Towards improved treatment of parameter uncertainty in hydrologic modeling

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SUMMARY (ENGLISH)

The research presented in this thesis has focused on the development of stochastic and recursive single- and multi-objective parameter estimation algorithms that combined with state-of-the-art data assimilation methods can be used to more completely treat input, output, parameter, and model structural uncertainty in environmental model calibration. The usefulness and applicability of these algorithms are demonstrated by application to vadose zone and surface hydrology, to improve understanding and predictions of unsaturated soil water flow, water uptake by plant roots, river water discharge, and heat and moisture fluxes at the land surface. What follows here is a short summary of each of the chapters in this thesis.

To state the case and illustrate a typical parameter estimation problem in hydrology, Chapter 2 discussed the inverse estimation of soil physical and root water uptake parameters in a physically-based three-dimensional unsaturated soil water flow model using measured spatial distributions of soil water content around a sprinkler irrigated almond tree. A multi-dimensional approach in root water uptake is needed if uptake is varying in space, thereby allowing a more accurate quantification of spatial variability of the soil water regime, including the water and solute flux densities below the root zone. After calibration of the selected root water uptake model and soil hydraulic parameters, the agreement between simulated and measured spatially distributed water contents during the 16-days calibration period was generally good. To evaluate the benefits of using a sophisticated three-dimensional vadose zone model, the results of this analysis were compared with numerical models describing soil water flow and root water uptake in one and two dimensions. For each of the considered models, independently measured soil water retention data agreed favorably with the optimized retention curves. Moreover, optimized root water uptake distributions between one-, two-, and three-dimensional flow models with corresponding root water uptake models were almost identical. However, major differences occurred for the spatial variation in root water uptake and drainage rates between one-dimensional and multi-dimensional models. This justifies the need for multi-dimensional root water uptake and flow models, especially when the fate and transport of chemicals below the rooting zone for single trees is of concern. Despite the good fit of each of the numerical models to the observed water content data, this chapter also highlighted some of the limitations of current parameter estimation methods: they are computationally very demanding when solving for high-dimensional parameter problems, and they do not provide any information about the probabilistic uncertainty associated with the final parameter estimates. This latter point is of
SUMMARY (ENGLISH)

particular relevance when assessing the identifiability of the model parameters or to diagnose how many parameters are supported by the calibration data.

To overcome the limitations of commonly employed parameter estimation algorithms, Chapter 3 presented a general-purpose code, entitled the Shuffled Complex Evolution Metropolis (SCEM-UA) global optimization algorithm, which is especially designed to provide an effective and efficient estimate of the traditional "best" parameter set and its underlying posterior distribution, within a single optimization run. The algorithm is a Markov Chain Monte Carlo sampler generating a sequence of parameter sets that converge to the stationary posterior distribution, for a large number of model simulations. The SCEM-UA algorithm is related to the successful Shuffled Complex Evolution (SCE-UA) global optimization algorithm, but uses the Metropolis-Hastings (MH) strategy instead of the Downhill Simplex method for population evolution. The stochastic nature of the MH annealing scheme avoids the tendency of the SCE-UA algorithm to collapse into a single region of attraction (local minima), while the information exchange (shuffling) between parallel sequences allows the search to be biased in favor of better regions of the solution space. These adaptive capabilities of the SCEM-UA algorithm significantly reduce the number of model simulations needed to infer the posterior distribution of the parameters when compared with traditional MH samplers. In the same Chapter the identifiability of the parameters in a rather parsimonious conceptual rainfall-runoff model, consisting of a relatively simple rainfall excess model, connected with two series of linear reservoirs was explored. Those results indicated that the entire model structure was well identifiable by calibration to runoff data, thereby supporting statements made in the literature that simple rainfall-runoff models with four to five parameters provide an adequate fit to the streamflow data and that the addition of more model structure and its associated parameters leads to no significant improvement in fit yet introduces poorly identified parameters.

While the capabilities and limitations of the inverse approach for the identification of soil hydraulic properties from laboratory soil cores or small field plots (e.g. Chapter 2) may be considered reasonably well understood, still little is known about the suitability of the inverse approach for the identification of vadose zone properties at larger spatial scales. Fortunately, in the past few years, computational capabilities have evolved to a point, where it is possible to use multi-dimensional physically based watershed models to study spatial and temporal patterns of water flow in the vadose zone. However so far, these models based on complex multi-dimensional governing equations have received only limited attention, in particular because of their computational, distributed input and parameter estimation requirements. In Chapter 4 the usefulness and applicability of the inverse approach for the estimation of spatially-distributed
vadose zone properties was explored, using the solution of a physically-based three-dimensional distributed model combined with spatially distributed measured tile drainage data from the 9700 ha Broadview Water District in the San Joaquin Valley of California. The inverse problem was posed within a single criterion Bayesian framework and solved by means of the computerized SCEM-UA global optimization algorithm, as presented in Chapter 3. To study the benefits of using a spatially distributed three-dimensional vadose zone model, the results of the three-dimensional model were compared with those obtained using a simple conceptual bucket model and a spatial-averaged one-dimensional unsaturated water flow model. Results presented in this Chapter demonstrate that measured spatially-distributed patterns of drainage data contains only limited information for the identification for the vadose zone model parameters, and are particularly inadequate to identify soil hydraulic properties at the larger spatial supports. The dominant hydrologic processes, controlling tile-drain discharge at the watershed scale are preferential flow and the properties of the drain system. Furthermore, results indicate that there are advantages of using physically-based hydrologic models to study spatial and temporal patterns of water flow at larger spatial scales as these mechanistic models not only generate consistent forecasts of spatially-distributed drainage during both the calibration and validation periods, but simultaneously also possess unbiased predictive capabilities of groundwater table depths not included during the calibration.

The primary focus of the Chapters 2-4 has been on the “batch” calibration approach, which aggregates error residuals over a large range of hydrologic behavior. These “batch” processing methods do not explicitly recognize differences in model sensitivity of the model parameters to the various measurements, and as such cannot be used to identify which sets of measurements are most informative for specific model parameters. In Chapter 5 a formal methodology is explicated, entitled the Parameter Identification Method based on the Localization of Information (PIMLI), which increases information retrieval from experimental data, by recursively assimilating and processing the information content in the calibration data. The PIMLI algorithm is a hybrid approach that merges the strengths of the Generalized Sensitivity Analysis (GSA) method, Bayesian recursive estimation, and the sampling efficiency of the Metropolis-Hastings algorithm to select those sets of measurements that contain the most information for the identification of the various model parameters. The usefulness and applicability of the PIMLI algorithm was demonstrated by application to the estimation of soil hydraulic parameters using soil water retention data and a more complex multi-step transient outflow experiment, and the calibration of a conceptual rainfall-runoff model. Each of these studies illustrated that the PIMLI algorithm was well suited to identify which parameters control
what part of model behavior, while providing insights into the importance of different kinds of calibration data in model parameter estimation. Moreover, the method revealed that only a very limited number of streamflow measurements were needed for a reliable calibration of a conceptual rainfall-runoff model.

The research presented in Chapters 2-5 focused on the use of a single-objective measure to extract all the information contained in the calibration data. Practical experience with the calibration of hydrologic models, however, suggests that single-objective functions are often insufficient to properly account for all of the characteristics of the observed data deemed to be important. One strategy to circumvent this problem is to define several optimization criteria (objective functions) that measure complementary aspects of the system behavior and to use a multicriteria optimization method to identify the set of nondominated, efficient or Pareto optimal solutions. While in the past several algorithms have been developed which can solve multi-objective calibration problems, these methods have two characteristic failing problems. In the first place, they tend to cluster the Pareto solutions in the compromise region among the objectives, thereby leaving the ends of the Pareto frontier unexploited. The second, perhaps more important, failure is the inability of these methods to converge to solutions within the “true” Pareto set for hydrologic models involving a large number of parameters and highly correlated performance criteria. In Chapter 6, therefore, the Multi-objective Shuffled Complex Evolution Metropolis (MOSCEM) global optimization algorithm is presented, which is capable of effectively and efficiently solving the multi-objective optimization problem for hydrologic models. The MOSCEM-UA algorithm combines the strengths of the complex shuffling employed in the SCE-UA algorithm, the probabilistic covariance-annealing search procedure of the SCEM-UA algorithm (see Chapter 3) and an improved fitness assignment concept to construct a uniform estimate of the Pareto solution set, thereby containing the single criterion end points. This Pareto set of solutions represent tradeoffs among the different incommensurable and often conflicting objectives, having the property that moving from one solution to another results in the improvement of one objective while causing deterioration in one or another. The MOSCEM-UA algorithm is the multi-objective relative of the SCEM-UA algorithm, but uses an innovative concept of Pareto dominance rather than direct single-objective function evaluations, to evolve the initial population of points towards a set of solutions stemming from a stable distribution (Pareto set). Application of the MOSCEM-UA algorithm to the Sacramento Soil Moisture Accounting Model of the US National Weather Service has demonstrated that there is considerable uncertainty associated with the percolation and recession processes in the model, which play a major role in determining the shape of the
hydrograph during periods without rainfall. A multi-criteria calibration of the bio-sphere atmosphere transfer scheme (BATS) land-surface model using measured heat and moisture fluxes from the Oklahoma ARM-CART site revealed that there are two disconnected regions in the parameter space which generate quite similar model behavior, indicating a interesting model structural issue that deserves further investigation.

With the availability of the stochastic and recursive SCEM-UA, MOSCEM-UA and PIMLI optimization algorithms, developed in Chapters 3, 5 and 6 we are now able to meaningfully and efficiently estimate single and multi-objective parameter uncertainty. However, uncertainties in the modeling procedure not only stem from uncertainties in the parameter estimates, but also from measurement errors associated with the system input (forcing) and output, and from model structural errors arising from the aggregation of spatially distributed real-world processes into a mathematical model. Not properly accounting for these errors during model calibration, results in model simulations and their associated prediction uncertainty bounds, which do not consistently represent and bracket the measured system behavior. This is usually evidenced by residuals, which exhibit considerable variations in bias (non-stationarity), variance (heteroscedasticity), and correlation structures under different hydrologic conditions. To more completely treat input, output, parameter and model structural uncertainty in hydrologic model calibration, Chapter 7 presented a Simultaneous parameter Optimization and Data Assimilation method entitled SODA, which combines the strengths of the parameter search efficiency and explorative capabilities of the SCEM-UA algorithm (see Chapter 3), and the power and computational efficiency of the Ensemble Kalman Filter to simultaneously estimate state variables and model parameters. Additionally, in this Chapter a nonparametric variance estimator is introduced, which is especially designed to estimate the measurement error of output data. The usefulness and applicability of SODA was demonstrated for two preliminary case studies. The first case study considered the highly nonlinear three-parameter Lorenz model, and demonstrated that SODA is indeed successfully able to simultaneously estimate state variables and model parameters when confronted with highly nonlinear model dynamics. The second case study explored the usefulness of SODA by application to hydrologic modeling using a simple conceptual watershed model and historical streamflow data from the Leaf River Watershed in Mississippi. The ability of SODA to properly deal with input, output, parameter and model structural errors, results in honest parameter and model prediction uncertainty ranges. Furthermore, detailed investigation of the computed state and output innovations as function of time, generates useful inspiration to improve our model concepts and as such our understanding of the functioning of hydrologic systems.
Finally, in Chapter 8 an epilogue is presented in which the most important research questions that can now be forcefully addressed with the availability of the SCEM-UA, PIMLI, MOSCEM-UA, and SODA parameter and state estimation are highlighted. Additionally, in this Chapter a short view on future research in model calibration is explicated.