Groundwater

# Generation of 3D Spatially Variable Anisotropy for Groundwater Flow Simulations

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## Abstract

Sedimentary units generally present anisotropy in their hydraulic properties, with higher hydraulic conductivity along bedding planes, rather than perpendicular to them. This common property leads to a modeling challenge if the sedimentary structure is folded. In this paper, we show that the gradient of the geological potential used by implicit geological modeling techniques can be used to compute full hydraulic conductivity tensors varying in space according to the geological orientation. For that purpose, the gradient of the potential, a vector normal to the bedding, is used to construct a rotation matrix that allows the estimation of the 3D hydraulic conductivity tensor in a single matrix operation. A synthetic 2D cross section example is used to illustrate the method and show that flow simulations performed in such a folded environment are highly influenced by this rotating anisotropy. When using the proposed method, the streamlines follow very closely the folded formation. This is not the case with an isotropic model.


## Introduction

Anisotropy in sedimentary rocks results from grain orientation, bedding, and lithological contrasts within the sedimentary sequence (e.g., successive strata of clay and sand horizons). Such anisotropy can be measured on rock samples (Renard et al. 2001; Clavaud et al. 2008) or estimated through upscaling procedures at the scale of a grid block for a numerical model (Bierkens and Weerts 1994). Accounting for anisotropy in groundwater flow simulations is required to represent accurately the flow systems. For example, Michael and Voss (2009) modeled the Bengal Basin aquifer system and showed the importance of anisotropy to understand the existence of deep groundwater flow systems and in particular how they can affect the presence or absence of arsenic.

In practice, accounting for anisotropy is made in two steps. First, one needs to use a code that includes a simulation technique able to handle full tensors. As discussed by Yager et al. (2009), several groundwater flow simulation techniques allow the consideration of the anisotropy. For example, finite elements can handle full tensors of hydraulic conductivity without difficulties. In the case of finite differences, the implementation is slightly more difficult but techniques are available (Li et al. 2010). The second step consists of providing a 3D field with hydraulic conductivity tensors varying in space. When the sedimentary units to be modeled are essentially sub-horizontal and follow the numerical mesh, most codes allow the definition of vertical and horizontal hydraulic conductivities. But, as soon as the sedimentary units are heavily folded, and could even possibly display reverse folds and faults, it becomes difficult to estimate the hydraulic conductivity tensor in every point of the 3D domain so that it accurately follows the geological structure and can be imported into a numerical solver.

In this paper, it is proposed to use the implicit 3D geological modeling technique to compute in a straightforward manner the hydraulic conductivity tensor everywhere in the domain. The results of this calculation can be used with any appropriate numerical modeling method to accurately describe groundwater flow even in complex geometries. After introducing the implicit approach, the paper describes the technique to compute the hydraulic conductivity tensor and illustrates its application on a simple anticline example.

## Methodology

### Implicit Geological Modeling

The first step in the proposed approach is to construct a 3D geological model that describes the geometry of the various formations. Over the last 20 years, different approaches and pieces of software have been


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developed to build geological models from incomplete data and geological interpretation. Among them, the implicit approach (Lajaunie et al. 1997) is particularly adapted to our problem.

As opposed to the explicit approach, which describes every geological interface explicitly (using for example a triangulated surface or a grid), the implicit approach is based on the interpolation of an abstract scalar quantity $P(x)$, defined as a potential, everywhere in the 3D domain $\Omega \in R^3$. A geological interface is defined in this approach as the set of points having identical value of the potential $P(x)$.

The orientation of any interface is directly given by the gradient of the potential $g_x$ which is the normal vector perpendicular to the geological interface. Using this framework, it is possible to interpolate the potential by cokriging field measurements of the position of the interface together with structural measurements (strikes and dips) that can be measured anywhere in the domain (Lajaunie et al. 1997). Finally a set of sub-parallel surfaces representing a stratigraphic series can be obtained.

When faults, unconformities, or thrusts are present, the model can be extended by using simultaneously a set of different potentials and erosion rules to represent those more complex structures (Calcagno et al. 2008). However the general approach remains unchanged and is therefore extremely powerful. In practice, to apply the implicit method, we have used the software Geomodeller3D® but other implementations are available, see for example Caumon et al. (2012).

### Computation of the Hydraulic Conductivity Tensor

Let us assume now that a 3D geological model has been built using the implicit method. In any point $x$ of the domain $\Omega$, the geological formation is known as well as the potential $P(x)$ and its gradient:

$$g_x = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix}\Bigg|_x = \begin{pmatrix} \frac{\partial P}{\partial x} \\ \frac{\partial P}{\partial y} \\ \frac{\partial P}{\partial z} \end{pmatrix}\Bigg|_x \qquad (1)$$

By construction, $g_x$ is perpendicular to the geological layers. It is defined everywhere within $\Omega$ and therefore can be used to rotate locally the hydraulic conductivity tensor.

To define the local anisotropy, two assumptions are made. First, the principal directions of anisotropy are supposed to be aligned with the layers and, second, no anisotropy is present parallel to the layers. Under those assumptions, it is sufficient to know the values of the hydraulic conductivities parallel $k_{||}$ and perpendicular $k_\perp$ to the bedding plane to define the conductivity tensor $\boldsymbol{K}_0$ in a local coordinate system aligned with the layers.

$$\boldsymbol{K}_0 = \begin{pmatrix} k_\perp & 0 & 0 \\ 0 & k_{||} & 0 \\ 0 & 0 & k_{||} \end{pmatrix} \qquad (2)$$

The next step consists in computing the components of the hydraulic conductivity tensor in the general coordinate system. For this purpose a rotation matrix is built and applied to the conductivity tensor.

The rotation matrix $R_x$ is constructed from a new orthonormal coordinate system composed by $\boldsymbol{i_x}, \boldsymbol{j_x}$ and $\boldsymbol{k_x}$ vectors:

$$R_x = (i, j, k)\,|_x \qquad (3)$$

where $\boldsymbol{i_x}$ is the unitary vector of the gradient of the geological field $\boldsymbol{g_x}$, $\boldsymbol{j_x}$ is the horizontal unitary vector, perpendicular to $\boldsymbol{i_x}$, and $\boldsymbol{k_x}$ is obtained by the vector product of $\boldsymbol{i_x}$ and $\boldsymbol{j_x}$:

$$i_x = \begin{pmatrix} i_1 = g_1/\|g\| \\ i_2 = g_2/\|g\| \\ i_3 = g_3/\|g\| \end{pmatrix}\Bigg|_x \quad j_x = \begin{pmatrix} j_1 = -i_2/\sqrt{i_1^2 + i_2^2} \\ j_2 = i_1/\sqrt{i_1^2 + i_2^2} \\ j_3 = 0 \end{pmatrix}\Bigg|_x$$

$$k_x = i_x \times j_x \qquad (4)$$

Finally the rotated conductivity tensor $\boldsymbol{K}$ is obtained by matrix rotation:

$$\boldsymbol{K_x} = \boldsymbol{R_x} \boldsymbol{K}_0 \boldsymbol{R_x^T} = \begin{pmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{pmatrix}\Bigg|_x \qquad (5)$$

The same steps are computed for each point in the 3D domain and always accounting for the local orientation of the layers. The result is a 3D field of hydraulic conductivity tensor. In the particular case when both $i_1$ and $i_2$ are zero (perfectly horizontal formation) the original values of $\boldsymbol{K_0}$ can be directly used.

Note that the values of the hydraulic conductivities parallel and perpendicular to the layers can either be considered constant within a specific geological formation, or vary in space within a formation following any stochastic model.

## A Simple 2D Example

In this section, a simple 2D example is presented to illustrate the method. The geological setup corresponds to a perched syncline with rocks of different ages (Figure 1a). The conductivity tensor is calculated using Equation 5. The lithology is considered to be uniform, that is, all layers are made of the same rock. Therefore the colored formations in Figure 1a do not represent a hydraulic conductivity contrast but simply highlight the internal geological structure within the fold. To compute the hydraulic conductivity tensor, values of $k_{||} = 10^{-6}$ [m*s$^{-1}$] and $k_\perp = 0.1 \times k_{||}$ are used.

Figure 2b through 2d show how the conductivity tensor components $k_{xx}$, $k_{xz}$ and $k_{zz}$ vary within the fold. As expected, $k_{xx}$ is close to $k_\perp$ (blue values in Figure 2b) in the regions where the layers are nearly vertical. On the contrary, the component $k_{zz}$ is high in the same region (red

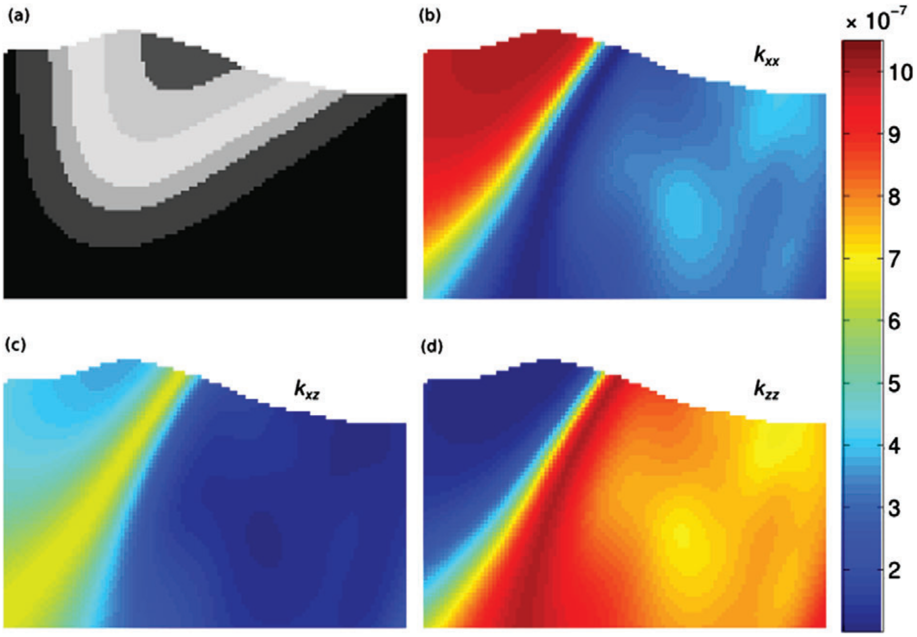


**Figure 1. (a) Geological model: a perched syncline. The lithology is assumed to be uniform but folded, the colors represent only the age of the formation; (b) $k_{xx}$ component of the hydraulic conductivity tensor; (c) $k_{xz}$ component, (d) $k_{zz}$ component. The color scale is given in [m/s] and is relative to b, c, and d subfigures.**

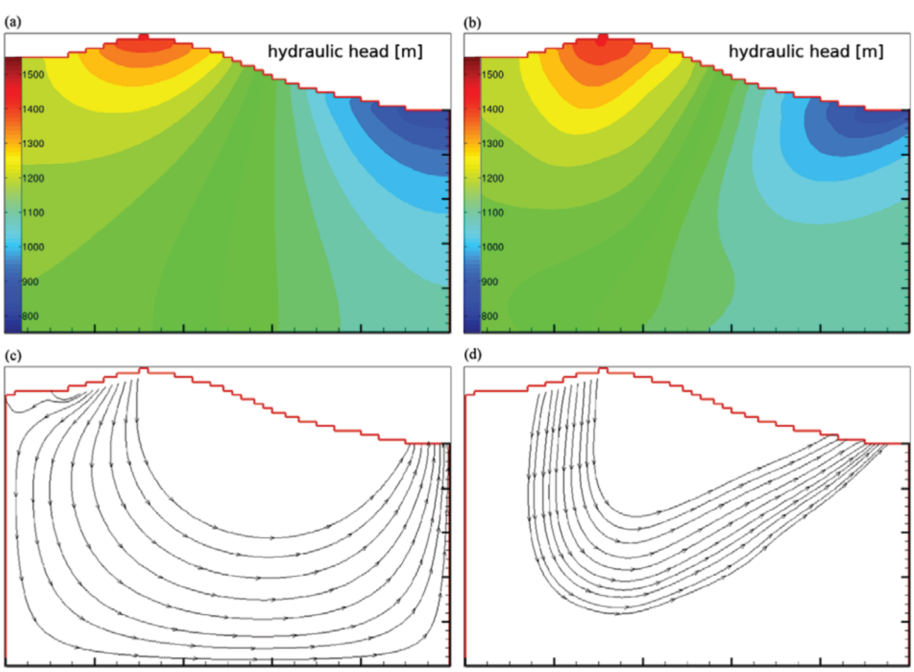


**Figure 2. Differences between a flow simulation that uses an isotropic K tensor and another that uses an anisotropic one which is consistent with the geological structure: (a) hydraulic head distribution, isotropic tensor; (b) hydraulic head distribution, anisotropic tensor; (c) flow lines, isotropic case; (d) flow lines, anisotropic case.**

values in Figure 2d). The interpretation of $k_{xz}$ (Figure 2c) is less intuitive: it has maximal positive (red) and negative (dark blue) values (maximal intensity) in both regions of the model where the formations show a dip close to a value of 45° and −45°. To highlight the hydraulic impact of using the proper rotating tensor, two steady-state regional flow system simulations were carried out using the finite element code Groundwater (Cornaton 2007). The same geometry and boundary conditions are used for both cases. A head equal to the topographic surface elevation is prescribed along the topography, and no flow conditions are prescribed on all the other boundaries. In the first simulation, the medium is assumed isotropic and its hydraulic conductivity is the geometric mean of $k_{||}$ and $k_{\perp}$. In the second simulation, the varying anisotropy tensors are used. Figure 2 shows the results of both flow simulations. Figure 2a and 2c correspond to the isotropic case; Figure 2b and 2d correspond to the anisotropic case.

The anisotropy strongly influences the result of the simulation both on head values (Figure 2a and 2b) and particle tracking results (Figure 2c and 2d). The flow lines in Figure 2d follow closely the geological structure as expected, while in the isotropic case (Figure 2c) they are mainly constrained by the no-flow boundaries of the model.

## Conclusions

In this paper, we propose a technique allowing the estimation of a 3D field of anisotropic hydraulic conductivity tensors consistent with the geological structure in order to improve flow simulations. The key step is to use an implicit approach to model the geological structure which allows the use of the stratigraphic gradient in every point of the 3D simulation domain. Because this gradient is perpendicular to the bedding, it can be used to orient the hydraulic conductivity tensor in every cell of the simulation grid. The proposed approach is simple to implement. It can be applied in a straightforward manner even for very complex geological structures as long as a consistent potential is defined everywhere in the domain as done in Calcagno et al. (2008).

Additional work should be conducted if some anisotropy between the two horizontal directions occur should be accounted for, because the method can handle only anisotropy between the directions perpendicular and parallel to the layers. However, in practice this situation is rarely considered.

As described earlier, accounting for anisotropy together with heterogeneity is feasible without difficulties by considering the variations in space of the $k_{||}$ and $k_{\perp}$ values. All the other steps remain unchanged. During the generation of heterogeneous models, let us note that the spatial correlations have then to be computed along the geological structures (following a layer and not simply using the Euclidean distance between the points). Those techniques are available and their application should not cause any difficulty.

Finally, one interesting feature of the proposed method is that it offers the possibility of modeling complex geological structures with any type of grids including structured or unstructured ones. The only requirement is that the value of the potential and its gradient must be available in any point of the domain. It is then expected that a better description of the anisotropy within the elements may allow to (at least partly) relax the need for complex meshing in the presence of a complex geological structure.

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