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# REFINEMENT AND COARSENING OF PARAMETERIZATION FOR THE ESTIMATION OF HYDRAULIC TRANSMISSIVITY

**Hend Ben Ameur**
Inria-Rocquencourt and
ENIT(LAMSIN), BP 37,
Le Belvédère, Tunis, Tunisia
Email: Hend.Benameur@inria.fr

**Guy Chavent**
Inria-Rocquencourt and
Ceremade, Université Paris-Dauphine,
Place du Maréchal De Lattre de Tassigny,
75775 Paris Cedex 16, France
Email: Guy.Chavent@inria.fr

**Jérôme Jaffré***
Inria-Rocquencourt, BP 105,
78153 Le Chesnay Cedex, France
Email: Jerome.Jaffre@inria.fr

## ABSTRACT

This paper deals with parameterization of hydraulic transmissivity during its estimation. Estimating transmissivity is based on the minimization of an misfit function defined as a least-squares misfit between measured data and the model output. The transmissivity is assumed to be a piecewise constant space dependent function. Refinement indicators, indicating the effect on the optimal data misfit of adding degrees of freedom to a current set of parameters, are calculated. Theses indicators lead to know where the hydraulic transmissivity needs to be made discontinuous and thus allows for the introduction of degrees of freedom one at a time, preventing from overparameterization.

## INTRODUCTION

When estimating hydraulic transmissivities, which are space dependent coefficients in a parabolic partial differential equations, we minimize a misfit function defined as a least-squares misfit between measurements and the corresponding quantities computed with a chosen parameterization of the transmissivities.

One of the difficulties in solving this problem is that, because of the high cost of experimental measurements, the data is usually insufficient to estimate the value of the hydraulic transmissivity in each cell of the computational grid. Therefore we have to find a parameterization of the transmissivity which reduces the number of unknowns. We refer to (Sun, 1994; Eppstein-Dougherty, 1996) for a presentation of the parameterizations which are the most commonly used in hydrogeology.

Lately multiscale parameterizations (Liu, 1993; Chavent-Liu, 1989) have provided a first answer to the problem of choosing the discretization of distributed parameters. With such an approach the parameter estimation problem is solved through successive approximations by refining the scale and the process is stopped when the refinement of the scale does not induce a significant decrease of the misfit function. This method has already brought interesting results in various problems of parameter estimation (Chardaire-Rivière et al., 1990; Chardighy et al., 1996). However, when going from the current scale to a finer one, degrees of freedom are added uniformly in the domain of calculation, and so this approach can lead to overparameterization in the case where only local refinements are needed.

The method using refinement and coarsening indicators, that we present in this paper, will avoid such a drawback. At a given refinement level the parameters are estimated by minimizing the least-squares misfit to the data. Then we compute refinement and coarsening indicators which indicate the effect on the optimal data misfit of adding or removing some degrees of freedom. A

* Address all correspondence to this author.

variant of this method has already been presented in (Chavent-Bissel, 1998).

We apply this technique to the estimation of the distributed transmissivity parameter $T$ in the partial differential equation

$$S\frac{\partial \Phi}{\partial t} + \text{div}\,(-T\ \text{grad}\,\Phi) = Q \text{ in } \Omega, \tag{1}$$

where $\Omega$ is a domain in $\mathbb{R}^2$. This equation governs a two-dimensional groundwater flow in an isotropic and confined aquifer, subject to initial and boundary conditions

$$\begin{aligned} &\Phi = \Phi_d \text{ on } \Gamma_D, \quad (-T\ \text{grad}\,\Phi)\cdot n = q_d \text{ on } \Gamma_N, \\ &\Phi(0) = \Phi_0 \text{ in } \Omega, \end{aligned} \tag{2}$$

where $\Gamma_D$ and $\Gamma_N$ is a partition of the boundary of $\Omega$ supporting respectively Dirichlet and Neumann conditions and where

$\Phi =$ piezometric head,
$S(x,y) =$ storage coefficient,
$T(x,y) =$ hydraulic transmissivity,
$Q(x,y,t) =$ distributed source term,
$\Phi_d, q_d$ given boundary piezometric head and source terms,
$\Phi_0 =$ given nitial piezometric head,
$n$ is the unit normal vector to $\Omega$.

The domain $\Omega$ is discretized with a mesh $T$ and equations (1),(2) are approximated by a mixed-hybrid finite element method, which is suitable to the case where the parameter $T$ have discontinuities (Chavent-Roberts, 1997).

Our problem is to search for a piecewise constant hydraulic transmissivity $T$. Both the zonation (the partition of $\Omega$ into zones where $T$ is constant) and the value of $T$ on each zone are to be determined and our aim is to be able to explain the data with a number of zones as small as possible.

We define our misfit function by:

$$J(T) = \frac{1}{2}\sum_{i,j} |\Phi(x_j,t_i) - \Phi^m_{i,j}|^2. \tag{3}$$

where $\Phi^m_{i,j}$ is the piezometric head measured in the point $x_j$ at the time $t_i$ and $\Phi(x_j,t_i)$ is the model output for current transmissivity values.

In order to have a computational cost independant of the number of transmissivity values to estimate, we use a Gauss-newton algorithm which is known to be an efficient optimization method in the case of large number of unknown parameters (Bonnans et al., 1997). The gradient of $J$ is computed by the adjoint state method (Sun, 1994).

Actual implementation of the calculation of the the piezometric head, the misfit function and its gradient has been achieved through automatic program generation (Jegou, 1997).

## 1 REFINEMENT AND COARSENING INDICATORS

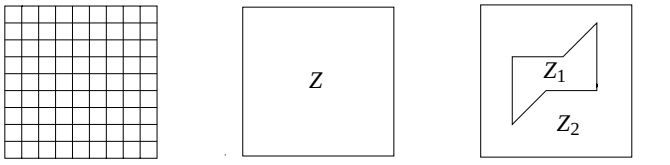
Usually the data are in insufficient quantity to estimate the unknown parameter in each cell of the computing mesh $T$. To every partition (zonation) $Z$ of $\Omega$, we associate the space of hydraulic transmissivities $T$ which are constant on each zone of $Z$. In practice we suppose that the boundary of a zone in $Z$ is made of edges or diagonals of cells of $T$. The degrees of freedom of the transmissivity to be estimated are the values of the transmissivity in each zone of $Z$. We want this number to be significantly lower than the number of elements in $T$.

Our goal is that the refinement and coarsening indicators technique will allow us to construct $Z$ with the lowest possible number of zones. Given a current parameterization partition, these indicators will tell us where to insert new discontinuities of the transmissivity and which ones can be removed.

### 1.1 Refinement indicators

We shall describe refinement indicators on an example. Let $(P_1)$ be an initial problem where the hydraulic transmissivity is constant in all the domain (figure 1(b)). So we have only one value of the transmissivity to estimate, which is done by minimizing the one variable misfit function $J$. We note $(P_2)$ the parameter estimation problem where we consider that the domain is made of two zones $Z_1$ and $Z_2$ having different transmissivities (figure 1(c)). We note $T^* = (T_1^*, T_2^*)$ the solution of $(P_2)$ obtained by minimizing the corresponding two variable misfit function. If $B = T_1^* - T_2^*$ were known, then the solution of minimizing $J$ under the constraints $T_1 - T_2 = B$ is necessarily $T^* = (T_1^*, T_2^*)$, the solution of $(P_2)$ and, if $B = 0$ then $T = T_1^* = T_2^*$ is the solution of $(P_1)$.

In general if we introduce $n$ new transmissivity values to estimate, the constraint condition $T_1 - T_2 = B$ is generalized to




(a) Computing mesh $T$ — (b) Partition $Z^1$ associated to problem $(P_1)$ — (c) Partition $Z^2$ associated to problem $(P_2)$

Figure 1. An example of parameterization refinement

$AT = B$ where $B$ is the discontinuity vector $(\sigma_{i,i+1})_{1\leq i\leq n}$ and $A$ is an $n\times(n+1)$ matrix with rank n defined by

$$A = \begin{bmatrix} 1 & -1 & 0 & 0 & . & . & . \\ 0 & 1 & -1 & . & . & . & . \\ 0 & 0 & 1 & -1 & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & . & . & 1 & -1 & \end{bmatrix}.$$

To the problem of minimizing the misfit function under these constraints $J(T^*) = \min_{AT=B} J(T)$, we associate the Lagrangian function defined by

$$L_B(T,\lambda) = J(T) + <\lambda, AT - B> \tag{4}$$

where $\lambda$ is the Lagrange multiplier associated to the constraint $AT = B$. Then the Lagrange condition ensures that $T^*$ is obtained by solving

$$\begin{aligned} &\frac{\partial L_B}{\partial T}(T^*,\lambda^*) = \nabla J(T^*) + A^T\lambda^* = 0, \\ &\frac{\partial L_B}{\partial \lambda}(T^*,\lambda^*) = AT^* - B = 0. \end{aligned} \tag{5}$$

If we denote by $J_B^* = J(T^*) = L_B(T^*,\lambda^*)$ the optimal misfit associated to the right hand side $B$ of the constraint, we deduce from (4) and (5) that

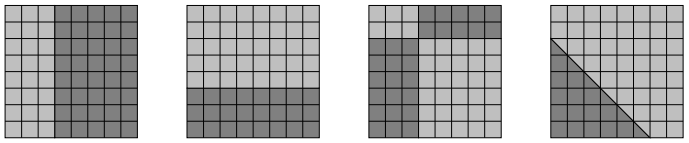
$$\frac{\partial J}{\partial B}|_{B=0} - \lambda^* = \frac{\partial L}{\partial B}(T^*,\lambda^*)|_{B=0} = 0. \tag{6}$$

Therefore the Lagrange multiplier gives us the sensitivity of the optimal data misfit $J_B^*$ to the perturbation $B$. For this reason we call $\lambda^*$ a refinement indicator. It can be easily deduced from equation (5). In the case of our example, to the refinement shown in fig. 1(c) we associate an indicator

$$\lambda^* = \frac{\partial J}{\partial T_1}(T^*) = -\frac{\partial J}{\partial T_2}(T^*). \tag{7}$$

And without solving $(P_2)$, this indicator indicates if the suggested refinement in figure 1(c) is likely to induce an important decrease of the misfit function.

One can see that we define such a refinement by introducing a curve (the boundary of $Z_2$ in fig. 1(c)). Such a curve is called a cut and divides the domain into only two zones of different transmissivities. In practice, we will use only the cuts shown in fig. 2.



(a) (b) (c) (d)

Figure 2. Four elementary cuts: (a) vertical, (b) horizontal, (c) checkerboard, (d) oblique

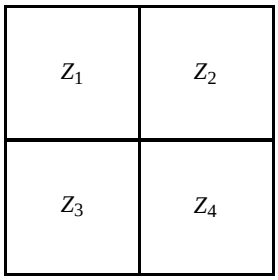



Figure 3. A four zone parameterization partition

The suggested refinement may also consist in dividing the domain in four zones of different transmissivities like in fig. 3. Then discontinuities between values of transmissivity in different zones can be writen:

$$\sigma_{1,2} = T_1 - T_2, \quad \sigma_{2,4} = T_2 - T_4, \quad \sigma_{3,4} = T_3 - T_4, \quad \sigma_{1,3} = T_1 - T_3.$$

These four equations are not independant, as we have $\sigma_{1,2} - \sigma_{3,4} = \sigma_{1,3} - \sigma_{2,4}$. Therefore they correspond to only three independant constraints which we write as

$$\begin{aligned} &(T_1 + T_3) - (T_2 + T_4) = \sigma_V \\ &(T_1 + T_2) - (T_3 + T_4) = \sigma_H \\ &(T_1 + T_4) - (T_2 + T_3) = \sigma_C. \end{aligned} \tag{8}$$

The first equation in (8) corresponds to a refinement given by a vertical line ($T_1 = T_3, T_2 = T_4$) dividing our domain into two zones, such line is called a "cut". The second one corresponds to a horizontal cut ($T_1 = T_2, T_3 = T_4$) and the third one corresponds to a checkerboard cut ($T_1 = T_4, T_2 = T_3$).
The matrix $A$ corresponding to constraints (8), is now

$$A = \begin{bmatrix} 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}.$$

Using the first equation in (5), we deduce that the associated La-

grange multiplier $\lambda = (\lambda_V, \lambda_H, \lambda_C)$ satisfies

$$\begin{aligned}
\lambda_V + \lambda_H + \lambda_C &= -\frac{\partial J}{\partial T_1}(T^*),\\
-\lambda_V + \lambda_H - \lambda_C &= -\frac{\partial J}{\partial T_2}(T^*),\\
\lambda_V - \lambda_H - \lambda_C &= -\frac{\partial J}{\partial T_3}(T^*),\\
-\lambda_V - \lambda_H + \lambda_C &= -\frac{\partial J}{\partial T_4}(T^*).
\end{aligned} \tag{9}$$

$\lambda_V$, $\lambda_H$ and $\lambda_C$ are the refinement indicators associated respectively to the vertical, horizontal and checkerboard cuts. Obviously we have

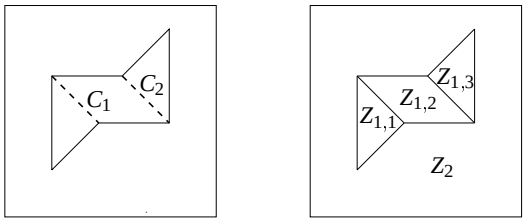
$$0 = \frac{\partial J}{\partial T_1}(T^*) + \frac{\partial J}{\partial T_2}(T^*) + \frac{\partial J}{\partial T_3}(T^*) + \frac{\partial J}{\partial T_4}(T^*) = \frac{\partial J}{\partial T}(T^*)$$

since $T^*$ is the minimizer for problem $(P_1)$ where the parameter is constant over the whole domain.

Given a current partition $Z$ and once the gradient of $J$ is calculated, refinement indicators can be calculated from (7) in a computationally inexpensive way for a large number of cuts. Only a few degrees of freedom corresponding to the cuts with the largest indicators $|\lambda^*|$ are selected. The degree of freedom finally added to the current parametrization is that which gives the largest actual decrease of the misfit function among those selected according to the size of $|\lambda^*|$.

### 1.2 Coarsening indicators

Consider the example shown in fig. 1, and suppose that in a first step the cut represented in fig. 1(c) is selected: the partition $Z$ contains two zones, an interior zone $Z_1$ and an exterior zone $Z_2$, with the corresponding optimal values of transmissivity $T_1^*$ and $T_2^*$. Suppose that refinement indicators corresponding to various positions and forms of cuts have been computed and that two cuts $C_1$ and $C_2$ in the interior zone have been selected (fig. 4 left). Therefore the cut defining the interior zone (its boundary) is divided into several subcuts, i.e. the boundaries $\partial Z_{1,1} \cap \bar{Z_2}, \partial Z_{1,2} \cap \bar{Z_2}$ and $\partial Z_{1,3} \cap \bar{Z_2}$ in fig. 4 right. The question now is " should we keep all the cuts, or are some of the subcuts sufficient to give the expected decrease of the misfit function?". Our goal now is not to choose new degrees of freedom to add, but to test if some of those considered are overabundant. Therefore we have to study the influence of removing each subcut on the optimal value of the misfit function.
With the current parametrization of fig. 1(c), minimizing the two variable misfit function is equivalent, with the parametrization




Two selected cuts  New parametrization to study

Figure 4. A refinement for figure 1(c)

of fig. 4 right, to minimizing $J(T_{1,1}, T_{1,2}, T_{1,3}, T_2)$ under the constraints

$$\begin{aligned}
T_{1,1} - T_2 &= T_1^* - T_2^*,\\
T_{1,2} - T_2 &= T_1^* - T_2^*,\\
T_{1,3} - T_2 &= T_1^* - T_2^*.
\end{aligned} \tag{10}$$

We can write these constraints using matrix form as

$$\begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} T_{1,1} \\ T_{1,2} \\ T_{1,3} \\ T_2 \end{bmatrix} = \begin{bmatrix} T_1^* - T_2^* \\ T_1^* - T_2^* \\ T_1^* - T_2^* \end{bmatrix}.$$

Aggregating for example the two zones $Z_1^1$ and $Z_2$ is equivalent to set to 0 the righthand side of the first constraint:

$$\begin{aligned}
T_{1,1} + T_2 &= 0,\\
T_{1,2} + T_2 &= T_1^* - T_2^*,\\
T_{1,3} + T_2 &= T_1^* - T_2^*.
\end{aligned} \tag{11}$$

The effect, at first order, of this aggregation on the optimal data misfit is measured by the corresponding Lagrange multiplier

$$\lambda_{1,1}^{2*} = -\frac{\partial J}{\partial T_{1,1}}(T_1^*, T_2^*). \tag{12}$$

Similarly the effects of aggregating $Z_{1,2}$ with $Z_2$ and $Z_{1,3}$ with $Z_2$ are measured respectively by

$$\begin{aligned}
\lambda_{1,2}^{2*} &= -\frac{\partial J}{\partial T_{1,2}}(T_1^*, T_2^*),\\
\lambda_{1,3}^{2*} &= -\frac{\partial J}{\partial T_{1,3}}(T_1^*, T_2^*).
\end{aligned} \tag{13}$$

Notice that one has

$$\lambda_{1,1}^2 + \lambda_{1,2}^2 + \lambda_{1,3}^2 = \frac{\partial J}{\partial T_2}(T_1^*, T_2^*) = 0.$$

The $\lambda_{1,i}^{2*}, i = 1..3$ are numbers associated to the subcuts of the cut defining the interior zone. Computing these indicators allows us to keep or to remove some subcuts, according to their values and their signs. For this reason we call these indicators "coarsening indicators".

### 1.3 Algorithm

We have used the refinement and coarsening indicators introduced above, for several numerical studies according to the following algorithm:

1. Choose an initial parameterization partition $Z$.

2. **Do** until data are satisfactorily fitted:

   3. Compute transmissivity with current parameterization partition $Z$ by minimizing $J$.

   4. **For** every part $Z_i$ of $Z$ **do**

      Compute the refinement indicators $I$ corresponding to tested cuts in $Z_i$.

      **Enddo**

   5. Compute $I_{max}$ the largest absolute value of all computed refinement indicators in all parts $Z_i$. Select all cuts corresponding to refinement indicators which are larger than 80% of $I_{max}$ (this percentage can be adjusted)

   6. **If** some of these cuts generate subdomains with more than one connected component **then**

      Compute the refinement indicators corresponding to the subcuts associated to each connected component.

      Update the set of selected cuts according to the 80% rule.

      **Endif**

   7. **If** the selected cuts or a priori information suggest a refinement pattern to the interpreter **then**

      Compute the corresponding refinement indicator, and update the set of selected cuts.

      **Endif**

   8. Minimize $J$ successively with all parameterizations associated to all selected cuts.

   9. Keep only the selected cuts which induce a decrease of $J$ larger than 80% of the largest one

   10. **If** two or more selected cuts divide the same part $Z_i$ **then**

      Compute the corresponding coarsening indicators.

      Aggregate the subdomains where coarsening indicators allow it.

      **Endif**

   11. Update the current partition by refining according to the selected refinement and coarsening indicators. This produces the new partition $Z$

12. **Enddo**

## 2 NUMERICAL EXPERIMENTS

Numerical experiments have been performed in several simple situations. There correspond to synthetic examples in which we try to recover two or three transmissivity values and the zones where they take these values (the range of this values go from 5 to 20). In all examples boundary and initial data are zero and the righthand side $Q$ of equation (1) is constant in space and time. The piezometric heads are measured in the whole domain and at all time.

In the following figures the transmissivity values are represented with a grey scale and the discretization of the domain – a $6 \times 6$ rectangular grid – is shown as well as the cuts or the parametrization partitions obtained.

### 2.1 Case of a central inclusion

We begin our numerical study by the case of a central inclusion (fig. 5). We suppose that the initial transmissivity is constant in the whole domain (fig. 6) and minimize the misfit function according to this parameterization.

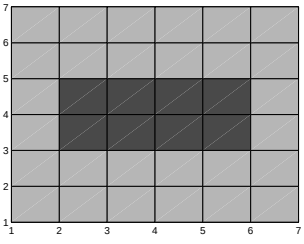



Figure 5. Exact transmissivity: unknown of the inverse problem

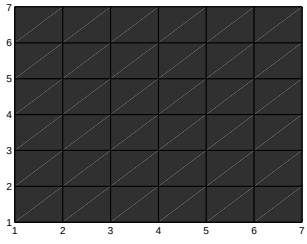



Figure 6. Initial transmissivity

The different absolute values of refinement indicators are represented in fig. 7. The largest values correspond to four checkerboard cuts, so we pass to step 6 of the algorithm, and we compute the refinement indicators corresponding to corner subcuts of the checkerboard cuts (there are four corner subcuts for each checkerboard cut).

Four of these subcuts represented by the symbols *, x, • and ∘, are selected (fig. 8). According to step 7 of the algorithm, we compute the refinement indicator corresponding the aggregated cut formed by these corners (symbol □ on fig. 7) and we observe that it has the largest absolute value of all computed refinement indicators. Therefore we select the corresponding cut and we obtain at the end of this first iteration the partition shown in fig. 9.

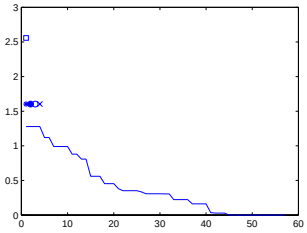
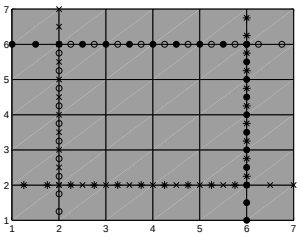


Figure 7. Computed absolute values of refinement indicators in decreasing order



∘: Top left, x: Bottom left
•: Top right, *: Bottom right

Figure 8. The 4 corner cuts corresponding to the largest absolute values of computed refinement indicators

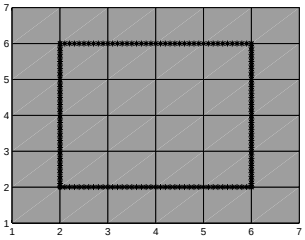


Figure 9. Partition obtained at the end of the first iteration

For the second iteration we begin by minimizing the misfit function, considering the parameterization partition obtained at the first iteration. Then we compute refinement indicators (fig. 10) and we observe that their highest absolute value corresponds to two cuts which divides the central zone into three parts (fig.11). The three corresponding coarsening indicators are computed, their absolute values showed in fig. 10 by the symbol $*$. Therefore only the middle part, corresponding to the largest value, is selected and we obtain the new partition shown in fig. 12.

At the beginning of the third iteration, after minimization, the misfit function vanishes up to machine precision, with transmissity values that correspond to the exact ones (fig.13).

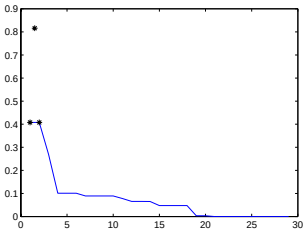


Figure 10. Computed absolute values of refinement indicators and three coarsening indicators (* symbol)

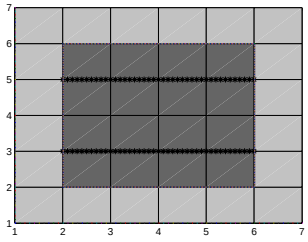


Figure 11. Computed transmissivity calculated on the partition shown in fig. 9 and selected cuts

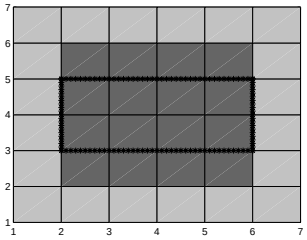


Figure 12. Partition obtained at the end of the second itération

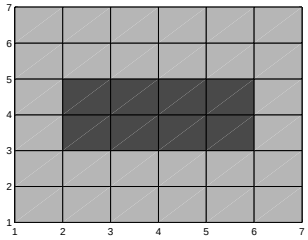


Figure 13. Optimal transmissivity computed with partition shown in fig. 12 is equal to the exact transmissivity

## 2.2 Case of an off center inclusion

An other case that we have studied is that of an off center inclusion (fig. 14). We start with the same constant initial transmissivity as in the previous case (fig. 6) and we proceed in the same manner as in the previous case. Figures 15, 16, 17, 18, 19 show the partitions obtained at each iteration and the transmissivity calculated on these partitions.

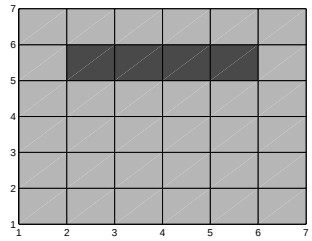


Figure 14. Exact transmissivity: unknown of the inverse problem

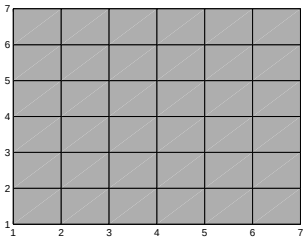


Figure 15. Transmissivity computed as a constant

We remark observing fig. 19 that the optimal transmissivity is recovered even though the partition has four zones instead of two. However we note that the number of zones (4) is quite smaller than the number of calculation cells (64), which shows the interest of the method.

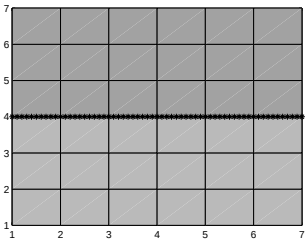


Figure 16. Partition obtained at the first iteration and the corresponding computed transmissivity

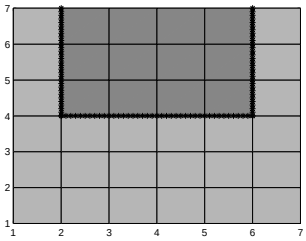


Figure 17. Partition obtained at the second iteration and the corresponding computed transmissivity

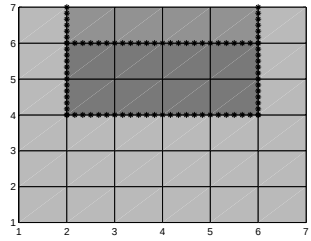


Figure 18. Partition obtained at the third iteration and the corresponding computed transmissivity

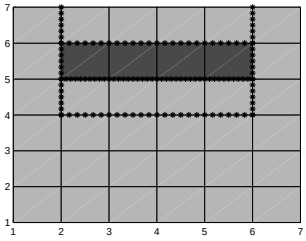


Figure 19. Partition obtained at the fourth iteration and the corresponding computed transmissivity

### 2.3 Case of a three zone transmissivity

The last case that we consider here is that of three zones of transmissivity as in fig. 20. Again we start with a constant transmissivity (fig. 6) and we follow the steps of the algorithm described in section 1.3. As in the previous case we show in figures 21, 22, 23, 24, 25 the partitions obtained at each iteration and the transmissivity calculated on these partitions.

In this case one notice, observing fig. 25, that only a close approximation of the exact partition and transmissivity is recovered.

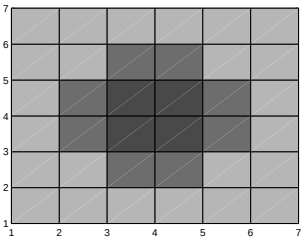


Figure 20. Exact transmissivity: unknown of the inverse problem

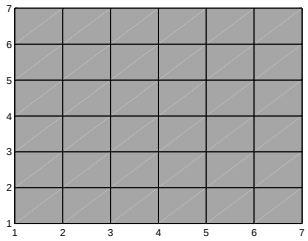


Figure 21. Transmissivity computed as a constant

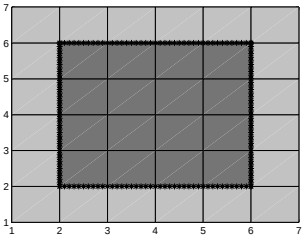


Figure 22. Partition obtained at the first iteration and the corresponding computed transmissivity

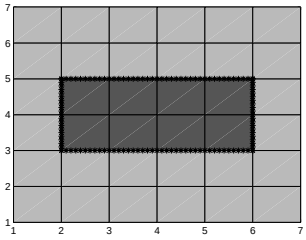


Figure 23. Partition obtained at the second iteration and the corresponding computed transmissivity

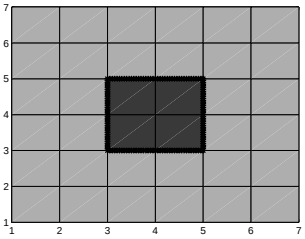


Figure 24. Partition obtained at the third iteration and the corresponding computed transmissivity

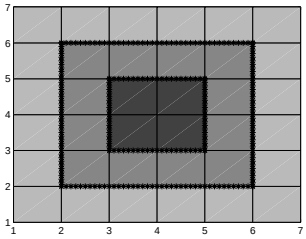


Figure 25. Partition obtained at the fourth iteration and the corresponding computed transmissivity

## 3 CONCLUSION

We presented a procedure for calculating transmissivity whose parameterization is constructed iteratively. The transmis-

sivity is a piecewise constant function of space defined on a partition of the domain which is also an unknown of the problem.

An algorithm based on indicators for refining or coarsening this partition has been tried with success in simple situations. Further work will attack more realistic situations.

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