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CONSTRAINING METHODS FOR DIRECT INVERSE MODELING

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Summary. We consider 3-dimensional groundwater flow models based on the block centered finite difference method. In a forward model the hydraulic conductivities are given in every grid block, and at each face on the boundary (including the wells) either the flow rate or the head is specified. In an inverse model conductivities are unspecified in a number of grid blocks, while both flow rate and head are specified in a number of boundary faces. Direct inversion means that the conductivities are obtained directly from Darcy's law. In the Double Constraint Method (DCM) grid block conductivities are initially estimated. From a forward run with flow rate boundary conditions all flow rates are calculated, and from a forward run with head boundary conditions all head gradients are calculated. Then, for each grid block the conductivity is updated using Darcy's law: conductivity is equal to minus the calculated specific flow rate divided by the calculated head gradient. Finally, artificial anisotropy is removed by iterations. DCM has been applied successfully and to make the method more flexible we have developed an extension called Hydraulic Impedance Tomography (HIT). A system of linear algebraic "back projection" equations for the grid block impedivities (the inverses of the conductivities) is based on flow rates calculated by a forward run with flow rate boundary conditions. This system is solved with head boundary conditions. Synthetic examples show that the method works well. In practical applications heads (obtained from observation wells) and flow rates (obtained from recharge data) are time-dependent. As a consequence, time series of impedivities obtained by HIT may be considered as noisy observations.

1 INTRODUCTION

3-Dimensional incompressible groundwater flow through an undeformable porous medium is governed by the continuity equation and Darcy's law

$$\nabla\cdot\mathbf{q} = 0 \tag{1}$$

$$\mathbf{q} = -k\nabla\varphi \tag{2}$$

The water table height is given by

$$z = h(x,y,t) \tag{3}$$

Defining $f(\mathbf{x},t)=h(x,y,t)-z$, the boundary conditions on the water table are

$$\theta \, \mathrm{d}f/\mathrm{d}t = r \tag{4}$$

$$\varphi = h \tag{5}$$

Since condition (4) is time-dependent, flux density $\mathbf{q}(\mathbf{x},t)$ and head $\varphi(\mathbf{x},t)$ are time-dependent too, while conductivity $k(\mathbf{x})$ is time-independent. $\theta(x,y,z{=}h,t)$ is the effective porosity (specific yield); $r(x,y,t)$ is the recharge (effective precipitation); x, y and z are respectively the two horizontal coordinates and the upward directed vertical coordinate; in this coordinate system, which is fixed to the earth, $\partial f/\partial t$ is the time derivative; $\mathrm{d}f/\mathrm{d}t \equiv \partial f/\partial t + (\mathbf{q}/\theta)\cdot\nabla f$ represents the time derivative in a coordinate system fixed to a flowing "fluid particle."

In a forward problem conductivity $k(\mathbf{x})$ is specified in each point of the modeling domain D, while in each point of its boundary ∂D either normal flux density $(\mathbf{q}\cdot n)_{\partial D}$ or head $\varphi_{\partial D}$ is specified (wells are considered as internal boundaries). When both normal flux density and head are specified in N_{FH} boundary "points" (including wells), conductivity can be determined in $N_{FH} - 1$ internal "points." This is generally called inverse modeling.

From now on we consider discrete models. In hydrological models the number of grid block conductivities, N_V, is generally greater than the number of specified flux-head pairs minus one, $N_{FH} - 1$. In that case $N_V - N_{FH} + 1$ conductivities have to be determined from "hydrological perception," similar to forward modeling where all N_V conductivities have to be "perceived" from other sources of knowledge.

Direct inversion means that the conductivities are derived directly from Darcy's law: conductivity is equal to flow rate divided by head gradient. Section 2 introduces the Double Constraint Method (DCM). Section 3 introduces Constrained Back Projection (CBP). We focus on Hydraulic Impedance Tomography (HIT); that is, the version of CBP compatible with models based on the block centered finite difference method (e.g. MODFLOW). Section 4 presents examples and section 5 summarizes and introduces future work.

2 THE DOUBLE CONSTRAINT METHOD

In the Double Constraint Method (DCM) estimated initial ("old") conductivities k^{old} are assigned to the grid blocks. From a forward run with the known fluxes as boundary conditions, all fluxes are calculated. The thus obtained flux densities q^F_i, i=1,2,3, honor the continuity equation and the known boundary fluxes. From another forward run honoring the known heads as boundary conditions, all heads φ^H are calculated. Darcy's law using q^F_i and $\partial\varphi^H/\partial x_i = -q^H_i/k^{old}$ for each grid block yields the improved ("new") conductivities $k^{new}_i = k^{old}\, q^F_i/q^H_i$. To avoid division by zero, q^F_i/q^H_i is replaced with $(q^F_i + q^\varepsilon)/(q^H_i + q^\varepsilon)$, where $q^\varepsilon \geq 0$ is a relatively small flux density

$$k^{new}_i = k^{old}\, (q^F_i + q^\varepsilon)/(q^H_i + q^\varepsilon) \tag{5}$$

A "mixing" rule, for instance

$$k^{new} = (k^{new}_1)^{\beta 1}(k^{new}_2)^{\beta 2}(k^{new}_3)^{\beta 3} \qquad (6)$$
$$\beta_i = [(q^F_i)^2+(q^\varepsilon)^2]/[\mathbf{q}^F\cdot\mathbf{q}^F+3(q^\varepsilon)^2]$$

yields isotropic conductivities that are used as "old" ones for a second iteration step, and so on until convergence to isotropy; that is, until convergence to $k^{new}_1 \cong k^{new}_2 \cong k^{new}_3 \cong k^{new}$.

The Double Constraint Method has been applied successfully.[1,2,3,4] However, it is sometimes difficult to remove artificial anisotropy.[5] Moreover, approximation of grid block fluxes from the calculated face-based fluxes introduces inaccuracies. Finally, DCM cannot handle accurately conductivities that are not allowed to be updated. For those reasons the related, but more flexible Hydraulic Impedance Tomography (HIT) is presented in section 3. However, DCM remains valuable as a preconditioner of HIT.[6]

3 CONSTRAINED BACK PROJECTION

Discretized groundwater flow equations are generally based on the block centered finite difference method, in which the heads are defined in the grid block centers. The resulting system of algebraic equations can be written as

$$\mathrm{DKD}^T\Phi = \mathrm{DK}\Pi \qquad (7)$$

DKD^T is the system matrix; Φ is the column of N_V block centered heads; Π is the column of N_{BF} boundary heads specified in the centers of the N_{BF} boundary faces (components of Π on internal faces equal zero); K is the conductance matrix; D is the incidence matrix relating grid blocks to grid faces.[7,8] The heads Φ can be pre-calculated by a constraining forward run with head boundary conditions, like in the Double Constraint Method (section 2). Then system (7) can be used with flux boundary conditions to determine the conductivities by back projection. However, conductance matrix K is nonlinear in the conductivities, which makes it unattractive to base Constrained Back Projection (CBP) on this system.

3.1 Hydraulic Impedance Tomography

Fortunately, we can construct a system of linear back projection equations based on the mathematically equivalent formulation of Darcy's law (2), $\nabla\times\gamma\mathbf{q}=\mathbf{0}$ ($\gamma=k^{-1}$), plus boundary conditions.[7,8] In discretized form this approach yields the system

$$\mathrm{R}^T\Gamma(\mathrm{Y})\mathrm{Q} = -\mathrm{R}^T\Pi \qquad (8)$$

Incidence matrix R relates the grid's edges to its faces, and Q is the column of fluxes through the faces. Impedance matrix $\Gamma = \mathrm{K}^{-1}$ is linear in the impedances $\gamma = k^{-1}$. That is, $\Gamma = \Gamma(\mathrm{Y})$, where $\mathrm{Y} = (\gamma_1,\ldots,\gamma_{Nv})^T$ is the array of grid block impedances. Therefore, this version of CBP is called Hydraulic Impedance Tomography (HIT). The fluxes Q are pre-calculated in a forward run (using MODFLOW, say) with the flux boundary conditions, like in the Double Constraint Method (section 2). These fluxes honor the continuity equation and the known boundary fluxes. Substitution of these fluxes into the above system results in the system of linear algebraic equations $\mathrm{AY} = \mathrm{B}$, from which the impedivities Y can be determined. Back projection matrix A is defined by $\mathrm{AY} = \mathrm{R}^T\Gamma(\mathrm{Y})\mathrm{Q}$, while $\mathrm{B} = -\mathrm{R}^T\Pi$ is the right hand side vector.[9,10,11]. Since the number of algebraic equations is generally greater than the number of impedances, a least squares solver is applied

$$(\mathrm{A}^T\mathrm{A} + \mathrm{I}^\varepsilon)\mathrm{X} = \mathrm{A}^T(\mathrm{B} - \mathrm{A}\mathrm{Y}^{old}) \tag{9}$$

where $\mathrm{X} = \mathrm{Y} - \mathrm{Y}^{old}$. I^ε is a diagonal regularization matrix with components equal to $(q^\varepsilon\Delta)^2$; $q^\varepsilon \geq 0$ is a relatively small flux density and Δ is a representative grid block dimension. Also other least squares methods may be attempted, e.g. QR decomposition. The least squares approach honors Darcy's law and the known boundary heads in a least squares sense. Outer iterations may improve point-wise honoring.

4 NUMERICAL EXAMPLES

In most hydrogeological models the number of grid blocks, N_V, is generally much greater than the number of measured flux-head data, $N_{FH} - 1$. Nevertheless, because of the mathematical challenge, the case $N_V << N_{FH} - 1$ has been chosen to test HIT for a number of synthetic problems.[9,10,11] In this case the solution of the inverse problem (i.e., the grid block conductivities) is independent from the initial conductivities. Moreover, if such an inverse problem is based on arbitrarily chosen flux-head boundary conditions, a solution exists only in a generalized sense. That is, application of the generalized conductivity solution to a forward problem with flux boundary conditions results in a head solution that honors the head boundary conditions only in a least squares sense (see section 4.1). Only if the flux-head boundary conditions are chosen consistent with the solution of a forward problem, the outer iterations converge to a classical solution, i.e., to conductivities in which the boundary conditions are honored point-wise (see section 4.2). In the examples presented below, the linear equations have been solved using conjugate gradients with diagonal scaling, without regularization ($\mathrm{I}^\varepsilon = 0$).

4.1 Example 1: Three layers

Example 1 considers three layers with reference conductivities of respectively 2, 4 and 3 m/d. Table 1 shows discretization characteristics. As reference boundary conditions we consider heads that decrease linearly from 5m on the west boundary to 0 on the east boundary. A forward run based on these reference conditions yields fluxes, Q, of respectively 10, 30 and 15 m^3/d through the three layers.

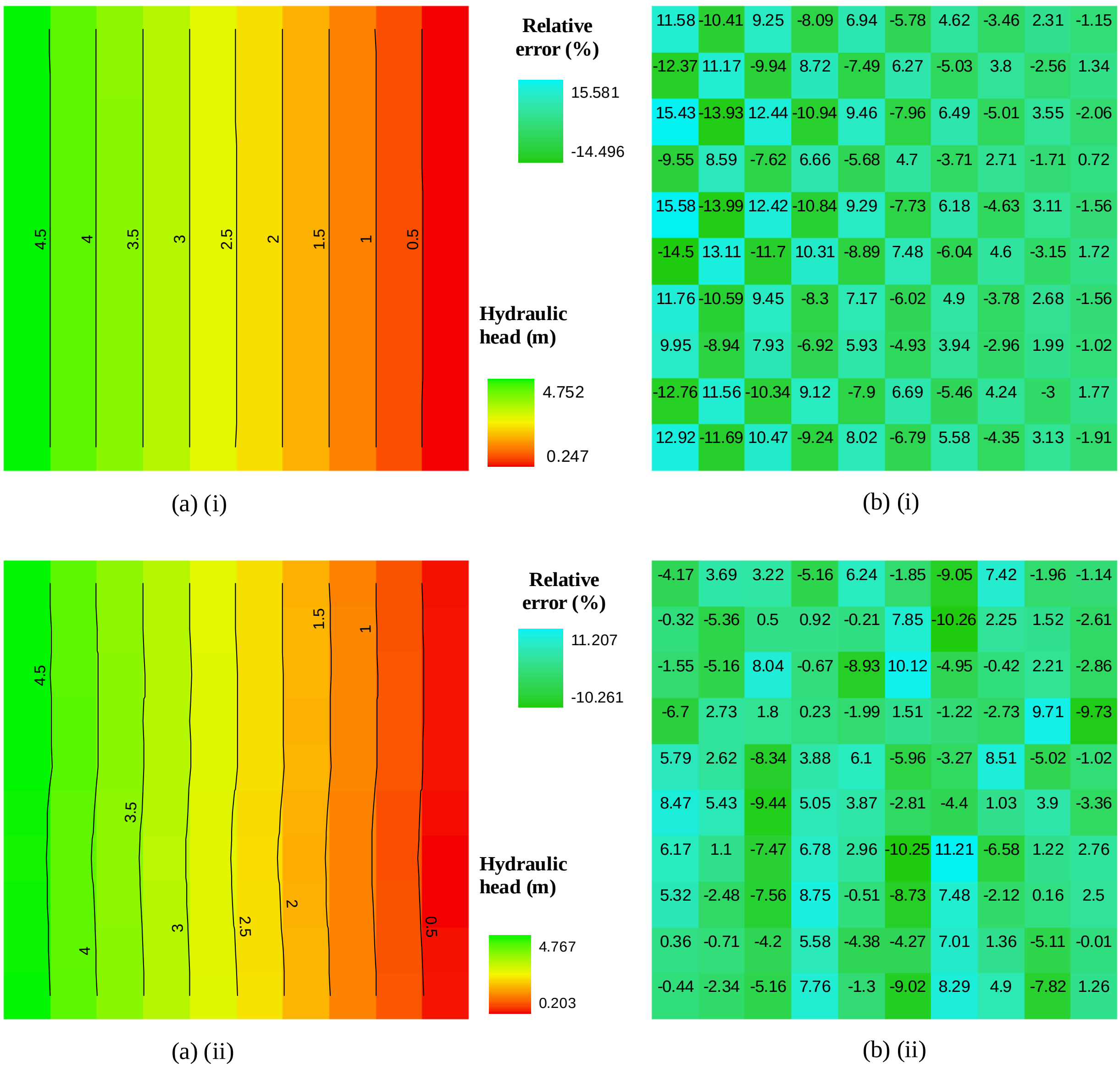
Table 1: Fine-scale grid and back projection equations for example 1

volumes, impedances	faces, fluxes	boundary faces, boundary heads	edges, equations $\mathrm{R}^T\Gamma(\mathrm{Y})\mathrm{Q} = -\mathrm{R}^T\Pi$	linearly independent equations
$N_V = 300$	$N_F = 1060$	$N_{FH} = 320$	$N_E = 1243$	$N_F - N_V = 760$

Now we forget the reference ("old") conductivities. Instead we consider "new" impedivities $\mathrm{Y} = (\gamma_1,\dots,\gamma_{Nv})^T$. Substitution of the calculated fluxes Q into the left hand side of equation (8) yields back projection matrix A multiplied by the unknown impedivities Y, i.e.,

$AY = R^T \Gamma(Y)Q$. Head boundary conditions Π are substituted into the right hand side of equation (8), $B = -R^T \Pi$. The back projection run based on system (9) yields the new grid block impedivities.

First we apply the reference head boundary conditions. In this case back projection yields new conductivities that are equal to the reference ones, as it should be.



(a) (ii) (b) (ii)

Figure 1: (a) block centered heads and (b) relative errors in top layer impedivities when using 1% noise in (i) west and (ii) top boundary heads

Secondly, we specify on the west boundary heads that are perturbed randomly with a relative standard deviation of 1% with respect to the reference boundary heads, while the other boundary heads are kept equal to the reference conditions. The new impedivities are calculated by back projection system (9). These impedivities are used in a forward run with the reference fluxes on the boundaries. The resulting internal fluxes (now deviating from the internal reference fluxes) are substituted into the left hand side of equation (8) to determine the new back projection matrix A. Again the impedivities are calculated by back projection. And so on. These outer iterations are terminated when the boundary heads calculated by the forward run do no longer come closer to the specified boundary heads. In this case only one iteration was needed. Near the west boundary, where the noise is introduced, the calculated impedivities have a relative deviation of 16% with respect to the reference impedivities (an absolute deviation of 0.08 d/m); close to the east boundary the deviation reduces to 2% (Figure 1b(i)). A forward run based on these impedivities shows that uniformity of flow is preserved: the heads in the grid block centers decrease globally from 4.5m west to 0.5m east, although they differ slightly from the reference values (Figure 1a(i)).

Finally we consider heads that are perturbed with 1% on the top boundary; the other boundary heads being equal to the reference conditions. The outer iterations were terminated after 3 iterations. Near the top boundary, where the noise is introduced, the calculated impedivities have a relative deviation of 11% with respect to the reference impedivities (an absolute deviation of 0.06 d/m) (Figure 1b(ii)). Close to the bottom boundary the deviation reduces considerably. The forward run based on these impedivities shows that the flow deviates from uniform flow: isolines of heads do no longer form straight lines. (Figure 1a(ii)). However, for the middle and bottom layer the head patterns come closer to uniform flow.

Many more examples have been tested. In all cases the inverse solution turns out to be stable under perturbations and the outer iterations always converge (never diverge).[10]

4.2 Example 2: Homogeneous medium and checkerboard pattern

Example 2 considers a case in which the flux-head pairs on the boundaries are consistent with a homogeneous porous medium having a conductivity of 10 m/d. That is, the truth pattern is homogeneous. However, the initial impedivity pattern has been chosen as a checkerboard pattern with conductivities of 1 m/d and 100 m/d. Figure 2 and Table 2 present the discretization characteristics.

Table 2: Fine-scale grid and back projection equations for example 2

volumes, impedances	faces, fluxes	boundary faces, boundary heads	edges, equations $\mathrm{R}^T \Gamma \mathrm{Q} = -\mathrm{R}^T \Pi$	linearly independent equations
$N_V = 1600$	$N_F = 6480$	$N_{FH} = 3360$	$N_E = 8241$	$N_F - N_V = 4880$

Notwithstanding the poor initial guess, HIT recovers the homogeneous impedivity image (the truth) after approximately 60 outer iterations.

Alternatively, we have also considered the case where the flux-head pairs on the boundaries are consistent with the checkerboard pattern (the truth pattern in this case). Now we have chosen a homogeneous initial impedivity pattern. Also here, in spite of the poor initial guess, HIT recovers the checkerboard pattern, again after approximately 60 iterations.[10]

5 SUMMARY, CONCLUSIONS AND FUTURE WORK

We have presented two related direct inversion methods: (i) the Double Constraint Method (DCM) and (ii) Hydraulic Impedance Tomography (HIT). The methods condition the grid block conductivities of a block centered finite difference model (MODFLOW, say) in such a way that the groundwater flow honors both specified heads and fluxes on the boundary. If the number of measured flux-head pairs minus one, $N_{FH} - 1$, is less than the number of grid block conductivities, N_V, the conductivities determined by inversion do not only depend on the specified flux-head pairs, but also on the initial conductivities. These initial conductivities reflect general hydrogeological knowledge. If, on the other hand, $N_{FH} - 1$ is greater than N_V, the conductivities determined by inversion are independent from the initial conductivities, as has been demonstrated by synthetic test examples.

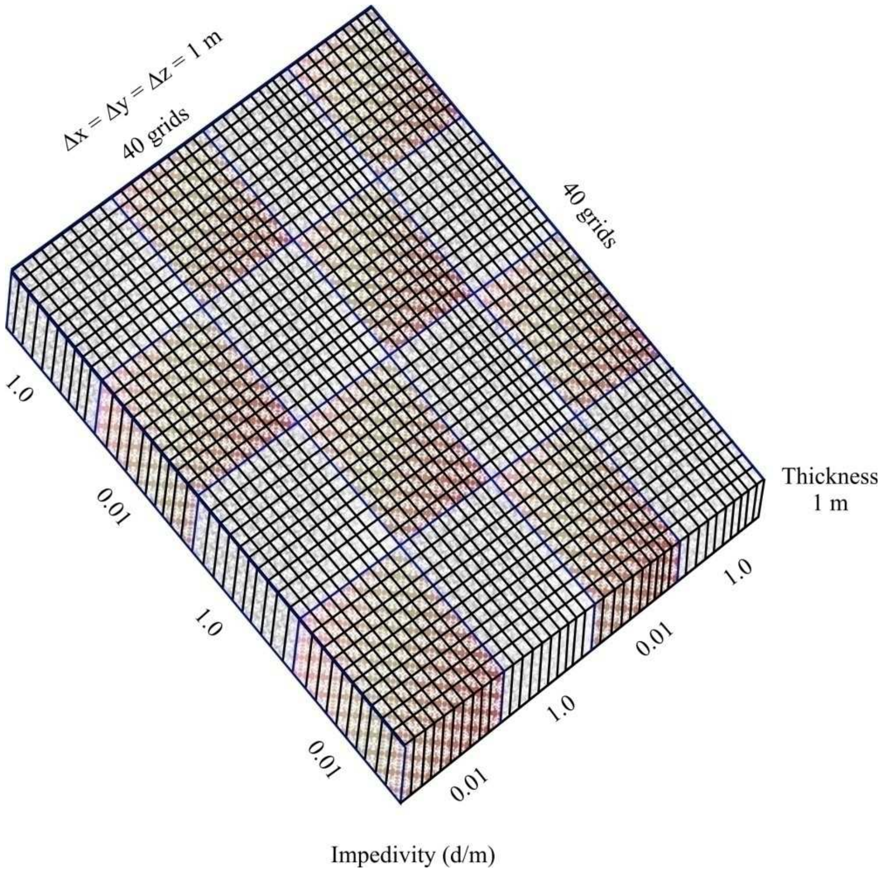


Figure 2: Dimensions of the fine-scale model example 2 with checkerboard impedivity pattern

DCM has been applied successfully since the 1980th.[1,2,3,4,5,6] However, its generalization to HIT is a relatively new development that promises to make DCM more flexible. Numerical optimization—for instance the use of DCM as a preconditioner for HIT—is considered as future research.

In practical applications heads (obtained from observation wells) and fluxes (obtained from recharge data) will be noisy (inaccurate). As a consequence, the conductivities determined by direct inversion will differ from measurement to measurement. We propose to consider the thus-obtained time-dependent conductivities as observations in the observation model of a Kalman Filter. The process model is: conductivities at time $t+\Delta t$ are equal to conductivities at time t. This way a time-independent conductivity estimate with uncertainty less than the noise level can be obtained. Kalman Filter inversion based on the above process model has been applied successfully already since the 1990th.[12,13] However, to ensure for the case $N_V >> N_{FH} - 1$ that hydrogeological perceptions be preserved, we propose to extend this Kalman Filter practice by introducing the above defined "observed conductivities".[14]

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