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Application of ensemble H-infinity filter in aquifer characterization and comparison to ensemble Kalman filter

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Abstract

Though the ensemble Kalman filter (EnKF) has been successfully applied in many areas, it requires explicit and accurate model and measurement error information, leading to difficulties in practice when only limited information on error mechanisms of observational instruments for subsurface systems is accessible. To handle the uncertain errors, we applied a robust data assimilation algorithm, the ensemble H-infinity filter (EnHF), to estimation of aquifer hydraulic heads and conductivities in a flow model with uncertain/correlated observational errors. The impacts of spatial and temporal correlations in measurements were analyzed, and the performance of EnHF was compared with that of the EnKF. The results show that both EnHF and EnKF are able to estimate hydraulic conductivities properly when observations are free of error; EnHF can provide robust estimates of hydraulic conductivities even when no observational error information is provided. In contrast, the estimates of EnKF seem noticeably undermined because of correlated errors and inaccurate error statistics, and filter divergence was observed. It is concluded that EnHF is an efficient assimilation algorithm when observational errors are unknown or error statistics are inaccurate.

Keywords: Data assimilation; Hydraulic parameter estimation; Ensemble H-Infinity filter; Ensemble Kalman filter; Hydraulic conductivity; Robustness

1. Introduction

Water shortage and pollution are common problems worldwide. For instance, in China a recent national water quality survey has shown that only 38.7% of groundwater from wells meets quality criteria for source water supplies (Yu et al., 2014), and toxic organic chemicals threaten groundwater supplies and human health in the U.S. (National Research Council, 2013). Aquifer characterization is always the first step to recognizing, managing, and protecting aquifers. Though a lot of pore- and fracture-scale studies manage to measure or characterize the exact geometries of porous or fractured media at small scales and simulate the detailed dynamics of flow and transport behaviors at such scales (Dou and Zhou, 2014; Chen et al., 2014), to date, small-scale techniques are not applicable to field-scale problems in practice, like aquifer characterization and modeling, because of a lack of sufficient measurements. Unfortunately, due to considerable spatial variability in geology and a lack of information, affordable and accurate characterization of aquifer properties is still a challenge. Efficient and accurate estimation of parameters in groundwater models is always one of the most significant focuses of hydrology, since reliability and predictability of models are greatly dependent on model parameters. The parameter estimation or inverse problems in

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subsurface modeling are commonly considered ill-posed, and the "non-uniqueness of inverse problems should be addressed as uncertainty in the solutions" (Yeh et al., 2015) and may sometimes be handled via optimization approaches (Carrera and Neuman, 1986).

In recent decades, filter methods used in data assimilation, which can combine and integrate different kinds of data, have drawn growing attention from hydrogeologists. These methods are capable of handling uncertainty with insufficient information in the framework of Bayes' theorem and improving the sensitivity of hydraulic variables (head, concentration, etc.) to hydraulic parameters (conductivity, dispersion coefficient, etc.) by introducing new kinds of data rather than simply adding more measurements of the same variable (McLaughlin and Townley, 1996); these are the fundamental reasons for the popularity of filter methods. As one of the most popular data assimilation techniques, the ensemble Kalman filter (EnKF) has received broad recognition, and has been verified, improved, and applied in many areas, including hydrogeology (Evensen, 2003; Chen and Zhang, 2006; Franssen and Kinzelbach, 2008; Sun et al., 2009; Nan and Wu, 2011; Panzeri et al., 2013; Assumaning and Chang, 2016). Applications show its capability of incorporating observations of various types from different sources to update the state of the model but expose its significant deficiencies as well. The performance of EnKF relies on accurate dynamic models of the system and on the premise that all the noises are Gaussian white noise whose statistical properties are clearly known. If the premise of accurate models or statistical properties of noises fails, the capability of the algorithm will deteriorate, and the method may even result in ridiculous system states (Sun et al., 2009; Nan and Wu, 2011). In practice, many measurement noises are not white noise. They are often correlative in time or space or even change with time. Thus, a uniform error model is prohibitive in many situations, let alone in the cases when their statistical properties completely unknown (Wang et al., 2004). EnKF encounters big problems in practice when only limited information on error mechanisms of many observational instruments for subsurface systems is accessible. This is especially true for many newly developed hydrogeophysical techniques (Chung and Lin, 2009; Tian et al., 2016). When water quality and security issues draw greater attention of the public, characterization of aquifer properties with a reliable risk control becomes a significant challenge, since variability of hydraulic properties and accuracy of parameter estimation are crucial for groundwater flow, solute transport, and incomplete mixing problems (Essaid et al., 2015; Tong et al., 2015).

The H-infinity (or H_∞) filter, which is used in signal processing and control theory to achieve stabilization with guaranteed performance, has good robustness against uncertain system noises (Shaked, 1990; Hassibi et al., 2000). It treats uncertain inputs and noises as random perturbations with limited energy and tries to minimize the H-infinity (H_∞) norm of the transfer function from perturbations to estimation errors or to make it less than a given positive number. A lot of work has been performed to develop and investigate theories and algorithms of H-infinity in linear spaces or spaces which can be transformed into linear spaces (e.g., Deng, 2013; Yoneyama, 2013; Zhang et al., 2014). Lü et al. (2010) used an H-infinity filter to estimate root zone water content by assimilating soil moisture data in a one-dimensional linearized Richards' equation.

To apply the H-infinity filter in nonlinear atmospheric systems, Han et al. (2009) combined the Monte Carlo method with the H-infinity filter and investigated the capability of the ensemble H-infinity filter (EnHF) in two synthetic data assimilation experiments. Luo and Hoteit (2011) proposed a time-local version of EnHF which utilized only the current state and observations of the system rather than the entire available history and found the equivalency between their algorithm and EnKF with covariance inflation. To the best of our knowledge, EnHF has not been studied in hydrogeology or parameter estimation fields. Accounting for its robust performance in the case of insufficient information on model or measurement errors, this algorithm may turn out to be a powerful and practical tool for integrating hydrogeophysical data into groundwater models and be worthy of more attention from the hydrogeology community. In this paper, we first formulate groundwater flow models and the algorithms of EnKF and EnHF, respectively. Afterwards, we examine the ability of EnHF to estimate aquifer properties with observations subject to uncertain (spatially and temporally correlated) errors, and compare it with that of the well-known EnKF.

2. Methods

2.1. Groundwater flow simulation

Transient groundwater flow in confined and isotropic aquifers is considered to satisfy the following basic equation:

$$\nabla \cdot [K(\boldsymbol{x})\nabla h(\boldsymbol{x},t)] + w(\boldsymbol{x},t) = S_{\mathrm{s}}\frac{\partial h(\boldsymbol{x},t)}{\partial t} \tag{1}$$

subject to the initial and boundary conditions:

$$h(\boldsymbol{x},0) = H_0(\boldsymbol{x}) \tag{2}$$

$$h(\boldsymbol{x},t) = H_{\mathrm{D}}(\boldsymbol{x},t) \quad \boldsymbol{x}\in\Gamma_{\mathrm{D}} \tag{3}$$

$$K(\boldsymbol{x})\nabla h(\boldsymbol{x},t)\cdot\boldsymbol{n}(\boldsymbol{x}) = Q(\boldsymbol{x},t) \quad \boldsymbol{x}\in\Gamma_{\mathrm{N}} \tag{4}$$

where $\boldsymbol{x}$ is the spatial vector, t is time, $K(\boldsymbol{x})$ is the hydraulic conductivity, $h(\boldsymbol{x},t)$ is the pressure head, $w(\boldsymbol{x},t)$ is the exchange between the element and outer space (source/sink term), S_{s} is the specific storage, $H_0(\boldsymbol{x})$ is the initial head distribution in the domain, $H_{\mathrm{D}}(\boldsymbol{x},t)$ is the prescribed head on the Dirichlet boundary segments Γ_{D}, $Q(\boldsymbol{x},t)$ is the prescribed flux across the Neumann boundary segments Γ_{N}, and $\boldsymbol{n}(\boldsymbol{x})$ is the outward