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Sparse data integration for the interpolation of concentration measurements using kriging in natural coordinates

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SUMMARY

Groundwater contaminant plumes often display a curvilinear anisotropy which conventional kriging and geostatistical simulation approaches generally fail to reproduce. In this paper, we use a physically relevant coordinate transformation in order to improve the kriging of contaminant plumes in 2D. The proposed coordinate transformation maps the Cartesian grid into the natural coordinates of flow: the hydraulic head and the stream function. This simplifies the specification of a nonlinear anisotropy by modifying the spatial relationships between grid points. The computation of the natural coordinates, however, requires the availability of a flow model, which often needs to be defined using limited data. For this reason, a data integration procedure is included in the methodology to support the use of the natural coordinate transformation in real cases. The performance of the approach is tested on two synthetic test cases where it produces concentration maps that are more accurate than those obtained with Cartesian coordinates kriging. These test cases also highlight some limitations of the approach. Whereas the transformation enables kriging to account for advection, results show the need to consider dispersion as well. Further work is also required to generalize the approach to 3D cases and to groundwater flow including wells and sources.

1. Introduction

Contaminant plume mapping is an important part of environmental characterization studies involving groundwater contamination. It is frequently used for tasks related to numerical fate-and-transport modeling, long-term monitoring network design and groundwater remediation (Reed et al., 2004; Michalak and Shlomi, 2007). Plume delineation is generally done using interpolation approaches, which can suffer many drawbacks as environmental studies often involve limited data, preferential groundwater sampling and complex heterogenous media (Reed et al., 2004). Thus, representative plume mapping requires the development of interpolation approaches that integrate efficiently secondary data to improve the description of the shape and extent of contaminant plumes in a sparse data context (Shlomi and Michalak, 2007).

Currently, plumes can be delineated using a large number of approaches, ranging from manual contouring of concentration data to inverse approaches combined with transport modeling. Hand drawing of concentration contours for plume mapping is rather simple to implement, especially in the case where only wide concentration intervals are required. However, this approach is subjective, as it is based on expert knowledge of the hydrogeological system.

Allowing delineated plumes to be coherent with mass transport equations requires advanced approaches involving the use of inverse modeling (Hendricks-Franssen et al., 2003; Shlomi and Michalak, 2007; Schwede and Cirpka, 2010). First, inverse modeling allows the estimation of flow parameters or source release history. Then, forward numerical mass transport modeling produces the concentration map. While a great number of plume mapping approaches make use of hydraulic head data, fewer allow conditioning on concentration data as well. Recent work presents such inverse modeling approaches as a framework for interpolating contaminant plume (Shlomi and Michalak, 2007; Schwede and Cirpka, 2010). These approaches outperform the other types (e.g. deterministic and geostatistical interpolation) in their ability to produce concentration fields coherent with the advection–dispersion equations. On the other hand, this gain is generally obtained at a high computational cost (Schwede and Cirpka, 2010), or under the assumption that an extensive knowledge is available about the flow and transport system being studied. Some approaches presume a full knowledge of the flow and transport conditions in the aquifer and focus on uncertainty associated with the source release history (Shlomi and Michalak, 2007), while other approaches consider uncertainty about flow parameters but not about the release history and most boundary conditions (Hendricks-Franssen et al., 2003; Schwede and Cirpka, 2010).

Deterministic (e.g. inverse-distance weighting) and geostatistical (e.g. kriging) interpolation methods make direct use of concentration

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measurements to produce concentration maps. Kriging, through its variants and extensions, allows the use of secondary information (Michalak and Shlomi, 2007) and soft data (Chilés and Delfiner, 1999). These additional constraints to the generally scarce concentration data can improve plume interpolation; nevertheless, the resulting interpolated plumes are often not coherent with the underlying transport equations and/or display interpolation artefacts. Moreover, as covariance models depend on Euclidean distance to describe inter-points continuity, it is well known that conventional kriging fails to reproduce long curvilinear features, such as those exhibited by meandering channels or by some contaminant plume (e.g. "diving plume" API, 2006). In the literature, solutions that arise from this problem consist in the use of either locally defined direction of anisotropy (Xu, 1996; te Stroet and Snepvangers, 2005), non-Euclidean distances calculated along the main direction of anisotropy (Curriero, 1996, 2006; Rathbun, 1998; Ver Hoef et al., 2006; Bailly et al., 2006; de Fouquet and Bernard-Michel, 2006) or some appropriate coordinate transform in which Euclidean distance can capture the continuity of the phenomenon (Dagbert et al., 1984; Deutsch and Wang, 1996; Christakos et al., 2000; Deutsch, 2002; Barabas et al., 2001; Legleiter and Kyriakidis, 2006). Representing local anisotropy requires a dense sampling of the studied variable for direct identification of local changes in orientation or else, the availability of directional data related to the variable being interpolated, such as dip, azimuth or gradient. Such requirements are seldom met in environmental studies. Computation of non-Euclidean distances share similar requirements as distances need to be calculated along the main direction of continuity. Further, the use of non-Euclidean distances is submitted to certain conditions regarding the covariance function to ensure the covariance matrix is positive definite (Curriero, 1996, 2006). This issue can be overcome using multidimensional scaling (MDS) which maps the points into a higher dimensional space where inter-points Euclidean distances correspond approximately to the computed non-Euclidean distances in the actual space (Sampson and Guttorp, 1992; Monestiez et al., 1993; Loland and Host, 2003; Almendral et al., 2008; Boisvert et al., 2009, 2010). Coordinate transformation based on MDS, however, does not provide a clear interpretation of the transformed space (Legleiter and Kyriakidis, 2006), contrary to transformations based on geographic features or physical processes. A general requirement for a coordinate transformation to be valid is that it provides an unambiguous "address" to points in the domain (Christakos et al., 2000). In other words, the transformation should be unique and reversible (Deutsch, 2002). Such coordinate transformations are used in various applications where a model, such as a river or a geological map, can serve as a basis for the deformation of the Cartesian grid.

Multiple-point geostatistics can produce simulated hydraulic conductivity fields for complex geological settings that include curvilinear features, provided a representative training image is available. Such multiple-point approaches, combined with groundwater flow and transport models, can be used to assess the uncertainty related to contaminant concentrations (Feyen and Caers, 2006; Huysmans and Dassargues, 2009; Blouin, 2010). However, they require the knowledge of the release history and cannot make direct use of concentration measurements.

In this paper, we present an approach that accounts for the non-linear anisotropy often displayed by contaminant plume to enhance groundwater contaminant kriging in 2D. It is based on a coordinate transformation that maps the Cartesian coordinates into the natural flow coordinates i.e. the hydraulic head and the stream function (Bear, 1972). This transformation is similar to that used for the principal direction technique proposed for numerical simulation of contaminant transport (Frind and Matanga, 1985), but adapted to kriging. The relationships between the stream function and the streamlines, as well as that with the hydraulic head, are presented in Section 2.1. The main objective of this paper is to present the coordinate transformation approach. The computation of the natural coordinates, however, requires the availability of a flow model, which often needs to be defined using limited data. For this reason, a data integration procedure is included in the methodology to support the use of the natural coordinate transformation in real cases.

2. Methodology

2.1. Dual formulation of flow

When governed by Laplace equation, two-dimensional groundwater flow can be described simultaneously using hydraulic head h and stream function u (also known as ψ). In 2D, the equation defining the streamline is (Bear, 1972):

$$q_y dx - q_x dy = 0 \tag{1}$$

where q_x and q_y are respectively the x and y components of specific discharge. The solution of Eq. (1) is given by:

$$u = u(x, y) = const \tag{2}$$

where u is the stream function, which takes constant values along streamlines. Derivatives of hydraulic head and stream function are related through the Cauchy–Riemann conditions:

$$K\frac{\partial h}{\partial x} = \frac{\partial u}{\partial y}; \qquad K\frac{\partial h}{\partial y} = -\frac{\partial u}{\partial x} \tag{3}$$

where K is the isotropic hydraulic conductivity. The approach treating h and u as two alternative ways of characterizing a flow regime is generally referred to as the *dual formulation of flow* (Frind and Matanga, 1985; Cirpka et al., 1999). Solving for both functions was found to be an efficient way of generating flow nets (Frind and Matanga, 1985; Fogg and Senger, 1985; Bramlett and Borden, 1990; Buxton and Modica, 1992), as stream function values can be obtained using the same numerical simulators as the hydraulic head (Frind and Matanga, 1985; Anderson and Woessner, 2002). Indeed, the hydraulic head and the stream function share the same form of governing equation:

$$\nabla \cdot K \nabla h = 0 \tag{4}$$

$$\nabla \cdot \frac{1}{K} \nabla u = 0 \tag{5}$$

Proper specification of boundary conditions for the stream function problem in the context of finite element modeling is discussed by Frind and Matanga (1985), Anderson and Woessner (2002). As an example, corresponding h (in bold) and u (in italic) boundary conditions are depicted on top of Fig. 1, which represents the model used in Test Case 2.

Further applications of the dual formulation stem from the fact that it can be used to define a streamline-oriented grid (Cirpka et al., 1999), as h and u define a natural, or intrinsic, coordinate system (Bear, 1972). This is used in the principal direction technique, in which the finite element equations for groundwater contaminant transport are formulated in terms of the natural flow coordinates (Frind, 1982). This way, mass fluxes are always oriented in the principal direction of the grid and the dispersion tensor is a diagonal matrix (Cirpka et al., 1999).

Kriging approaches can also benefit from the dual formulation of flow. Whereas the curvilinearity shown by a contaminant plume could also be accounted for using a locally varying anisotropy in the actual space, a coordinate transformation based on the dual formulation simplifies the specification of anisotropy in the transformed space.

2.2. Flow data integration

The transformation into natural coordinates requires the availability of a flow model to compute the hydraulic head and