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A comparison of discrete versus continuous adjoint states to invert groundwater flow in heterogeneous dual porosity systems

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ABSTRACT

Dual porosity models become increasingly used for simulating groundwater flow at the large scale in fractured porous media. In this context, model inversions with the aim of retrieving the system heterogeneity are frequently faced with huge parameterizations for which descent methods of inversion with the assistance of adjoint state calculations are well suited. We compare the performance of discrete and continuous forms of adjoint states associated with the flow equations in a dual porosity system. The discrete form inherits from previous works by some of the authors, as the continuous form is completely new and here fully differentiated for handling all types of model parameters. Adjoint states assist descent methods by calculating the gradient components of the objective function, these being a key to good convergence of inverse solutions.

Our comparison on the basis of synthetic exercises show that both discrete and continuous adjoint states can provide very similar solutions close to reference. For highly heterogeneous systems, the calculation grid of the continuous form cannot be too coarse, otherwise the method may show lack of convergence. This notwithstanding, the continuous adjoint state is the most versatile form as its non-intrusive character allows for plugging an inversion toolbox quasi-independent from the code employed for solving the forward problem.

1. Introduction

Various hydrological studies are increasingly employing dual porosity models that fully overlap two matrix and fracture continua for the purpose of performing tractable calculations of flow and transport in underground fractured systems as exemplified by Neuman (2005), Bourbiaux (2010), and Lemonier and Bourbiaux (2010a,b). The homogenization of fracture fields provided by the continuous approach (Warren and Root, 1963; Gerke and Van Genuchten, 1993) is conducive to investigate the dynamics of large-scale systems such as regional groundwater reservoirs (e.g., Follin and Thunvik, 1994; Cornaton and Perrochet, 2002; Trottier et al., 2014). Nevertheless, conditioning these large-scale homogenized problems regarding, for instance, their hydrodynamic parameters is often plagued by the absence of data or the non-representativeness of measures at the mesh scale of a regional model. For example, Noetinger and Estebenet (2000), and Landereau et al. (2001), clearly showed via homogenization techniques or numerical experiments that an important amount of information on a fracture network was needed to assign correctly hydraulic parameters to a dual porosity model. Therefore, modeling highly heterogeneous media has to be flanked with inversion procedures that seek model parameters, most often by relying upon history-matching exercises, in the sense of a comparison between model outputs and available flow data. To mention a few: steady-state or transient hydraulic heads in natural flow conditions, interference testing between wells during forced flow conditions (e.g., Pourpak et al., 2009; Ackerer and Delay, 2010), and hydraulic tomography (e.g., Brauchler et al., 2013; Illman, 2014).

The parameterization of a model, taken here as the way to diminish the number of parameters sought by inversion is also a key to retrieve the heterogeneity of the modeled system (e.g., Hendricks-Franssen et al., 2009; Zhou et al., 2014). Many techniques exist such as zonation (e.g., Roggero and Hu, 1998; Hayek et al., 2009; Pasetto et al., 2013), pilot-points (de Marsily et al., 1984; Ramarao et al., 1995; Alcolea et al., 2006), master points (Gomez-Hernandez et al., 1997; Capilla et al., 1998), and various interpolations of local seed parameter values (Mantoglou, 2003; Hassanne and Ackerer, 2017). In many cases, parameterization still asks for large numbers of parameters as degrees of freedom to the inversion of the flow model. These large numbers are not suited to the implementation of optimization techniques employing the class of evolutionary algorithms such as genetic algorithms (e.g., McKinney and Lin, 1994; Karpouzos et al., 2001), particle swarm optimizations (Robinson and Rahmat-Samii, 2004) and Markov Chain Monte Carlo (e.g., Vrugt et al., 2009); all these being usually applicable

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to weakly parameterized problems, with few exceptions. One of them involves Markov Chains coupled with parameter field decompositions and application to heterogeneous hydrological systems (mainly, hydraulic conductivity fields, e.g., Laloy et al., 2013; Mara et al., 2015). Finally, classical descent direction methods as exemplified in, e.g., Carrera and Neuman (1986b), Carrera (1988), and Tarantola (2005), appear better suited to highly parameterized problems. Nevertheless, descent methods require precise calculations of directions in the parameter space along which a set of parameters is moved toward a solution that fits the model to data.

Since their origin, dual porosity models have been enhanced, with, for example, the studies by Pruess and Nakasimhan (1982,1985) initiating the multiple interacting continua (MINC) models, then revisited in the last ten years, mainly on the complexity of mass exchanges between fracture and matrix compartments (Karimi-Fard et al., 2006; Tatomir et al., 2011; De Dreuzy et al., 2013). This notwithstanding, dual porosity model inversion did not receive much attention except for a few recent works (Kaczmaryk and Delay, 2007; Ray et al., 2012; Trottier et al., 2014; Ackerer et al., 2014). The point is that in dual porosity models the strong heterogeneity of parameters, associated with highly variable sensitivity of the model to parameters, hinder inversion techniques relying upon descent directions calculated with model sensitivities (Delay et al., 2007). Since each sensitivity calculation requires solving equations similar to that of the forward problem, duplicating the procedure over a whole set of parameters with "unstable" sensitivities may render the inverse problem intractable with numerous iterations that hardly converge into a valuable solution.

Fortunately, descent methods manipulating high numbers of parameters can also rely upon Quasi-Newton optimization algorithms, the latter simply asking for the calculation of the gradient components of the objective function (e.g., Carrera and Neuman, 1986b; Carrera, 1988; Carrera et al., 2005; Tarantola, 2005). In that case, the adjoint state (i.e., a set of Lagrangian multipliers associated with model equations as the additional constraints to the minimization of the objective function; see hereafter for details) may help in evaluating the gradient components (e.g., Townley and Wilson, 1985; Yeh, 1986). Evaluating the adjoint state requires a single calculation similar to that of the forward problem, irrespective of the number of sought parameters. The downside is that Quasi-Newton algorithms are far less efficient than methods based on model sensitivities and may show very slow convergence.

Even though fundamentals of the adjoint state calculations were posed between the late sixties and the mid-seventies (Lions, 1968; Chavent 1971; Chavent, 1975), the technique has not been employed intensively in the domain of hydrology. A few pioneering illustrations are available in Neuman (1980), Townley and Wilson (1985) or Yeh (1986) for seeking (with success) hydraulic parameters under steady-state flow. They were followed by, for example, Sun (1994) who developed the adjoint states for various configurations of flow and transport in groundwater systems, Medina and Carrera (2003) who inverted source terms in a flow-transport coupled problem, and Ackerer and Delay (2010), Ackerer et al. (2014) who inverted flow in a limestone aquifer on the basis of interference data. One can distinguish between the continuous form (e.g., Chavent 1975) and the discrete form (e.g., Townley and Wilson, 1985) of the adjoint state but it is worth noting that most applications rely upon discrete approaches. However, the discrete adjoint state has the drawback in its implementation of requiring the complete structure of the (discrete) equations of the forward model (see hereafter). The discrete adjoint state must be developed specifically for the code of the forward problem, and therefore, cannot be seen as part of a separate inversion toolbox plugged into a numerical model to seek optimal model parameters. This is probably the main reason why discrete adjoint state techniques are not widely available and used.

The continuous adjoint state is grounded in a variational formulation of the continuous equations that rule the forward model (see hereafter), this formulation then being discretized and calculated by any means, eventually independent of the way the forward problem is solved. This feature renders the technique versatile. Notably, calculations of both the adjoint state and gradient components of the objective function need for results imported from the forward model. This exchange of information between two separate models, eventually calculated differently, may result in a slight denaturation of the exchanged information that has been made compatible between the two models. In addition, most developments of continuous adjoint states are not generic, meaning that they are built to invert a specific type of parameter in a model (e.g., Sun, 1994).

We propose in this study a fair comparison between discrete and continuous forms of adjoint states by assessing their ability to assist a Quasi-Newton descent algorithm that inverts a flow problem in a heterogeneous dual porosity system. To our best knowledge, this type of comparison has never been undertaken, the eventual discrepancies and inaccuracies of the continuous adjoint state being generally conjectured and not demonstrated. We first propose a discussion on the fundamentals that define both the discrete and continuous adjoint states. These are in general not well known, even though they clearly picture the main differences between the two forms of adjoint states (Section 2).

In the comparison, we employ a discrete adjoint state formalism already developed by some authors of the present contribution (Ackerer et al., 2014). The continuous adjoint state applied to flow in a dual porosity model is here fully developed because no attempt on the topic appeared to date in the literature and because the proposed form is applicable to the assessment of any type of parameter in a dual porosity model (Section 3). We do not cope with the inversion of boundary conditions, even though it can be noted that these specific evaluations, as for the discrete adjoint state (see Ackerer et al., 2014), do not require more than the development proposed for inverting model parameters. We acknowledge however that we did not consider the inversion of sink-source terms.

Discrete and continuous adjoint states are compared on the basis of synthetic test cases of inversion that allow us to know the reference solution to the flow problem investigated (Section 4). We can therefore clearly evaluate to what extent the different forms of adjoint states are useful to retrieve the heterogeneity of parameter fields, how the sought solutions generate model outputs that fit conditioning data; and finally, how the inversion procedure is repeatable in the sense that it provides multiple solutions close together even though they have been initiated at different locations in the parameter space. We acknowledge that this type of study employing synthetic tests cases is problem dependent, and the cases analyzed only represent an illustration of the strengths and weaknesses of discrete versus continuous adjoint states. Nevertheless, these cases are aimed at the representation of a wide range of problems in relation with, e.g., groundwater flow in chalk and limestone fractured aquifers.

2. Discrete versus continuous adjoint states

Before detailing how to derive a continuous adjoint state for inverting dual porosity models of flow in porous fractured rocks, it may be useful to review the general context of inversion under constraints and the main differences in the formalism of adjoint states, either discrete or continuous. Let us take for the sake of simplicity a groundwater flow problem handling Darcian flow under steady-state conditions in a single porosity system. As is very well known, this problem is modeled in a finite domain Ω by the following equation:

$$\nabla.\,(-\mathbf{K}\nabla h) + q = 0$$

$\mathbf{K}$ [LT^{-1}] is the hydraulic conductivity of the system corresponding to the model parameter, h [L] is the hydraulic head corresponding to the state variable of the problem, and q [T^{-1}] is a local sink-source term corresponding to volumetric fluxes extracted/injected per unit volume