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Estimating initial conditions for groundwater flow modeling using an adaptive inverse method

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ABSTRACT

Due to continuous increases in water demand, the need for seasonal forecasts of available groundwater resources becomes inevitable. Hydrogeological models might provide a valuable tool for this kind of resource management. Because predictions over short time horizons are foreseen, the reliability of model outputs depends on accurate estimates of the initial conditions (ICs), as well as the estimated parameter values, boundary conditions and forcing terms (e.g., recharge, as well as sinks and sources). Here, we provide an inverse procedure for estimating these ICs. The procedure is based on an adaptive parameterization of the ICs that limits over-parameterization and involves the minimization of an ad hoc objective function. The quasi-Newton algorithm is used for the minimization, and the gradients are computed with an adjoint-state method. Two test cases based on a real aquifer that are designed to evaluate the capability of the method were addressed. It is assumed that the boundary conditions, hydraulic parameters and forcing terms are known from an existing hydrogeological model. In both test cases, the proposed method was quite successful in estimating the ICs and predicting head values that were not used in the calibration. 50 calibrations for each test case have been performed to quantify the reliability of the predictions.

1. Introduction

Seasonal forecasts of groundwater resources are increasingly required for optimal management, especially to cover agricultural water needs during summer periods. Because seasonal forecasts usually cover a short period of time (one month or so), their production is very challenging because of groundwater system inertia, which may retain the memory of the initial conditions (ICs) in the simulation results over the entire period covered by the forecast.

The need for accurate ICs for operational forecasting is well known in climate modeling (*e.g.,* Collins and Allen, 2002) and in modeling of seasonal surface flow (*e.g.,* DeChant and Moradkhani, 2011). The relative importance of ICs for seasonal hydrologic forecasting has been analyzed by Li et al. (2009), who showed that the reliability of predictions depends on the uncertainties related to the ICs, and that the impacts of the ICs are influenced by the variability in the physical characteristics of the basins and the forcing terms acting on them.

Because groundwater modeling usually addresses either steady-state conditions or covers long periods of time, the estimation of ICs has received very little attention compared to the efforts that have been dedicated to model parameter estimation (Sun, 1994; Carrera et al., 2005). ICs are usually set using a steady-state solution (Hill and Tiedeman, 2007) computed with average inflows and outflows. Alternatives include the use of interpolated measured heads based on contour maps (Ting et al., 1998), the use of more elaborate interpolation techniques, such as kriging (Nobi and Das Gupta, 1997) or the use of computed heads from a previous simulated stress period (Cheng et al., 2011). However, inaccurate ICs can significantly impact simulation periods for years in confined aquifers or for decades in unconfined aquifers (Rushton and Wedderburn, 1973) and can lead to inaccurate parameter estimates (Liu et al., 2009).

ICs are reference head values for the computation of changes in heads (Franke et al., 1987), and the results of simulations that cover short time horizons are strongly correlated with these reference values. Therefore, the reliability of this type of predictions is strongly dependent on the reliability of the ICs. This motivates our work, which develops an inverse methodology to estimate ICs on the basis of head observations. We assume that a hydrogeological model already exists, in which the hydrodynamic parameters have been calibrated beforehand over a long period of time, and that the effects of approximations related to boundary conditions can be neglected. We also assume that the parameters

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employed for seasonal predictions (short periods of time) are identical to those estimated for simulations covering long time periods (typically several years). These assumptions avoid the correlations between ICs and parameters that may appear when ICs and parameters are estimated simultaneously, as shown by Liu et al. (2009).

The first section of the paper is dedicated to the adaptive inverse procedure that we apply to estimate the ICs. As an IC solution has essentially the same size as the flow grid used to solve the forward problem, a multi-scale parameterization technique that uses local parameter values as seeds for interpolation over the whole flow domain is employed. Gradients of the objective functions are approximated via a purposely derived adjoint-state method. Numerical experiments are then presented in the second section. With the aim of evaluating the accuracy and robustness of the method, the latter is tested against two examples derived from an actual setting involving a heterogeneous limestone aquifer that differ in terms of the number of observation wells and the number of reference heads per well. Changing the amount of information included in the inversion for ICs is expected to influence, at a minimum, the accuracy of the solutions.

2. Mathematical model and estimation of initial conditions

For the sake of simplicity, we address here a situation involving two-dimensional flow in a confined aquifer. We note that the developments proposed hereafter would hold for three-dimensional problems in either confined or unconfined systems. The usual mathematical model is depicted by the following equations:

$$\begin{cases} S\frac{\partial h}{\partial t} = \nabla\cdot(\mathbf{T}\nabla h) + f & \textit{in } \Omega, t\in[0,T_f] \\ h(x,y,0) = h^0(x,y) & \textit{in } \Omega \\ h(x,y,t) = h^D(t) & \textit{on } \partial\Omega_D t\in[0,T_f] \\ -\mathbf{T}\nabla h(x,y,t)\cdot\mathbf{n} = \mathbf{q_N(t)} & \textbf{on } \partial\Omega_\mathbf{N}, \mathbf{t}\in[\mathbf{0},\mathbf{T_f}] \end{cases} \quad (1)$$

where S is the storativity [–], h is the head [L], $\mathbf{T}$ is the transmissivity tensor [$L^2\,T^{-1}$], and f is the sink-source term [LT^{-1}]. Ω is the model domain, $\partial\Omega_D$ and $\partial\Omega_N$ are partitions of the domain boundaries $\partial\Omega$ that correspond to Dirichlet and Neumann conditions, and $\mathbf{n}$ is the unit vector normal to the boundary, counted positive outward. $h^D(t)$ are the prescribed head values at the Dirichlet boundaries, $q_N(t)$ are the prescribed fluxes at the Neumann boundaries and $h^0(x,y)$ represent the ICs defined over the whole domain Ω. T_f is total simulated period.

Due to the complexity of the parameter distribution and the time varying sink-source terms, the flow equation is solved numerically, which leads to a discretized form that is written as:

$$\mathbf{A}\mathbf{h}^k = \mathbf{b}^{k-1} \quad (2)$$

where k is the time step counter, $\mathbf{h}$ is the vector of hydraulic heads, $\mathbf{A}$ is the system matrix, which depends on the model geometry and parameters, and $\mathbf{b}$ is the right hand side vector, which depends on the boundary conditions, sink-source terms and heads at the previous time step $k-1$.

The ICs $\mathbf{h}^0$ are estimated by minimizing an objective function written in the maximum likelihood framework that is defined as:

$$J\left(\mathbf{h},\mathbf{h}^0\right) = \sum_{k=1}^{N}\left(\mathbf{h}^k-\hat{\mathbf{h}}^k\right)^T[\mathbf{W}^{-1}]\left(\mathbf{h}^k-\hat{\mathbf{h}}^k\right) + \mu\left(\mathbf{h}^0-\tilde{\mathbf{h}}^0\right)^T[\mathbf{V}^{-1}]\left(\mathbf{h}^0-\tilde{\mathbf{h}}^0\right) \quad (3)$$

where $\mathbf{h}$ represents the computed heads, $\hat{\mathbf{h}}$ represents the measured heads, and N is the number of time steps. $\tilde{\mathbf{h}}^0$ represents prior estimates of the initial heads, and $\mathbf{h}^0$ represents the computed initial heads. The index T stands for the transpose operator. $\mathbf{W}$ represents a prior estimate of the covariance of the measurement errors associated with the heads, whereas $\mathbf{V}$ represents a prior estimate of the covariance of measurement errors associated with the ICs. Both terms in the objective function represents the quadratic errors between computed and measured heads at different locations and for N different times. The quadratic errors for the initial conditions are explicitly expressed to provide them a significant weight for the minimization. For this reason, we also set $\mu = N$ to balance the two terms in the objective function.

Assuming that the measurement errors are known and uncorrelated in space and time, the matrices $\mathbf{W}$ and $\mathbf{V}$ are defined by:

$$\mathbf{W}^{-1} = \mathbf{V}^{-1} = 1/\sigma_h^2\mathbf{I} \quad (4)$$

where σ_h^2 is the estimated variance of the measurement errors, and $\mathbf{I}$ is the identity matrix. μ is a weighting coefficient that allows the balancing of the two terms in the objective function.

Depending on the numerical method used to solve (1), the ICs have to be determined for each node or element of the discretized domain. Since groundwater flow models require several thousand nodes or elements, the optimization problem minimizing (3) is over-parameterized. To overcome this problem, we rely upon the adaptive parameterization technique suggested by Ackerer et al. (2014) and Hassane and Ackerer (2017). This approach was applied initially to parameter estimation; here, it is extended to IC estimates on a grid (that is, the IC grid), which is independent of the grid used to solve the flow model (that is, the flow grid). Because hydraulic heads vary smoothly in space, we assume that the ICs over Ω can be approximated as a sum of piecewise linear functions, with each function being defined over a single triangle. Therefore, the IC grid is a triangulation of Ω and is chosen to be very coarse at the beginning of the algorithm (Fig. 1). During optimization, the IC grid is progressively refined (Fig. 2) whenever the value of the objective function remains too high. It is worth noting that the flow grid beneath the IC grid can be of any type, and that other methods for approximating the ICs could be chosen. The ICs on the flow grid are obtained by mapping the ICs defined on the IC grid to the flow grid using linear interpolation, to be consistent with the approximation of the IC. The details of the algorithm can be found in Ackerer et al. (2014) and Hassane and Ackerer (2017).

After successive refinements of the IC grid, the number of degrees of freedom of the optimization problem (one per vertex of the IC grid) may increase strongly, which renders the adjoint-state method (*e.g.,* Sun and Yeh, 1992; Townley and Wilson, 1985) preferable to standard sensitivity approaches, which require considerable computing time when many parameters are sought (Medina and

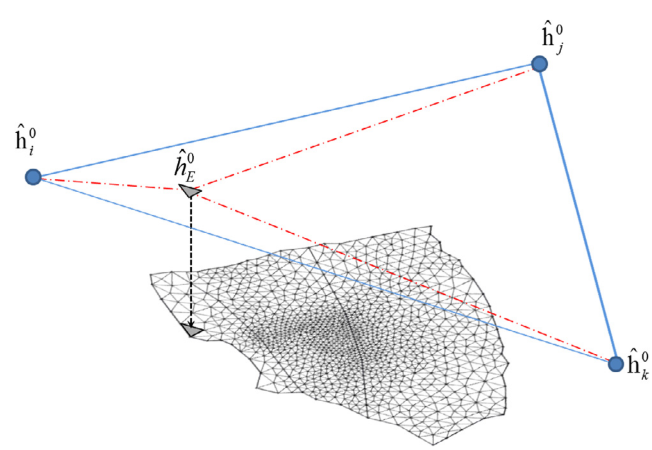

Fig. 1. IC grid (in blue) and flow grid (in black) during the first step of the parameterization.