the surrounding area of the contaminated plume, is relatively common (Mehl and Hill, 2002; Mehl et al., 2006). However, grid telescoping requires a well defined inner domain of interest and an outer domain from which conditions can be extracted and used as boundary conditions for the inner domain. This is not suitable in all situations, e.g., it cannot be used for large nonpoint contamination problems, such as agricultural nitrate leaching from cultivated land.

Recently, more attention has been given to the influence of spatial discretization on model calibration of *pde*-based hydrological model. For example, Wildemeersch et al. (2014) analyzed parameter sensitivity, i.e., the influence of model parameters on the simulation output, and the linearized confidence interval for various spatial discretizations. These quantities were found to be very similar for all grid sizes, in this synthetic case study based on a Belgian catchment of approximately 300 km².

In the present study, we also focus on the links between model calibration and grid resolution. We propose a methodology to accelerate calibration in fully coupled *pde*-based hydrological models. Our main objective is to reduce simulation time, while obtaining a final model with a precise description of topography. To reach this objective, we vary the resolution of spatial discretization during the calibration. Moreover, we analyze how the changing grid resolution affects the model outcome and test the validity of our method in a case study in North-East Spain.

A prerequisite of the present analysis is that the subsurface structure and land-use at the surface is represented by zonation, which – in principle – is represented on all grid levels. Important questions of coarse-graining fine-scale information onto the resolution scale of larger grids are beyond the scope of the present study. Calibrating systems that account for internal heterogeneity

would require a multi-scale representation of the domain, robust coarse-graining rules, and the provision of fine-scale proxy data used in the calibration, which has been done in conceptual hydrological modeling (Samaniego et al., 2010) but not yet in *pde*-based catchment-scale models.

The remainder of this paper is structured as follows: First, we describe the principles of the proposed calibration method. Then, we present the governing equations of the numerical model HydroGeoSphere (Therrien, 2006), used in this study, and the study area. This is followed by the construction of the conceptual model for the test case. Afterward, we compare the outputs of the model when using different computational grids. Finally, we report the results of the sensitivity analysis and the calibration of our calibration method.

2. Proposed calibration strategy

The proposed method to accelerate calibration utilizes a set of coarser grids on which simulations run faster than on the original fine grid. The coarser grids should be coarse enough to noticeably decrease computation time while capturing enough system behavior to be useful for calibration. We suggest to use two auxiliary grids, a coarse grid and an intermediate one.

The coarse grid is used to largely constrain model parameters in the full parameter space. The model outputs based on simulations using this grid and the fine grid should be comparable but may still show large differences, for example a consistent bias in model prediction along the parameters sets. Model results from simulations with the intermediate grid should be more comparable to those of the fine grid than the coarse-grid results, but differences may prevail. Indeed, if the intermediate grid would yield identical results in comparison to the fine grid, the latter grid would be unnecessary. We will show in the following that, upon grid refinement, hydraulic head and low flow can be adequately represented in a coarse grid while peak flow, evapotranspiration and saturation needs to be modeled on a finer grid, at least in the catchment under consideration in this study.

Conceptually, the proposed calibration method consists of the following seven steps, summarized in Fig. 1:

- 1. Set up of three computational grids:
 - a fine grid used in the final model,
 - an intermediate grid used to restrict the possible parameter space,
 - and a coarse grid used to estimate the possible parameter space.
- 2. Systematic comparison of the simulation results using different computational grids.
- 3. Parameter sensitivity analysis on the intermediate grid.
- 4. Constraining the feasible parameter space using the coarse grid.
- 5. Calibration of model parameters on the intermediate grid.
- 6. Transfer of the model parameters to the fine grid and eventual final parameter adjustments.
- 7. Model validation and evaluation on the fine grid.

The choice of the discretization for the coarse and intermediate grids depends on the impact of the grid coarsening on the model outputs used for calibration, such as stream flow hydrographs or hydraulic heads. This therefore also depends on catchment characteristics such as the topography or soil-hydraulic parameters. However, the size of the grid cells used in our case study, described in Section 6, may serve as a starting point in other applications. The method can be adapted to use more or less than three grids, depending on the complexity of the problem.

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