# DOWNSCALING: A COMPLEMENT TO HOMOGENIZATION

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**Abstract.** A groundwater flow model based on a specified hydraulic conductivity field in the modeling domain has a unique solution only if either the head or the normal flux component is specified on the boundary. On the other hand, specification of both head and flux as boundary conditions may be used to determine the conductivity field, or at least improve an initial estimate of it. The specified head and flux data may be obtained from measurements on the boundary, including the wells. We have presented a relatively simple, but instructive approach: the Double Constraint (DC) method. The method is exemplified in the context of upscaling and its inverse: downscaling. The DC method is not only instructive, but also easy to implement because it is based on existing groundwater modeling software. The exemplifications shown in this paper relate to downscaling and demonstrate that the DC method has practical relevance.

**Key Words.** Double Constraint Method, Downscaling, Inverse problems, Conductivity

# 1. Introduction

The Double Constraint (DC) method is a relatively simple, yet very instructive approach to inverse modeling. In this paper the DC method has been applied to downscaling, which can be considered as a practical complement to upscaling. However, the DC method is applicable in a wider range of settings, especially in applications in which wells play a role. The DC method is instructive, because it shows all the ingredients required for inverse modeling: measured heads and fluxes at the same location on the closed boundary, as well as estimated conductivities — the priors. At the same time, the method can be easily implemented, provided that groundwater modeling software is available.

In the context of groundwater flow, a forward model is a model in which the hydraulic conductivity is specified everywhere in the modeling domain. A forward model has a unique solution provided that appropriate boundary conditions are imposed. Considering groundwater flow this is the case only if either the head on a part of the boundary of the modeling domain, or the flux through that part of the boundary is specified in any point. Specification of both head and flux at that part of the boundary over-specifies the problem and has, therefore, no solution. However, such an over-specification may be used to improve the initially estimated conductivity field by conditioning it to the measured hydraulic data head and flux, in such a way that downscaling is meaningful. Determination of conductivities from additional boundary data is generally called inverse modeling. In our approach we follow the main steps of a method that has proved its applicability in Eletrical Impedance Tomography, [1, 4, 6, 9].

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After an introduction to downscaling in section 2, the double constraint method is presented in section 3. An exemplification of downscaling for a grid block far removed from wells is shown in section 4, where two isotropization equations — Wexler's equation and the square root equation — have been compared. A similar example is briefly presented in section 5. Section 6 presents a summary, conclusions and discussion, while section 7 shows the references.

For reasons of simplification, 2-dimensional problems will be considered. Extension to 3D problems is straightforward.

# 2. Downscaling

In this paper downscaling is considered as a practical complement to upscaling with application in groundwater flow modeling.

Upscaling starts with a fine-scale model with heterogeneous fine-scale conductivities in the elements (triangles, grid blocks) of a gridded rectangular upscaling cell. From these fine-scale conductivities the homogeneous effective coarse-scale conductivity of the upscaling cell is determined. A variety of upscaling methods has been applied and published, starting from well-known arithmetic and harmonic averages for flow respectively parallel and normal to layers, as well as the geometric average for fine-scale isotropic checkerboard patterns. For more complex fine-scale conductivity configurations the renormalization method can be applied, or a large class of methods based on fine-scale solution of the flow equation - see [7] for a review. Then based on specific discharge rates and head gradients in the fine-scale elements, the upscaled conductivity may be computed.

With respect to the latter class of methods, the question of boundary conditions to impose on the upscaling cell arises. Homogenization, probably the most popular method from this class, assumes periodicity of the porous medium and, as a consequence, periodic boundary conditions. Presumably, boundary conditions that are consistent with the actual flow might appear superior above the more-or-less arbitrarily chosen periodic boundary conditions. However, when using boundary conditions derived from an actual flow pattern, there is no consistency between different possible definitions of a large-scale conductivity, [11]. It should be mentioned that there exists another category of methods capable of dealing directly with a multiscale structure of the medium. A wide overview of such methods is given in [5]; this topic will not be further addressed in this paper.

A coarse-scale model consists of grid blocks (in a finite difference setting) in which each grid block has a coarse-scale conductivity that is obtained by upscaling from fine-scale conductivities. Once the solution of the flow problem in the large scale is computed, the modeler (the geohydrologist) may want to zoom in into the details of the groundwater flow in one or more coarse-scale grid blocks. If the original finescale conductivity distribution — from which the coarse-scale conductivity was derived by homogenization — is still known, we can run a fine-scale flow model on one large-scale cell with boundary conditions derived from the flow pattern calculated by the coarse-scale model. The fine-scale boundary conditions should be such that: (i) the total inflow through the boundary of the fine-scale model should be equal to the inflow calculated by the coarse-scale model, and (ii) the average head on each boundary node of the fine-scale model should be equal to the average head calculated by the coarse-scale model. Also wells may be considered as boundaries. Since specification of two types of boundary conditions — both flux (discharge rate) and head — over-constrains a groundwater flow problem with specified conductivity distribution, we have to modify, or condition, the original fine-scale conductivities (the priors) in such a way that the conditioned conductivities honor both the flux and the head boundary conditions. The Double Constraint (DC) method presented here may be considered as a practical engineering approach to apply results obtained from simple homogenization methods to realistic, non-periodic media.

### 3. The Double Constraint method

The aim is to find conductivities that satisfy Darcy's law, the continuity equation, as well as both the flux and the head boundary conditions. Below we discuss the Double Constraint method, which presents, in a conceptually simple way, the ingredients of an inverse modeling technique: *both* measured boundary head *and* measured boundary flux complemented by prior conductivities in the flow domain. The DC method consists of three steps: (i) a head run with a forward model, (ii) a flux run with a forward model, and (iii) a post processing step. Simplicity is one of its great advantages: the method is based on standard finite difference or finite element groundwater flow models; therefore the main additional effort consists of implementing the post processing step. Our implementation is based on the finite element method.

Run 1: head constraining step. The original fine-scale conductivities (referred to as the priors) in the elements (triangles) of our finite element model are contained in system matrix A of the finite element model, while the specified heads (derived from the coarse-scale model) in the boundary nodes are contained in the righthand side array B. Then the nodal heads X on the whole finite element mesh are calculated from solving the system of linear algebraic equations AX = B, from which the fluxes in the elements follow too. The calculated total flux through a boundary will generally differ from the total flux found by the coarse-scale model.

Run 2: flux constraining step. Now the boundary fluxes are specified resulting in the right-hand side array B. The original fine-scale conductivities (the priors), similarly as in the run 1, are now contained in system matrix A. The nodal heads X on the whole mesh are calculated from solving the system of linear algebraic equations AX = B, from which the fluxes in the elements follow. The calculated average head on a boundary will generally differ from the average head found by the coarse-scale model.

Post processing. In each element we determine the flux densities  $q'_x$ ,  $q'_y$  obtained from flux-constraining run 2, as well as minus the head gradients  $h_x = -\partial \phi / \partial x$ ,  $h_y = -\partial \phi / \partial y$  obtained from head-constraining run 1. These fluxes and head gradients satisfy the measured flux and head boundary conditions, while the fluxes also satisfy the continuity equation (in discrete finite element form). To satisfy Darcy's law we define the conditioned conductivities (the posteriors) as  $k_x = q'_x / h_x$ and  $k_y = q'_y / h_y$ . The thus-calculated conductivities are the fine-scale conductivities that belong to fine-scale flux densities  $q'_x$ ,  $q'_y$  and heads  $\phi$  in which we are interested.

Isotropization. If we prefer to avoid anisotropy, we define for each triangle an isotropic conductivity, either by Wexler's isotropization rule  $k = -(q_x h_x + q_y h_y)/(h_x^2 + h_y^2)$ , [6, 9] or by square root isotropization rule  $k = \sqrt{k_x k_y}$ , [3]. The above-described steps are repeated using the isotropized k's as priors until convergence to sufficient isotropy is obtained  $(k_x/k_y \to 1)$ . **3.1. Wexler's method.** Wexler's isotropization rule goes back to a class of methods generally referred to as Electrical Impedance Tomography (EIT), [1, 2, 4, 6, 9]. The term 'impedance' is taken from circuit theory where it denotes the ratio of the voltage (electric potential difference) across a circuit element to the electric current through that element. Originally, the method comes from medical imaging, where it is aimed at reconstruction of distribution of electric conductivity inside a human body, [4, 9]. As such, the Wexler's method falls into a broad category of inverse problems.

To give an argument for Wexler's isotropization formula we focus again on the two forward runs. Flux-constraining run 2, with Neumann boundary conditions, yielding the flux densities  $q'_x = -k \partial \phi' / \partial x$ ,  $q'_y = -k \partial \phi' / \partial y$  and head-constraining run 1, with Dirichlet boundary conditions, yielding the negative head gradients  $h_x = -\partial \phi / \partial x$ ,  $h_y = -\partial \phi / \partial y$ . One cannot generally expect that  $\mathbf{q}' + k \nabla \phi$  vanishes everywhere inside the region. As a consequence, a residual is obtained.

The optimization problem is then defined as minimization of the square of the residual over the computational domain; that is,  $R = \int_{\Omega} (\mathbf{q}' + k\nabla\phi)(\mathbf{q}' + k\nabla\phi)d\Omega$  is minimal, where  $\Omega$  denotes the modeling domain. In a finite element method  $\mathbf{q}'$  and  $\nabla\phi = -\mathbf{h}$  are defined element-wise, which means that the integral over  $\Omega$  can be replaced with a summation of integrals over the elements (triangles)  $\Omega_i$ :  $R = \sum_i \int_{\Omega_i} (\mathbf{q}' + k_i \nabla\phi) (\mathbf{q}' + k_i \nabla\phi) d\Omega_i.$ 

Since conductivity  $k_i$  is assumed constant in each element, minimization of R by modifying the  $k_i$  requires  $\delta R/\delta k_i = 2 \int_{\Omega_i} (\mathbf{q}' \cdot \nabla \phi + k_i \nabla \phi \cdot \nabla \phi) d\Omega_i$  to be equal to zero for all elements  $\Omega_i$ . Since in triangular elements  $\mathbf{q}'$  and  $\nabla \phi$  are constant, the integrand is constant yielding  $\delta R/\delta k_i = 2 (\mathbf{q}' \cdot \nabla \phi + k_i \nabla \phi \cdot \nabla \phi) A_i = 0$ , where  $A_i$  is the surface area of triangle  $\Omega_i$ . This results in the formula for the new conductivity value in each triangle:  $k_i = -\mathbf{q}' \cdot \nabla \phi / (\nabla \phi \cdot \nabla \phi)$ , which is the same as already given formula for Wexler's isotropization. An important distinction from other inversion procedures is that the error to be minimized by adjustment of the conductivity distribution is the difference between the interior current densities calculated from the Neumann and Dirichlet problems.

It should be remarked, however, that when choosing the residual to be minimized as  $R' = \int_{\Omega} (\gamma \mathbf{q}' + \nabla \phi) (\gamma \mathbf{q}' + \nabla \phi) d\Omega$ , where  $\gamma = k^{-1}$  is the resistivity, we would end up with isotropization equation  $\gamma_i = -\mathbf{q}' \cdot \nabla \phi/(\mathbf{q}' \cdot \mathbf{q}')$ . In this case the error minimized by adjustment of the resistivity distribution is the difference between the interior potential differences calculated from the Neumann and Dirichlet problems.

The minimization approach presented above is also referred to as equation-error approach [2, 6]. The process is a least-square process which carries with it a measurement-error averaging property as well as stability. In [6] a slightly different formula for the updated  $k_i$  can be found:  $k_i = \sqrt{\mathbf{q}' \cdot \mathbf{q}' / (\nabla \phi \cdot \nabla \phi)}$ .

**3.2. Differences with the EIT approach.** Finally, it is important to emphasize the differences between our target and the aim originally addressed in the problems related to electrical impedance tomography (EIT). We are less restrictive in looking for the 'shape' of the conductivity distribution, in particular the problem of smoothed boundaries between areas of different conductivity, [2, 6], is not that crucial in downscaling groundwater flow patterns. Our main aim is to get a consistent formulation of a problem defined within the upscaling (downscaling) cell, with a simultaneous fulfillment of the two sets of boundary conditions. Also, the area of application has an influence on the quality of solution needed. On the other hand, in our case only one set of boundary conditions is applied, as opposed to



FIGURE 1. Homogenization square with checkerboard conductivity pattern.

classical EIT problems, where several measurements for different boundary fluxes and potentials are performed.

The approach presented in this paper has been successfully applied to match statistically generated permeability fields to data measured in wells, [3]. A square root method has been applied, with forward runs based on the finite difference flow model Modflow.

# 4. Example 1: Far field downscaling

**4.1. Problem definition.** In this section we present results obtained with the double constraint method. We consider a synthetic 2-dimensional case for which we apply respectively Wexler's and the square root isotropization. In the two constraining steps the flow equation is solved with a standard, conformal-nodal Finite Element Method with linear triangle-based elements. Conductivities are assumed constant within the triangles.

Let us consider a coarse-scale grid block that is far removed from a well. The square has a size of  $[0, 4] \times [0, 4]$ . The initial fine-scale conductivities within this square represent a checkerboard pattern with conductivities  $k_1 = 1$  and  $k_2 = 100$ , as shown in Fig. 1. The discrete model is based on a grid with 1681 nodes, 4880 edges and 3200 triangles.

The aim is to condition the initial fine-scale conductivities in such a way that the two sets of boundary conditions dictated by the coarse model, one given as nodal boundary heads, the second given as boundary fluxes, are honored simultaneously.

The exact upscaled conductivity is equal to  $\sqrt{k_1 \cdot k_2} = \sqrt{100 \cdot 1} = 10$ , [8]. However, in case of a high contrast between  $k_1$  and  $k_2$  it is hard to obtain this value by discrete methods, such as finite elements or finite differences, [11]. If the homogenization procedure is performed for a square with the heterogeneity pattern shown in Fig. 1, even a relatively fine mesh consisting of 1681 nodes and 3200 triangles yields a computed effective permeability value equal to approximately 23 and is thus more than twice the exact value. This is important because the coarse-scale model acts on numerically upscaled conductivity values (here approximated as 23), whereas the fine-scale model exemplified here is based on exact conductivities (1 and 100 in checkerboard pattern). The great difference between the numerically



FIGURE 2. Solutions of the forward problems and conditioned conductivities. Solid lines: isolines of heads from  $run\ 2$  (specified boundary fluxes). Dashed lines: isolines of heads from  $run\ 1$  (specified boundary heads). a) after first iteration, b) after iteration 3, c) after iteration 8.

upscaled conductivity (K = 23) and the exact upscaled conductivity (K = 10) may have an additional influence on the discrepancy between the flux and/or potential boundary values of the coarse-scale and fine-scale model.

On the left and right sides of the domain fixed fluxes and fixed potential boundary conditions have been applied. On the horizontal sides the no flow boundary condition has been applied for the flux run and a linear difference in potential for the head run. These conditions are considered to come from a large-scale model.

The coarse-scale model yields heads in each node of the coarse-scale grid square, with a linear interpolation along the grid square's boundaries. The fine-scale boundary conditions do not follow that linear interpolation. They have been specified inversely proportional to the fine-scale conductivities of the triangles bordering at the boundaries, in such a way that the boundary averaged fine-scale head equals the boundary averaged coarse-scale heads. The coarse-scale model yields constant fluxes through the grid square's boundaries. Fine-scale boundary fluxes have not



FIGURE 3. Distribution of conductivity values within the elements of the mesh during iterations. Far field case, Wexler's method.

been chosen equal to this constant flux. They have been specified proportional to the conductivities of the triangles bordering at the boundaries, in such a way that the total coarse-scale flux equals the total fine-scale flux through a boundary.

There is a question of compatibility of coarse-scale pressure and flux boundary conditions. If such compatibility is 'lacking', large changes in prior conductivity values occur during the iterations required for isotropization. A certain 'balance' among: flux conditions, head boundary condition and prior conductivities is established during iterations. This means that, if the two sets of boundary conditions are not 'equivalent' in quantity of flow, this will be obtained through generating changes in the conductivity field. On the other hand, if a consistent set of boundary conditions is given, then no change in priors occurs.

**4.2.** Wexler's isotropization. The results presented in Figs. 2 have been obtained with the DC method combined with Wexler's isotropization formula.

In Figs. 2 conductivities are visible only schematically. In order to get more insight in the values taken by the conductivities, Fig. 3 shows the distribution of the conductivities values obtained in the 3rd and 8th iteration.

A range of values taken by conditioned conductivity values may be considered as one of the characteristics of the performance of a method. It has been observed that there are a number of cells in which conductivities tend to relatively high and relatively small values. Conductivities generated after the 1st iteration were from the interval (0,32, 667), after the 3rd iteration from the interval (0,11, 2137), to become (1,24E-04, 2098) after the 8th iteration. The number of elements with such extreme values is not large, still this effect is highly undesirable because of the tendency of growing in subsequent iterations. Apart from this effect, the conductivities in the majority of elements does not change much in further iterations.

During the iterations it happens that negative values of the conductivity occur. This is mostly the case for regions with low conductivity and thus of a very slow



FIGURE 4. Solutions of the forward problems and conditioned conductivities. Solid lines: isolines of heads from  $run\ 2$  (specified boundary fluxes). Dashed lines: isolines of heads from  $run\ 1$  (specified boundary heads). a) after first iteration, b) after iteration 3, c) after iteration 8.

flow. In such a case the conductivity value obtained in a previous iteration was taken instead of the new prior. The number of negative values appearing at a given iteration step may be viewed as a measure of convergence of a method. In the computations performed for the case test presented in this section the number of negative conductivities varied from 20, during the 1st iteration, to 4 in the 8th iteration. It is important to note that in 2nd and 3rd iterations the number of negative conductivities was equal to zero. The deviation from isotropy cannot be measured in Wexler's method, but can in the square root method (Sec. 4.3).

**4.3.** Square root isotropization. Computations for the same initial conductivity pattern have been performed again, with a post-processing step based on square root isotropization. The results are presented in Figs. 4.

In the course of this method conductivities in x and y directions are computed independently. It is interesting to study the level of anisotropy created with the method. Fig. 5 gives a graphical comparison of anisotropy ratio obtained during



FIGURE 5. Distribution of conductivity values along elements of a mesh during iterations. Far field case, square root method.



FIGURE 6. Anisotropy ratio during iterations. Far field case, square root method.

the 1st, 3rd and 8th iterations. A tendency of decreasing the number of elements with anisotropic conductivity has been observed, Fig. 6.

As compared to the Wexler's method, the square root method seems to be less stable in the sense of a tendency to create extremely high conductivity values.



FIGURE 7. Picture in Cartesian plane of checkerboard conductivity pattern circular coordinate plane's square.

Moreover, special care must be taken while computing the conditioned conductivities  $k_x = q'_x/h_x$  and  $k_y = q'_y/h_y$  in regions of low conductivities (which results in low potential gradients).

# 5. Example 2: Near well downscaling

In this section the Double Constraint method will be exemplified for a nearwell problem. Let us consider a domain of a circular shape, as shown in Fig. 7. Although in a Cartesian x, y coordinate plane this shape is not a square, it does again represent a square  $([1, 2] \times [\pi/6, 2\pi/6])$  in the  $r, \phi$  coordinate plane of a circular coordinate system. In that case the apparent conductivities do not only contain the ordinary conductivities, but also the metrical factors (or scale factors) of the circular coordinate plane, [10].

Results obtained with the Wexler's isotropization method will be presented together with results computed with the square root method, Figs. 8.

Differences in the distribution of conductivities obtained with the two methods visible in Figs. 8 reflect already mentioned 'smoothing' property of Wexler's isotropization method, as compared to the square root method. The conductivity distribution obtained during iterations for the Wexler's method are presented on Fig. 9, whereas Fig. 10 gives analogous results obtained for the square method. The anisotropy ratios obtained for the square root method are shown in Fig. 11.

As in the former case, in a certain number of cells large and very small conductivities appeared. Conductivities generated after the 1st iteration were from the interval (0,20, 634), after the 3rd iteration from the interval (0,06, 1910), to become (4,69E-04, 4722) after the 8th iteration. Our observation is that once conductivity in an element becomes too large or too small, there is a tendency of unlimited growth or decrease. Apart from this effect, conductivities in the majority of the elements does not change much in further iterations. A very small number of negative values of conductivity occurred. The number of negative values appearing at a given iteration step may be viewed as a measure of convergence of the method. In the computations performed for the case test presented in this section the number of negative conductivities varied from 10, during the 1st iteration, to 3 in the 8th iteration.



c) Wexler's method

Square root method

FIGURE 8. Solutions of the forward problems and conditioned conductivities. Solid lines: isolines of heads from  $run\ 2$  (specified boundary fluxes). Dashed lines: isolines of heads from  $run\ 1$  (specified boundary heads). a) after first iteration, b) after iteration 3, c) after iteration 8.



FIGURE 9. Distribution of conductivity values within elements of the mesh during iterations. Near well case, Wexler's method.



FIGURE 10. Distribution of conductivity values within elements of the mesh during iterations. Near well case, square root method.

# 6. Summary, conclusions and discussion

In the context of groundwater flow, a forward model is based on a specified hydraulic conductivity field in the modeling domain. A forward model has a unique solution only if, on a part of the modeling domain's boundary, either the head or



FIGURE 11. Anisotropy ratio during iterations. Near well case, square root method.

the normal flux component is specified. Specification of both head and flux at that part of the boundary over-specifies the problem and has, therefore, no solution. However, such an over-specification may be used to improve the initially estimated conductivity field by conditioning it to the measured hydraulic head and flux data. Determination of conductivities from such additional boundary data is generally called inverse modeling.

Here we have presented a relatively simple, but very instructive approach to inverse modeling, the Double Constraint (DC) method, in the context of upscaling and its inverse: downscaling. In the DC method a well is considered as a boundary and an observation well is a well with exactly zero flow rate and measured head. The DC method is instructive, because it shows all the ingredients required for inverse modeling: measured heads and fluxes at the same parts of the closed boundary, as well as prior knowledge on conductivities. In addition, the method can be implemented easily, because it is based on existing groundwater modeling software.

From the exemplification shown in this paper we observe that the DC method has practical relevance in the context of upscaling and downscaling. We observe that the DC method may be viewed as a kind of a smoothing procedure: large contrasts in conductivity are smoothed, still preserving the original flow pattern. We have also observed that a small percentage (less than 1%) of the conditioned conductivities is negative. Provided that the specified head at the inflow point of a stream tube is higher than the specified head at the outflow point of that stream tube, the effective resistance of that stream tube is positive. A negative resistivity (resistivity = 1/conductivity) means that most of the positive resistivities along the stream tube are too large, in such a way that one or a few negative resistances have to compensate in order to obtain the correct resistance (which is the weighted sum of the resistances along the stream tube). Therefore, if wanted, negative values could be cured by "renormalization"; that is by making all positive resistances along the stream tube lower while making the negative resistivities along that tube positive, in such a way that the weighted sum of the resistivities yields the correct effective resistance. Such refinements will be the subject of a forthcoming paper.

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