Limitations to upscaling of groundwater flow models dominated by surface water interaction

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Different upscaling methods for groundwater flow models are investigated. A suite of different upscaling methods is applied to several synthetic cases with structured and unstructured porous media. Although each of the methods applies best to one of the synthetic cases, no performance differences are formed if the methods were applied to a real three-dimensional case. Furthermore, we focus on boundary conditions, such as Dirichlet, Neumann, and Cauchy conditions, that characterize the interaction of groundwater with, for example, surface water and recharge. It follows that the inaccuracy of the flux exchange between boundary conditions on a fine scale and the hydraulic head on a coarse scale causes additional errors that are far more significant than the errors due to an incorrect upscaling of the heterogeneity itself. Whenever those errors were reduced, the upscaled model was improved by 70%. It thus follows that in practice, whenever we focus on predicting groundwater heads, it is more important to correctly upscale the boundary conditions than hydraulic transmissivity.

1. Introduction

Although faster computers have been developed in recent years, they tend to be used to solve even more detailed problems. Examples of decreasing problem scales are pollution problems, and conservation of small nature conservation areas. One of the drivers is that the information scale has increased enormously. For example, the online available database in the Netherlands (http://www.dinoloket.nl) contains ~400,000 drillings (~10/km²) of the subsoil (0–100 m). This makes it possible to define an accurate description of the geology on a local scale (<250 m).

Moreover, due to modern observation techniques (e.g., land use by satellite images, digital terrain models obtained by laser altimetry) we are able to map and level the surface water most accurately (see Figure 1).

A recent development is that detailed numerical models are build that address small problem scales for very large areas. These models seek for optimal strategies in management of regional water problems. In many cases this will yield enormous models that cannot be resolved within acceptable time constraints. It is worthwhile mentioning that the time efficiency of a simulation model can be increased by (1) using a more time-efficient solver [Mehl and Hill, 2001] and/or (2) formulating a reduced model that is capable of simulating the important behavior of the original model [Vermeulen et al., 2004]. The first technique acquires extra computer resources (i.e., memory and disk space) and becomes impracticable whenever the model under consideration contains too many nodes (more than a million). The second method is restricted since it assumes a limited application of the model, e.g., it cannot compute other scenarios than those that are closely related to the ones that were used to compute the reduced model.

A coarsening (upscaling) of grid blocks in each direction reduces the computational times and disk space significantly since it relates almost quadratic to the number of grid blocks. In this paper we refer to this type of coarsening as uniform upscaling. In standard usage, uniform upscaling usually means that a global solution is used to determine upscaled parameters [Holden and Nielsen, 2000], however, in this paper we use this term to express that the entire model domain is subject to coarsening (see Figure 2a). However, it reduces the overall scale of detail, and if that is not desired, the alternative is to keep the fine-scale grid in the area of interest, and coarsen only those areas that are further away from it. We refer to this as nonuniform upscaling (see Figure 2b). For both of these coarsening approaches we need to obtain model parameters that are referred to as upscaled, effective, equivalent and/or homogenized parameters. They are defined such that they reproduce the global behavior of the aquifer while keeping the local behavior as close as possible to “reality”. The term reality is here referred to as that model solution that would have been obtained whenever we were able to compute the entire model without coarsening. Unfortunately, the coarsening of grid blocks is not without any consequence because detail will be lost that relates to subgrid heterogeneity of geology and the boundary conditions.

Excellent reviews on upscaling geology and hydraulic parameters are given by Renard and de Marsily [1997], Farmer [2002], Sánchez-Villa et al. [1995], and Neuman and Di Federico [2003]. However, this literature does not
provide a comparison between different upscaling methods on a range of different hydraulic transmissivity distributions. Moreover, many papers are devoted to upscaling of hydraulic transmissivities in reservoir engineering [Durlofsky, 1991; Durlofsky et al., 1997; Chen et al., 2003; Wen et al., 2003; Holden and Nielsen, 2000]. These type of models are often focused on an accurate prediction of oil production at the boundaries of the reservoir, and model impulses are rather simple as they are formed by an injector and a producer (i.e., closed loop simulations). Moreover, the quality of these upscaled models is often assessed by comparing the total flow rate for a specified pressure difference between injector and producer. In groundwater hydrology, however, we have a densely distributed system of boundary conditions that appear throughout the model domain. To ensure that the flow rate for these boundary conditions is correct, we urge to have local agreement. Our statement is that one cannot simply upscale the surrounding and assume that these boundary conditions are met. Since this is common practice, especially in hydrologic modeling, our paper should be an eye-opener for those that construct models with an overwhelming number of (nonlinear) boundary conditions. Although the global quantity might satisfy a criterion, the local quantities are also important. So, in regional groundwater models for water management the upscaling of these boundary conditions is important for which no literature exists.

The objective of this paper is to present a review of existing upscaling techniques and test their performances to single-phase groundwater flow which is discretized by means of finite differences (i.e., rectangular volumes). It tries to answer for which type of media which upscaling method performs best, and if there is a single method that performs ‘‘best’’ in practice. Furthermore, this paper addresses the issue of upscaling boundary conditions and quantifies the importance of this.

The paper is structured as follows: section 2 briefly gives the governing equation that describes three-dimensional groundwater flows for the fine and coarse blocks. It also defines several error criteria for quantifying the performances of the upscaling methods. Section 3 is devoted to upscaling techniques for the hydraulic transmissivity and illustrates their performances to several synthetic cases. Section 4 describes the consequences of block coarsening on Dirichlet and Neumann conditions. Section 5 shows the overall performance of the upscaling methodologies to a large-scale real-world application. Finally, conclusions and recommendation are formulated in section 6.

2. Governing Equations and Error Measures

2.1. Fine-Scale Equations

The equation that describes steady state incompressible, single-phase groundwater flow in three-dimensional porous media can be represented by the combination of the equation of continuity \( \nabla \cdot \mathbf{u} = -q \) and Darcy’s Law \( \mathbf{u} = -K \nabla \phi \) [Strack, 1989]

\[
\nabla \cdot [K(x) \nabla \phi] = q(\phi) ; \mathbf{x} \in \Omega,
\]

where \( \phi [\text{L}] \) is the hydraulic head, \( \mathbf{u} \) is the Darcy velocity \([\text{LT}^{-1}]\) (also called specific discharge), \( q \) is a source/sink term \([\text{LT}^{-2}]\) that can be hydraulic head dependent, and \( K \) is the hydraulic tensorial permeability \([\text{LT}^{-1}]\) for a fine-scale point \( \mathbf{x} \) subject to domain \( \Omega \). The tensor can be represented by its matrix of components

\[
K = \begin{bmatrix}
    k_{xx} & k_{xy} & k_{xz} \\
    k_{yx} & k_{yy} & k_{yz} \\
    k_{zx} & k_{zy} & k_{zz}
\end{bmatrix}.
\]

From a macroscopic point of view [Bear, 1972] it can be shown that \( K \) is symmetric \((k_{xy} = k_{yx}, k_{xz} = k_{zx}, k_{yz} = k_{zy})\) and positive definite \((k_{xx} k_{yy} k_{zz} \geq k_{xy}^2, k_{xz}^2, k_{yz}^2; k_{xx}, k_{yy}, k_{zz} > 0)\). This assures that energy is always dissipated during flow. However, most of the models assume quasi three-dimensional flow, i.e., the head gradient does not vary vertically within aquifers and does not vary horizontally within aquitards (Dupuit-Forchheimer flows). As a consequence of this, the tensor components \( k_{xx} = k_{yy} = k_{zz} = k_{xy} = 0.0 \) and the model is simulated by the quantity \( T [\text{LT}^{-1}] \) which is the transmissivity defined as \( T = kh \), where \( h [\text{L}] \) is the thickness of the aquifer/aquitard. A solution for these Dupuit-Forchheimer flows can be obtained by means of a grid-centered finite difference discretization [McDonald and Harbaugh, 1988]. However, this is already an important choice since there are

![Figure 1](image1.png) **Figure 1.** Detailed layout of the surface water elements (white) in a “polder” region (below sea level) in the Netherlands. Resolution of the grid is 25 x 25 m.

![Figure 2](image2.png) **Figure 2.** Schematic showing fine- and coarse-scale grid blocks for (a) uniform upscaling of the entire model domain, and (b) nonuniform upscaling of parts of the domain.
many different types of numerical model schemes available. They can be grouped into methods that use the arithmetic mean (upper bound method [Penman, 1988] or harmonic mean (lower bound method [Duvaut and Lions, 1976]) of the hydraulic block conductances C between grid nodes. However, the difference between these methods vanishes whenever the mesh refines infinitely (see Figure 3). Zijl and Trykozko [2001] used both methods in order to capture the absolute hydraulic transmissivity of the medium. However, the discussion whether the upscaled hydraulic parameters reflect the intrinsic property of the medium is not the purpose of this paper. Our only objective is to reproduce the fine-scale solution with a coarse-scale equation most optimally.

2.2. Coarse-Scale Equations

[9] It has been shown by Bourgeat [1984] under certain conditions (a uniform flow within an infinite domain), that the coarse-scale equation for the hydraulic head is of the same form as the fine scale equation, but for which the fine-scale hydraulic permeability tensor K is replaced by the coarse-scale hydraulic permeability tensor KC. This in itself is a significant finding, as a homogenized version of a partial differential equation is not necessarily of the same form as the original equation. The coarsening itself can be given by

\[ x = \xi \cdot x^c \quad ; \quad x, x^c \in \Omega, \]

where \( \xi \) is the upscaling factor in two directions (x, y), and \( x^c \) is a coarse-scale point within the identical domain \( \Omega \). We denote each coarse-scale variable by \( (\cdot)^c \) to distinguish them from their fine-scale equivalents. Furthermore, \( K^c \) itself is positive definite and symmetric, just as the fine-scale hydraulic permeability [Mei and Auriault, 1989]. An important aspect of coarsening is that \( K^c \) becomes often anisotropic, even if the original hydraulic permeability \( K \) is isotropic. Recently, methods became available that cope with the off-diagonal components in a tensor [Aavatsmark et al., 1996; Lee et al., 1998; Anderman et al., 2002].

2.3. Error Measures

[10] A complete equivalence, however, between the fine and coarse model is never possible since the grid coarsening introduces numerical errors simply because the degrees of freedom are reduced (factor \( \xi^2 \)), and the flow follows a different “path”. Ames [1992] stated that the size of the grid blocks should be about the inverse of the gradient of the logarithm of transmissivity, in order to prevent numerical dispersion. This error is negligible for the hypothetical case of uniform flow that is aligned to a network. Therefore several methods align their meshes to the local flow conditions [Cao and Kitanidis, 1999; Mansell et al., 2002]. However, an accurate and efficient implementation for a large-scale, multilayered systems is often limited since the final mesh becomes a mixture of concessions that will not guarantee an overall improvement. In general, however, this error will be smaller than other errors discussed in the following sections.

[11] To quantify the error, we use three criteria.

[12] 1. First is conservation of the hydraulic head: Ultimately, the upscaled hydraulic head \( \phi^c \) should be equal to the spatial averaged hydraulic head on the fine scale:

\[ \varepsilon^o(x^c) = \left[ \phi(x^c) - \frac{1}{V(x^c)} \int_{V(x^c)} \phi(x) dx \right]^2, \]

where \( V(x^c) \) corresponds to a coarse grid block volume.

[13] 2. Second is conservation of continuity: This requirement is especially important in transport problems, where velocity plays a dominant role. It prescribes that the upscaled Darcian flow \( u^c \) equals the averaged Darcy flow of the corresponding fine-scale model [Renard and de Marsily, 1997]. We define it as a relative error:

\[ \varepsilon^u(x^c) = \frac{\| u(x^c) - \frac{1}{V(x^c)} \int_{V(x^c)} u(x) dx \|}{\| \frac{1}{V(x^c)} \int_{V(x^c)} u(x) dx \|} \cdot 100\%. \]

[14] 3. Third is conservation of dissipation: This criterion is the equality of energy dissipated by the hydraulic head [Bar, 1994]. It is defined as the rate of dissipation of mechanical energy per unit weight of fluid. The relative dissipation error is given by

\[ \varepsilon^d(x^c) = \frac{\| -\nabla_x \phi u(x^c) - \frac{1}{V(x^c)} \int_{V(x^c)} [-\nabla_x \phi u(x)] dx \|}{\| \frac{1}{V(x^c)} \int_{V(x^c)} [-\nabla_x \phi u(x)] dx \|} \cdot 100\%. \]

Unfortunately, energy is lost when discretizing the flow domain, so that the numerical dissipation is always larger than the exact dissipation for discrete block-centered schemes. This leads to having a \( K^c \) that should be larger than \( K \) for isotropic homogeneous domains [Sánchez-Villa et al., 1995; Duvaut and Lions, 1976].
3. Upscaling Hydraulic Parameters

This section describes the most common upscaling techniques as mentioned in literature, for the hydraulic permeability \( k \), and the conductances \( C^x \), \( C^y \), \( C^z \). They can be roughly categorized into (semi) problem-dependent and problem-independent techniques.

3.1. Power Averaging (GEO Method)

It is known, from analytical solutions, that the upscaled hydraulic permeability for flow parallel to the strata is the arithmetic mean of the fine-scale hydraulic permeabilities, and for flow perpendicular to the strata, the harmonic mean [e.g., Wiener, 1912; Matheron, 1967]. Journel et al. [1986] proposed the general equation

\[
\bar{k}(x^f) = \left\{ \frac{1}{V(x)} \int_{V(x)} k(x)^p dV(x) \right\}^{1/p}, \tag{7}
\]

where \( p = -1 \) corresponds to the harmonic mean, \( p = 1 \) to the arithmetic mean. Desbarats [1992] demonstrated that, for moderately heterogeneous two dimensional systems, the upscaled hydraulic permeability could be estimated accurately by means of a spatial optimized \( p \) that best fit numerical simulations.

However, one of the few exact results, for two-dimensional flow, is the rule of geometric averaging \((p = 0)\) [Matheron, 1967]:

\[
k^g(x^f) = \exp \left\{ \frac{1}{V(x)} \int_{V(x)} \ln[k(x)] dV(x) \right\}. \tag{8}
\]

The rule of geometric averaging is only satisfied for an isotropic lognormal medium and a checkerboard binary design [Warren and Price, 1961]. Moreover, it holds only for uniform (parallel) flow fields and is not satisfied for example for radial flow that is discretized by rectangles.

3.2. Darcian Methods (HNF Method)

This approach is like laboratory measurements of local properties of the porous medium, but using simulated experimental results. This method was first introduced by Warren and Price [1961], and after all, it simply consists of numerically simulating the experiment of Darcy upon a coarse grid block isolated from the total model domain (see Figure 4). The advantage of Darcian methods is that the shape of hydraulic transmissivities affects the final upscaled hydraulic transmissivity, that power averaging lacks (section 3.1).

The coarse-scale conductance \( C^{cx} \) between adjacent blocks along the column direction would now be obtained by simulating a coarse grid block with domain \( \Omega_x^c \times \Omega_y^f \) having “sealed-off” boundary conditions along \( \Omega_y \), and a constant pressure drop along \( \Omega_x \). The conductance will be the ratio between the averaged local flow and the averaged gradient in the coarse grid block [Rubin and Gómez-Hernández, 1990], so

\[
C^{cx}(x^f) = \frac{\langle u^x \rangle \Omega_y}{\langle \nabla \phi^x \rangle |\Omega_x|}. \tag{9}
\]

The averaged quantities along the \( x \) direction are defined as:

\[
\langle u^x \rangle = \frac{1}{V(x)} \int_{V(x)} u^x(x) dx \tag{10}
\]

\[
\langle \nabla \phi^x \rangle = \frac{1}{V(x)} \int_{V(x)} \nabla \phi^x(x) dx, \tag{11}
\]

with \( x \in \{ \Omega_x \times \Omega_y \} \). The coarse-scale block conductance along the row direction \( C^{cy} \) is derived analogously.

Gomez-Hernandez and Journel [1990] suggested that “jacket cells” (i.e., extension of the flow region larger than the coarse block, see Figure 4) will improve the upscaled hydraulic transmissivity. It is possible that these extra “border rings” will improve the results [Wen et al., 2003]; however, there is a simple example that illustrates the risk of using those jacket cells or border rings. Consider a case where zero hydraulic transmissivity barrier divides a coarse cell into two pieces and extends unto the boundary of the coarse cell. Whenever no jacket cells were used, the upscaled hydraulic transmissivity will become zero, if they will be used, then some flow will be allowed, and a nonzero hydraulic transmissivity results.

3.3. Homogenization (TEN and PTEN Methods)

A disadvantage of Darcian methods (section 3.2) is that they yield an upscaled hydraulic transmissivity that depends on the imposed boundary conditions. In contrast to this, homogenization is an upscaling method [Bensoussan et al., 1978], that yields a homogenized hydraulic transmissivity that is independent of the chosen boundaries. These boundary conditions assume that the region under study is immersed in a large-scale pressure field and the system itself is surrounded by periodic replications of itself on all sides [Durlofsky, 1991]. It seems an unrealistic situation
since there is no natural medium periodic. However, there is no reason to believe that these periodic boundary conditions are less arbitrary than sealed-off type, uniform type of boundaries, or effective flux boundary conditions [Wallstrom et al., 2002].

Periodic boundaries prescribe specific correspondences between pressure and velocity on opposite faces of an isolated coarse grid block. This means that the fluxes through opposite boundaries should be equal and opposite, and the heads along that direction equal to each other minus a given drop in pressure. Perpendicular to this, the heads for opposing boundaries should be equal. A model with these boundary conditions needs to be solved twice, a) with a hydraulic gradient in the x direction, and b) in the y direction. From these solutions we compute the averaged velocities (10) and pressure gradients (11) and obtain the components of the tensorial hydraulic permeability by solving:

\[
\begin{bmatrix}
(\nabla \phi_x)_a & (\nabla \phi_y)_a & 0 & 0 \\
0 & (\nabla \phi_x)_a & (\nabla \phi_y)_a & 0 \\
(\nabla \phi_x)_b & (\nabla \phi_y)_b & 0 & 0 \\
0 & (\nabla \phi_x)_b & (\nabla \phi_y)_b & 0
\end{bmatrix}
\begin{bmatrix}
k_{xx} \\
k_{xy} \\
k_{yx} \\
k_{yy}
\end{bmatrix}
= -\begin{bmatrix}
(u_x)_a \\
(u_y)_a \\
(u_x)_b \\
(u_y)_b
\end{bmatrix},
\]

where \( \langle \cdot \rangle^a \) represents the average quantities obtained by the first simulation, and \( \langle \cdot \rangle^b \) those from the second. A solution of (12) yields always a symmetric and positive definite tensor [Duruľošky, 1991]. Instead of flux averaging, we can apply dissipation averaging and whenever they distinct minor, it is a measure for the necessity of periodic boundary conditions [Bensousan et al., 1978].

Periodic boundaries are not completely general as they assume periodicity for a block scale which is not equivalent to the intrinsic property of the medium. Again, border rings can be expected to provide an improved tensorial hydraulic permeability because the effects of larger-scale hydraulic transmissivity connectivity are accounted for [Wen et al., 2003]. Nevertheless, the size of the grid block should essentially capture the intrinsic property of the medium (Representative Elementary Volume REV). To approach this condition slightly, we introduce a different strategy (PTEN) by applying periodic boundary conditions to all fine-scale grid blocks and include 1 jacket cell. We assume that the intrinsic property of the medium could be described by those 3 × 3 cells. The upscaled tensorial hydraulic permeability within a coarse-scale grid block becomes the geometric mean as defined in (8).

### 3.4. Local-Global Method

The local-global method [Chen et al., 2003] is a slight adjustment to the previously mentioned methods (see sections 3.2 and 3.3). It can be seen as a minimization problem, whereby the upscaled hydraulic transmissivity minimizes the differences in the velocity fields generated by the coarse and fine scale [Holden and Nielsen, 2000]. The method can be briefly summarized by stating that the boundary conditions for the local model domains are extracted from subsequent iterations of the global solution. The local model domain is extended toward the center of the neighboring grid blocks, and the global heads \( \phi^a \) are projected on the fine-scale boundary domain (see Figure 4).

Those boundary pressures \( \phi^b \) are weighted harmonically by the transmissivities, so the \( i \)th column along the \( x \) direction yields

\[
\phi^b_i = \phi^a_i + \frac{x_i - x^*_i}{x^*_2 - x^*_1} \left( \phi^a_i - \phi^*_i \right) \frac{T^*}{T_i} : x^*_1 < x_i < x^*_2,
\]

where \( T^* \) is the total harmonic conductance along the current direction between \( x^*_1 \) and \( x^*_2 \). Chen et al. [2003] solved the local problem twice by assuming a global flow along the \( x \) direction (interpolating linearly in one direction and harmonically in the perpendicular direction), and a global flow along the \( y \) direction. They state that by doing so the upscaled hydraulic transmissivity will be representative for more different cases.

The method is efficient whenever the effort put into the local flow simulations is less than a single simulation of the original fine-scale model. Chen et al. [2003] suggested therefore to apply these simulations only for areas with a significant drop in pressure.

### 3.5. Global-Local Methods

As shown in the previous subsections, the upscaled hydraulic transmissivity is not unique and depends on the local flow conditions. So, the best thing we can do is using these local flow conditions in order to compute the upscaled conductances as the ratio between the averaged flux and averaged pressure gradient in each coarse-scale grid block (9). The upscaled parameters are optimal for the used boundary conditions and are, however, no guarantee that different flow conditions will be simulated correctly [Bierkens and van de Gaast, 1998]. This is the major disadvantage of this global-local strategy as it leads to the paradoxical situation where one has to know a priori the local solution on a global scale, in order to determine the upscaled block hydraulic conductance. In this chapter, we assume that we have the “luxury” of knowing the exact fine-scale solution and therefore the results obtained by this method should be interpreted as being the best possible for this method.

### 3.6. Vertical Hydraulic Conductance

The 3-D domain is often discretized as quasi-3-D, which means that stratified layered media are assumed which is as a set of two-dimensional models that exchange water vertically over intermediate layers with poor hydraulic conductance without horizontal flow components (Dupuit-Forchheimer flows). The assumption of quasi-3-D flow behavior holds if the vertical conductance of the separate layers (aquitard) is very small compared to the horizontal transmissivity of the aquifers. The amount of water that is vertically exchanged over a coarse grid block, should be equal to the total exchange in the fine-scale model, so

\[
C^{k}_{k} (\phi_{k} - \phi_{k+1}) = \int_{V(x)} \{ C^{l}_{k} (\phi_{k} - \phi_{k+1}) \} (x) dx,
\]

where \( k \) denotes the model layer, and \( C^{l}_{k} \) is the vertical conductance between two overlaying aquifers \( k \) and \( k+1 \). Again, it follows that the upscaled vertical conductance is a function of the fine-scale solution. This could be easily implemented for the GL method. For the LG method we have extended the “local” model toward 3-D in order to...
apply Equation (14). The other methods, however, compute the vertical conductance as

\[ C_{zc} = \int_{V(x)} C_z(x) \, dx \]  

which is only valid whenever \( d(\phi_k - \phi_{k+1})/dx \approx 0 \).

### 3.7. Examples

[29] This section describes the performance of the upscaling techniques mentioned in the previous subsections for different heterogeneous media. We denote the different techniques by their acronyms.

#### 3.7.1. Distribution of Heterogeneity

[30] We have defined three synthetic cases with different distributions of hydraulic heterogeneity. All of these cases are two-dimensional (102 columns by 102 rows with \( \Delta x = \Delta y = 10 \text{ m} \)) and possess a Dirichlet condition around the entire model domain. In the middle of the model we have positioned an extraction well with rate \( q = 100 \text{ m}^3/\text{day} \). Since upscaling is most sensitive to the amount of distortion of the flow direction compared to the axis of the network, we simulated a diagonal flow from the lower left corner unto the upper right corner.

[31] The first transmissivity field is that of a strong anisotropic medium (see Figure 5a). It yields a strong preferential flow that is rotated 45° clockwise to the axis of the network (Figure 6a). The second case, is a multi-Gaussian random field (http://www.math.umd.edu/bnk/bak/generate.cgi) (see Figure 5b) that has an irregular shaped drawdown (Figure 6b). The last synthetic case is that of a dual hydraulic transmissivity system that is derived from a real-world channeling system [Snepvangers and te Stroet, 2005] (Figure 5c). The flow field shows sharp irregular shaped discontinuities (Figure 6c).

#### 3.7.2. Results

[32] We have increased the size of the grid blocks subsequently by the upscaling factors \( \xi = 2, 3, 4, 5, 6, 7, 8, 10, 15, 20 \), without upscaling those grid blocks that possess Dirichlet conditions. We have computed the errors for the hydraulic head (\( \langle \phi^0 \rangle \)) for all these cases and plotted them in Figures 7a–7c.

##### 3.7.2.1. Anisotropic Medium

[33] The tensorial methods TEN and PTEN, yield the most accurate results since the medium is anisotropic and diagonal preferential flow is present (see Figure 7a). The PTEN method performs better than TEN since it captures the intrinsic periodicity of the medium (i.e., \( 3 \times 3 \) grid blocks) instead of periodicity on a coarse block scale. The worst performance for this medium is given by the HNF and GEO methods since they cannot cope with the anisotropic character of the flow field. The performance of HNF increases with \( \xi \), which sounds rather contradictory but can be explained by the fact that the effects of the sealed-off boundaries reduces as the isolated block increases. Therefore the GL method performs better since realistic boundary conditions are used. However, it cannot cope with the diagonal preference of the flow which is the main reason why the LG method does not converge properly.

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**Figure 5.** Different maps of the fine scale: (a) an anisotropic medium with \( T = 1 \text{ m}^2/\text{day} \) (black) and \( T = 100 \text{ m}^2/\text{day} \) (white), (b) a multi-Gaussian random field with lognormal distribution between \( T = \exp(-2) \text{ m}^2/\text{day} \) (black) and \( T = \exp(2) \text{ m}^2/\text{day} \) (white), and (c) a channeling system with a dual hydraulic transmissivity identical to Figure 5a.

**Figure 6.** Different maps of the hydraulic head that migrates by a 45° rotation through (a) an anisotropic medium, (b) a multi-Gaussian random field, and (c) a channeling system (see Figures 5a–5c).
3.7.2.2. Multi-Gaussian Medium

For this type of medium, there is no upscaling method that performs significantly better than another method (see Figure 7b). All methods perform rather accurately for \( \xi \leq 5 \) and perform worse beyond. This case shows best the error that is caused by the artificial shift of the source term, it influences the graph least at \( \xi = 5 \) and \( \xi = 10 \). In section 4.2 we mention a strategy to minimize this error. However, it is a remarkable finding that for such a medium the choice of upscaling is irrelevant and upscaling of boundary conditions might be of more importance.

3.7.2.3. Channeling Medium

For this synthetic case the HNF performs rather well (see Figure 7c). A reason for this is that the system shows strong drops in pressure that are mainly aligned to the network, the harmonic mean is therefore a good approximation. A similarity exists for the TEN that yields almost identical homogenized parameters because no anisotropic conditions are distinguishable. At the same time, this phenomena causes the GEO method to perform poorly. Again, the performance of the LG and GL methods are the best. The PTEN performs rather inaccurate since it assumed an REV size of \( 3 \times 3 \) cells for the entire model domain which is, however, incorrect for most parts of the model field. In this context, the TEN method performs slightly better since it uses an REV size which is based upon the coarse grid blocks, which is often larger than \( 3 \times 3 \) cells.

3.8. Conclusions

From the results obtained by the synthetic cases, it is obvious that the inaccuracy of a coarsened model increases rapidly with the upscaling factor \( \xi \). The smallest upscaling of \( \xi = 2 \) results in errors \( \langle \epsilon^2 \rangle > 0.1 \) m. The anisotropic medium can be most successfully upscaled over a wide range of upscaling factors by using tensors (e.g., complex cross beddings, dipping layers not aligned to the coordinate system). There is no upscaling method favorite for the Multi Gaussian Medium, all methods perform rather well until \( \xi \leq 5 \). For the channeling system best results were obtained with the LG and GL methods for at least small-scale factors \( \xi \leq 5 \). Unfortunately, real-world media are a “mixture” of the above mentioned hydraulic transmissivity fields. So there is no single “best” upscaling method! which is also confirmed by a practical application in section 5. Therefore it should be locally determined which technique describes the current hydraulic transmissivity most optimally. Moreover, the network configuration should be a function of the hydraulic transmissivity variance [Garcia et al., 1990] and/or existing periodic structures [Zijl and Trykozko, 2001], which is, however often impossible or difficult to implement.

4. Upscaling Boundary Conditions

This section is devoted to the treatment of boundary conditions in the process of upscaling meshes. These conditions can be divided into three categories that are often used in hydrological modeling. These are (1) Neumann conditions that are used to model fixed source terms (e.g., wells), (2) Dirichlet condition that are used to model the interaction with the world outside the model domain, and (3) Cauchy condition that simulate the interaction between surface water and groundwater. This section describes the

![Figure 7](image-url)
consequences of grid coarsening to the behavior of Dirichlet, Neumann, and Cauchy conditions. Especially the last condition is very important in the process of upscaling meshes.

4.1. Dirichlet Conditions

Dirichlet conditions are “open” boundary conditions that exchange flow $u^b$ with the world outside the model domain $\Omega$. It is modeled by keeping the hydraulic head “fixed” on the boundary and the boundary flux along the column direction becomes:

$$u^b = C^x(\phi^b - \phi),$$

(16)

Whenever we apply a grid coarsening we transform each coarse grid block into a Dirichlet condition whenever there is at least one fine-scale Dirichlet condition in it. Therefore the shape and the individual boundary parameters $C^x, \phi^b$ need to be replaced by averaged quantities, such that the coarse Dirichlet conditions yields a similar Darcy flow $u^{cb}$ by a comparable flow field, so

$$u^{cb} = \sum_{i=1}^n u^b_i(x) ; x \in x^c,$$

(17)

where $n$ is the number of fine-scale Dirichlet conditions within a single coarse grid block. To approximate $Q^{cb}$, we define a local fine-scale model between the coarse grid block with Dirichlet conditions and its adjacent grid block along the column direction (see Figure 8a). The model is determined by no-flow boundaries perpendicular to the columns, and Dirichlet conditions for all rows at the right boundary (see Figure 8b).

The head $\phi^{cb}$ at the right boundary is the averaged head for all Dirichlet conditions within the coarse grid cell, minus an arbitrary chosen $\Delta \phi$. The coarse boundary conductance $C^{cb}$ along the column direction follows from

$$C^x = \frac{u^{cb}}{\Delta \phi},$$

(18)

The conductance along the $y$ direction $C^{cy}$ is defined analogously. In this paper we refer to these computations as Dirichlet simulations, and we observed an improvement of the dissipation and hydraulic head whenever we applied them (see Figure 9). However, since the actual flow at these Dirichlet conditions was radial, we overestimated the flow by assuming sealed-off boundaries along the axis of the local fine-scale model.

4.2. Neumann Conditions

Neumann conditions are head-independent point sources (e.g., precipitation, extraction wells) that guarantee a similar flux exchange for the fine-scale and coarse-scale model. Nonetheless, the actual position of a Neumann condition can be shifted in the coarse scale model, simply because the node does not need to resemble the actual well position. We can reduce this error by distributing the well strength among neighboring coarse grid blocks, such that they resemble the center of gravity for the well. In this paper we refer to this as Neumann displacements.

Figure 8. (a) Schematic showing the local model domains ($\Omega^x_{col} \times \Omega^y_{row}, \Omega^x_{row} \times \Omega^y_{col}$) for computing the coarse grid block conductances aligned to (1) the column and (2) the row direction of the model network, subject to fine-scale Dirichlet conditions (*). (b) Schematic showing the isolated fine-scale model with sealed-off boundaries and a drop in pressure $\phi^{cb} - \Delta \phi$.

Figure 9. Graph showing the mean relative error in dissipation ($||\epsilon||^2$) versus the upscaling factor $\xi$ for a uniform upscaling with and without Dirichlet Simulations for a homogeneous medium ($T = 100$ m$^2$ day$^{-1}$).
A simple method is to compute a distribution index \( \omega_i \) by a numerical simulation whereby the model domain is determined by the centers of the coarse-scale blocks that neighbor the specific well (see Figures 10a and 10b). The amount of water that will be released from each corner determines the corresponding well index \( \omega_i \), and the well strength for each neighboring coarse grid block becomes, \( q_i = \omega_i \cdot q \). The strategy shows some resemblance to the method proposed by Durlofsky et al. [2000], however, they related the conductances of the coarse block to the well instead.

Applying Neumann Displacements showed to improve an upscaled model significantly (almost an order of magnitude; see Figure 11). More improvement can be expected whenever the local fine-scale model is extended with jacket cells and/or simulated in 3-D. However, it should be mentioned that the method can have a drawback too, since nonactiveness within the local fine-scale model can cause an unbalanced distribution of the well indexes. In the worst case, no indexes can be computed as all corner points are inactive on a fine scale.

**4.3. Cauchy Conditions**

The most important boundary condition in lowland areas such as the Netherlands is the surface water system (see Figure 1). The flux \( q_i \) between surface water and groundwater is modeled as a Cauchy condition. Moreover, often this condition is nonlinear, e.g., a drainage flux is limited to a specified drainage level, and infiltration from rivers is often easier than exfiltration. They can be generally formulated as

\[
\Delta h_i = h_i - \phi_i
\]

\[
q_i = C_i(\Delta h_i)\Delta h_i,
\]

where the conductance \( C_i \) is specific for the considered external force and is a nonlinear function of \( \Delta h_i \) (Figure 12a). Most iterative solvers use a Picard iteration that sequentially reformulates and solves a linear system after reexamining \( \Delta h_i \). Whenever we coarsen the grid blocks, this evaluation takes place between coarse- and fine-scale parameters and yields an overestimation or underestimation of the interaction, see \( \Delta h^c \) in Figure 12b. However, it is only possible to compute an averaged coarse scale \( h^c \) whenever the conductances \( C_i \) on the fine scale are equal, which is rarely the case.

An alternative is to use the fine-scale solution (or a good approximation of it) \( \phi_i \) and obtain a prior estimation of the coarse-scale solution \( \delta^c \). We are now able to approximate a corrected level \( h^c \), such that the coarse-scale solution exchanges approximately the same flux within the external system, thus

\[
\Delta h^c = \left( \phi^c - \phi_i \right)
\]

\[
q^c = C_i\left( [h_i + \Delta h^c] - \phi_i \right) \approx q_i
\]

We refer to this method as Cauchy corrections, and we show in section 5.2 that these corrections yield a significant improvement of an upscaled model of a real-world case.

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**Figure 10.** (a) Local model domain \((\Omega_x \times \Omega_z)\) for encountering well (diamond) displacement onto neighboring nodes (crosses) within a coarse mesh. (b) Corresponding isolated fine-scale model used to compute the distribution index \( \omega_i \) for the four Dirichlet conditions positioned in each corner (asterisks).

**Figure 11.** Graph of the mean absolute error of the hydraulic head \( (\varepsilon^0)^t \) versus the minimal distance between the exact well location to the nearest coarse grid block, i.e., the “misfit” \( (\xi = 20) \).

**Figure 12.** Schematic showing the pressure differences for the computation of a drainage flux \( q_1 \), \( q_2 \) within (a) a fine-scale model and (b) a coarse-scale model where \( \phi^c \) represents the coarse-scale solution.
Table 1. Statistics for the Horizontal and Vertical Transmissivities for the Regional Groundwater Flow Model of the Province of Noord-Brabant in the Netherlands

<table>
<thead>
<tr>
<th>Layer</th>
<th>Horizontal Transmissivity in the Aquifers, m² d⁻¹</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>SD</th>
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<tr>
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<table>
<thead>
<tr>
<th>Layer</th>
<th>Vertical Transmissivity Between Aquifers, m² d⁻¹</th>
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<th>Maximum</th>
<th>Mean</th>
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<td>2.75E-04</td>
<td></td>
</tr>
</tbody>
</table>

However, they yield correction factors that are based upon a prior simulation and it is questionable whether these factors remain valid for different scenarios.

4.4. Conclusions

The errors of upscaling boundary conditions emerges simply because we coarsen a mesh and the boundary conditions (Dirichlet, Neumann and Cauchy conditions) need to be grouped or clustered together. This yields an inaccuracy that could be reduced by computing average quantities that ensures that fluxes from boundary conditions are more or less equal to those within the fine-scale model. This is a new line of research that has not been reported on before. As will shown in the following section, errors due to upscaling of boundary conditions is often much larger than those of hydraulic parameters.

5. Real-World Case

5.1. Introduction

The real-world case is a regional steady state threedimensional groundwater flow model that describes the entire region of the province of Noord-Brabant in the Netherlands (≈10,700 km²). The model consist of 320 rows, 535 columns and 9 model layers, so the total number of nodes is 1,540,800. Each grid block is a square with Δx = Δy = 250 m. The first model layer contains the influence of an intense surface water network that consists of “polders” (i.e., specific lowland areas where a fixed surface water level is maintained) and natural drainage systems situated in higher areas. Absolute levels for these nonlinear boundary conditions were obtained by accurate laser altimetry. The model is furthermore characterized by a detailed description of the precipitation and evapotranspiration rate. These were obtained by combining data from rain gauge stations throughout the model domain with accurate land use classification from satellite images. The subsurface modeling was based upon thousands of drillings that were available for the region under consideration (http://www.dinoloket.nl).

The statistics of the hydraulic transmissivities for the aquifers and the vertical resistances of the aquitards are given in Table 1, and two maps of the hydraulic head are given in Figures 13a and 13b. The maps show the irregularity of the boundary conditions and the highly detailed solution of the hydraulic head.

5.2. Results

We have sequentially solved the real-world case for different upscaling factors 2 ≤ ξ ≤ 10. We applied a variety of upscaling techniques for the hydraulic transmissivities (subsection 3) and depicted the error for the hydraulic head in Figure 14a. As we expected, the hydraulic transmissivity field of the real-world case is of such a mixture of periodic media, Multi Gaussian distributions and sharp discontinuities that all upscaling methods perform almost identical. In fact, we should say “just as bad” since the smallest upscaling factor ξ = 2 yields an error of η² ≈ 0.1–0.25 m. Herein, the GL, LG (more or less plotted over GL) and the PTEN performed best, followed by the GEO, TEN and HNF methods. Furthermore, the relative-mean-averaged error in the Darcy flow (η²) does not distinguish significantly between the upscaling methods too. A small upscaling of ξ = 2 yields an error of the Darcy flow of ≈30% (see Figure 14b). These bad performances are mainly caused by significant errors due to upscaling of the boundary conditions such as Dirichlet, Neumann and Cauchy conditions. In section 3 we suggested several techniques for the upscaling of these conditions and we have added these techniques and plotted their improvements in Figure 14c.

Techniques that proved to work rather well for synthetical problems, appear to be of low relevance for our real-world case. The error reduction given by Dirichlet simulations is maximal 0.02 m and the error becomes even worse for ξ ≥ 8. A reason for this is that the coarse grid blocks increases such that the assumed

Figure 13. Map of the hydraulic head [m + MSL] within (a) model layer 1 and (b) model layer 9 for the real-world case. Shading ranges from 5 m-MSL (black) to 30 m + MSL (white).
sealed-off boundaries become more and more invalid. The Neumann displacements have, however, a negligible effect. The regional scale of the model with grid blocks of 250×250 m causes the irrelevance of the artificial shift for these Neumann conditions. In contrast, the Cauchy corrections have a significant effect and improve the upscaled model ranging from 0.06 m unto 0.33 m for 2 ≤ ξ ≥ 10, respectively. This means that the Cauchy corrections yield an error reduction of ≈40%. This again shows that reliable upscaling for groundwater flow models is only possible whenever we know the fine-scale solution. Since a fine-scale solution cannot be computed, however, it can be approximated by subsequently solving an upscaled model with a local refinement (nonuniform upscaling; see Figure 2b), and collect the results from those fine regions only to form a limited part of the global solution. It is important that the models overlap to determine the zone for which the solution can be copied. Again, it should be understood that this type of upscaling needs to be carried out with care since there is a clear trade-off between efficiency (ratio between the number of nodes in the original fine-scale model and the upscaled model) and accuracy of the hydraulic head in the fine part of the coarsened model. High efficiencies increase the error significantly, especially for aquifers that have a significant resistance to the boundary conditions (in our case that appeared to be ≈20,000 days; see Figure 14d).

6. Conclusions and Recommendations

This paper describes the error due to upscaling of meshes in groundwater flow modeling that uses block centered finite differences. The paper consists of two parts. 

The first part describes the upscaling of hydraulic transmissivities by means of the most important and promising techniques, mentioned in literature. For three synthetic cases that all differ in their heterogeneity distribution, it is clear that the different upscaling techniques have their preferences for which type of distribution they perform optimally.

The second part is devoted to the error that evolves due to the upscaling of boundary conditions. This error emerges because we coarsen a mesh and reduce the degrees of freedom. Therefore the model forces (Dirichlet, Neumann and Cauchy conditions) within a model need to be grouped or clustered together. This yields an inaccuracy that was, for several synthetic cases, successfully reduced to acceptable levels by computing average quantities that ensures that the fluxes from the upscaled boundary conditions are more-or-less equal to the fluxes in the fine-scale model. Errors due to upscaling of boundary conditions are often much larger than those caused by upscaling of hydraulic parameters. This is a new line of research that has not been reported on before.

We applied the above mentioned techniques to a real-world three-dimensional case and observed that the differences between the upscaling techniques for the hydraulic transmissivity were negligible. Since real-world media are a mixture of different distributions of heterogeneity, there is no single upscaling technique that performs best. In practice we should vary between different techniques throughout the model domain which is, however, impractical. Moreover, all techniques performed poorly. The techniques we introduced for the upscaling of Dirichlet and Neumann conditions were
not relevant too. The major improvements were obtained by using the Cauchy corrections that increased the accuracy of the upscaled model for ≈40%. Nonetheless, it needs the entire fine-scale solution which is often not available. So, in order to achieve a reliable coarsened model, we need to know the fine-scale solution. However, this implies a paradoxical situation where one has to know the solution in order to acquire it. A possible option is to use an a priori analysis of localized “small” models in order to acquire this fine-scale solution. With these results an accurate global model can be constructed for the current application, however, it is questionable for which other applications this upscaled model can be still used.

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References

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