Hierarchical coarse-graining transform

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We present a hierarchical transform that can be applied to Laplace-like differential equations such as Darcy's equation for single-phase flow in a porous medium. A finite-difference discretization scheme is used to set the equation in the form of an eigenvalue problem. Within the formalism suggested, the pressure field is decomposed into an average value and fluctuations of different kinds and at different scales. The application of the transform to the equation allows us to calculate the unknown pressure with a varying level of detail. A procedure is suggested to localize important features in the pressure field based only on the fine-scale permeability, and hence we develop a form of adaptive coarse graining. The formalism and method are described and demonstrated using two synthetic toy problems.

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I. INTRODUCTION

A combination of phenomena taking place at multiple scales in time and space is ubiquitous in many fields of science. The hierarchical transform that will be presented in this paper can be applied to a wide variety of problems that can be expressed by a matrix eigenvalue problem deriving from the discretization of a differential equation. The method is applied to Laplace-like differential equations where flux is proportional to a spatially varying quantity multiplied by a potential gradient. This is the case when calculating flow through a porous medium with varying permeability, when calculating current through a mesh of resistors or heat transfer in a material of varying thermal conductivity and also in the calculation of mechanical properties of solids. In general terms, whenever a Dirichlet boundary condition is given in the calculation of the potential in such systems, this method will allow one to obtain this potential with an adaptive spatial resolution, keeping details only where needed and reducing the computational time. Having an approximation for the potential, the flux will be easily calculated on the desired scale. It is possible that the same approach could be successful when tackling other kinds of differential equations, leading to interesting applications.

Certainly a good example where such an approach is desirable are the geological systems that are the focus of attention of flow in porous media studies. Commonly, the information available on these systems is at a scale different from the one which is relevant for the purpose of understanding or modeling the systems dynamics. For this reason, a very well studied problem in the field is that of upscaling, where a fine-scale geological model is substituted by a coarser, more tractable model, on which flow calculations can be carried out efficiently. An error is inherent in all upscaling procedures, and often choosing the correct level of coarse-graining is key to preserving the model accuracy. A recent attempt to estimate the optimal scale-up factor is presented in Zhang *et al.* [1]. An alternative to upscaling is multiscale flow simulation, where an attempt is made to capture the flow at the large scale while including the effects of the small-scale heterogeneity. A key concept in both these approaches is that of adaptive gridding—that is, the idea of keeping a finer grid around the areas where important flow patterns need to be captured and using a coarser mesh away from them [2]. Aarnes and Efendiev [3] pointed out the importance of large-scale features and barriers to guide the adaptivity of the grids. One of the important factors in assessing the quality of a grid is whether the properties within the cells are sufficiently uniform. An adaptive grid refinement strategy, in which the grid is dynamically adapted to ensure convergence, was discussed in [4]. The starting point is a Cartesian grid with anisotropic refinement around connected high-permeability flow paths [5,6]. One issue in designing adaptive grids arises when trying to identify the areas which require a fine mesh. Intuitively, regions where the flow is high will likely have important details that have a major influence on the flow pattern [7]. This requires a preliminary single-phase flow simulation to identify the areas of high flow. There are also advantages in orienting the grid according to this approximate flow scenario, which sometimes justifies performing the flow calculation as a first step of an upscaling method. In the present work we will assume that no flow information is known before the upscaling is performed.

Aarnes *et al.* [8] present an elegant extension of the multiscale mixed finite-element method formalism to deal with hierarchical corner-point grids. These types of grids are the preferred choice to represent complex reservoir geology, but it could be argued that adaptivity with anisotropic refinements is an equally valid approach. Recently, a promising upscaling scheme suggests to use adaptive stencils in the finite-element calculation of fluxes. Lambers *et al.* [9] use a multipoint flux approximation where the stencil varies to revert to two-point flux approximation where the flow is more

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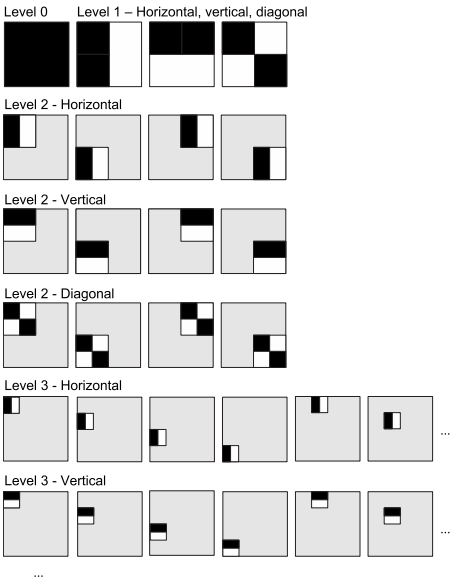

FIG. 1. A pictorial representation of the hierarchical scheme underlying the structure of **H**. Each row of this diagram is composed of squares of equal size. Each of the squares refers to a single row in the **H** matrix. We will consider each row as acting independently on the pressure vector. Each square contains the elements of the corresponding row, written as a matrix (see Appendix B). The square in the top left corner contains the coefficients in the first row of **H**. These are all 1s. The result of multiplying this row by the pressure vector is the sum of all the pressures. On level 1, the system is grouped into 2×2 blocks. The three types of differences (horizontal, vertical, and diagonal) are calculated for each subset of the system (weights: 1=black, −1=white, 0=gray). For example, the level 1 horizontal difference is the difference between the averages of the pressure on the left and right halves of the system (see Appendix B). The number of rows assigned to level 2 is $2^2\times 3=12$—that is, 4 subsystems multiplied by 3 types of differences. Similarly at level 3, here only partially represented, there will be 48 rows, $(2^{3-1})^2$ subsets multiplied by 3 types of differences. At level i there will be $3\times(2^{i-1})^2$ rows and the total number of rows of the matrix for a $2d$ system of linear size N will be N^2, exactly the size of the pressure expressed as a vector. The matrix is then divided by N to ensure the top row gives the pressure average, and finally the rows must be normalized such that they are all orthonormal to the first one.

homogeneous. Here we will only consider Cartesian grids and for the moment only isotropic coarse graining. However, there is reason to believe that the following ideas could be applied in the context of corner-point geometries as well.

Whether the system of choice for solving the equations is finite volumes or finite differences, all these methods naturally lead to a hierarchical description of the system. Berg and Øian [10] propose a hierarchical approach to modeling faults and conclude that all scales are important for correct modeling of the flow. Even in the absence of faults, heterogeneities in the permeability play a similar role. It could be argued that it is actually fluctuations away from the average pressure at different scales which are responsible for the nontrivial flow patterns that can be observed in geological systems. Recently, a multiresolution approach based on *Fup* basis functions which guarantee an adaptive solution to problems with different spatial and temporal scales, has been proposed [11].

Wavelets are often used to highlight the hierarchical components of a signal, and indeed the transform we propose is inspired by a discrete Haar wavelet transform [12]. The Haar basis, the simplest of wavelet bases, decomposes a function into averages and differences at different scales. When this is applied to a two-dimensional field, it gives rise to three types of differences, which we have called vertical, horizontal, and diagonal for simplicity. Contrary to a two-dimensional Haar wavelet transform, our hierarchical transform can be applied with a single matrix product and can therefore be used in a formalism similar to the one introduced in [13]. We refer the reader to [14] for a similar Haar wavelet approach to hierarchical coarse graining.

The paper is organized as follows: Section II is a brief introduction to single-phase flow in porous media. In Sec. II A, the transform is introduced and the formalism to apply it to Darcy's equation is shown; in Sec. III, an approach to calculating the pressure solution at different scales is demonstrated. Section IV shows how the method can be used to obtain nonuniform adaptively coarse-grained pressure profiles, while Sec. V discusses the advantages and problems of the method and possible further developments. In Appendix A, more details on the implementation of the transform are given.

II. PROBLEM

To illustrate the application of the hierarchical transform to a specific problem, we will calculate pressure in a porous medium with single-phase flow and known permeability values. This is done by setting to zero the divergence of flux, which is given by Darcy's law: $\mathbf{q}=-\mathbf{K}\cdot\nabla P$, where $\mathbf{q}$ is the flux, $\mathbf{K}$ is permeability, and ∇P is the gradient of pressure. Imposing flux conservation $\nabla\cdot\mathbf{q}=0$ gives rise to a Laplace-like differential equation $\nabla\cdot(\mathbf{K}\cdot\nabla P)=0$. In the most general case, permeability is a tensor, but we will consider it a diagonal tensor, as would be true for isotropic media. We consider the case where we solve this equation on a discretized Cartesian grid, approximating it with a five-point finite-difference scheme. The discretization is performed by specifying the permeability values at the cell centers and assuming pressure to be piecewise linear across the cell. In the following we will use transmissibility, which is equal to permeability in the case of unit volume of the discretization grid cell: $t_i=k_i/\Delta x$, where $\Delta x=1$ is the size of the grid cell. Assuming transmissibility t_i to be piecewise constant with an interface between t_i and t_{i+1} at the cell boundary and imposing flow conservation, the intercell transmissibility t_{ij} is found to be the harmonic mean of t_i and t_j. This constitutes a satisfactory approximation if the properties do not change excessively between adjacent cells [15]. The flow equation under this discretization scheme can thus be expressed with the matrix equation

$$\mathbf{TP}=\mathbf{R}. \tag{1}$$

Here, for a d-dimensional system of linear size N, $\mathbf{T}$ is a $N^d\times N^d$ transmissibility matrix, $\mathbf{P}$ is an $N^d\times 1$ pressure vector, and $\mathbf{R}$ is an $N^d\times 1$ boundary condition vector [15,16]. The calculation of pressure can thus easily be performed inverting the transmissibility matrix.

A. A hierarchical transform

Many hierarchical transforms can be defined. To start with, we focus on the requirements imposed by the fact that

we need to apply it to the finite-difference form of the single-phase flow equation, described above. We need to apply the transform to a pressure vector, which contains the pressure values of a two-dimensional system of linear size N, arbitrarily vectorized columns first, such that pressure value 1 is in the top left corner of the grid, pressure 2 is just below it, and pressure $N+1$ is to the right of pressure 1, leaving pressure N^2 in the bottom right corner. This will be the numbering scheme used throughout the paper for the pressure. We require that the transform be a simple matrix operation and that its order be equal to the square of the linear system size.

B. H matrix and its properties

The aim of using this transformation is to represent each value of pressure as the sum of a pressure average plus fluctuations at different scales, given by differences. The Haar basis is at the heart of the transformation, and this, in two dimensions, leads to three possible types of differences: horizontal, vertical, and diagonal. These differences are used to describe the type of fluctuations in different areas of the system and at different scales. The system is thus described at different levels, where we define a level for a system of linear size N in the following manner: level 0 will correspond to a single value, an estimate of the spatial average of the pressure over the whole system; at level 1, we will be able to distinguish 4 values of pressure, as in a 2×2 system, level 2 will give us 16 values of pressures, as in a 4×4 system, and in general, level i will be equivalent to a system of size $2^i\times2^i$ (see Fig. 2). The highest level corresponds to the fine scale and varies in size depending on the original system. A scheme of the different levels, representing the system at different scales, can be seen in Fig. 2. At level 0 we do not consider the differences; the pressure is approximated by a constant value which is an approximation of the pressure average. At level 1, we imagine the system to be on a 2×2 grid. Now, in addition to the pressure average, we can either take the difference between the two values on the left and the two on the right, which we call the horizontal difference, and the difference between the top two values and the bottom two, which is the vertical difference—respectively, the second and third squares in the first row in Fig. 1. Finally we can take the difference between the sum of the upper left and lower right blocks minus the sum of the lower left and upper right ones, the fourth square in the first row in the figure. At level 2 we imagine the system on a 4×4 grid and we consider the same type of differences on each 2×2 set, horizontal for the four sets, then vertical, and finally diagonal, rows 2, 3, and 4 of Fig. 1. We can repeat the operation until the system is at the fine scale. The operation of taking these differences on the pressure is encoded in the different rows of the transform matrix **H**, which has terms equal to 0, 1, or -1 with a normalization factor that ensures that the average is given by a row with all ones and that each row is orthonormal to the top one.

The **H** matrix for a 4×4 system is

$$\mathbf{H} = 1/4 \begin{bmatrix}
0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 \\
0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & 0.25 & -0.25 & -0.25 & -0.25 & -0.25 & -0.25 & -0.25 & -0.25 & -0.25 \\
0.25 & 0.25 & -0.25 & -0.25 & 0.25 & 0.25 & -0.25 & -0.25 & 0.25 & 0.25 & -0.25 & -0.25 & 0.25 & 0.25 & -0.25 & -0.25 \\
0.25 & 0.25 & -0.25 & -0.25 & 0.25 & 0.25 & -0.25 & -0.25 & -0.25 & -0.25 & 0.25 & 0.25 & -0.25 & -0.25 & 0.25 & 0.25 \\
0.5 & 0.5 & 0 & 0 & -0.5 & -0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.5 & 0.5 & 0 & 0 & -0.5 & -0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5 & 0.5 & 0 & 0 & -0.5 & -0.5 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5 & 0.5 & 0 & 0 & -0.5 & -0.5 \\
0.5 & -0.5 & 0 & 0 & 0.5 & -0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.5 & -0.5 & 0 & 0 & 0.5 & -0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5 & -0.5 & 0 & 0 & 0.5 & -0.5 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5 & -0.5 & 0 & 0 & 0.5 & -0.5 \\
0.5 & -0.5 & 0 & 0 & -0.5 & 0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.5 & -0.5 & 0 & 0 & -0.5 & 0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5 & -0.5 & 0 & 0 & -0.5 & 0.5 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5 & -0.5 & 0 & 0 & -0.5 & 0.5
\end{bmatrix}$$

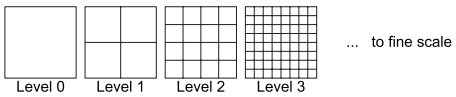

FIG. 2. A schematic representation of the different levels. Level 0 is always given by a single value for pressure. The highest level corresponds to the original fine-scale system.

On the largest scale, level 0, all the elements are 1. At level 1 the elements will be either 1 or −1 multiplied by the factors that ensure normalization. For the higher levels, only one block in the system is considered at any one time. The numbering scheme is always from left down first and then right (see Fig. 1). The three types of differences calculated at all the levels produce a transform matrix of order N^2 for a $2d$ system of linear size N, which matches our requirement that it must multiply a vector of size $N^2 \times 1$ (see Fig. 3).

One very important property of the **H** matrix is that it is a unitary matrix; that is, its transpose is identical to its inverse. For this reason, when we require the inverse of **H**, instead of performing a matrix inversion, we can simply use its transpose instead, saving considerable computational time. Moreover, the transform is linear, so the transform of the sum of two vectors is the same as the sum of the transforms.

Another useful property of this matrix is that its elements can be determined based on the binary representation of the number of the cell to which they refer (see Appendix A for a detail explanation of the algorithm to generate the transform matrix).

C. Transforming the transmissibility matrix

The question we would like to address is whether we can obtain a good estimate of the pressure without solving for it

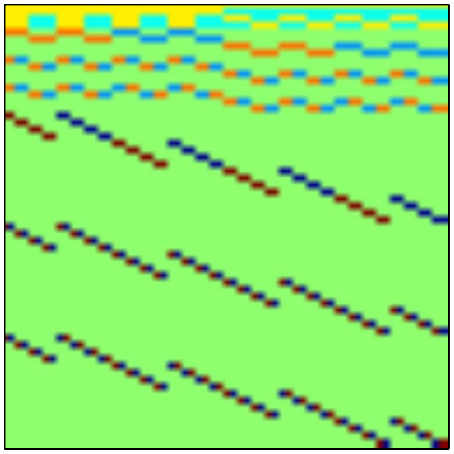

FIG. 3. (Color online) The hierarchical transform matrix **H** for an 8×8 system. We see here a 64×64 matrix. The first row refers to level 0, where the pressure average is recovered and the elements are all equal to 1. The next three rows correspond to the level-1 differences: horizontal, vertical, and diagonal, respectively. The rows at level i are ordered by type of difference and by location, down then right. The different colors indicate the different size of the elements due to the normalization acting on the coefficients that are either 1 or −1. Green areas (uniform gray background in black and white) are elements equal to zero.

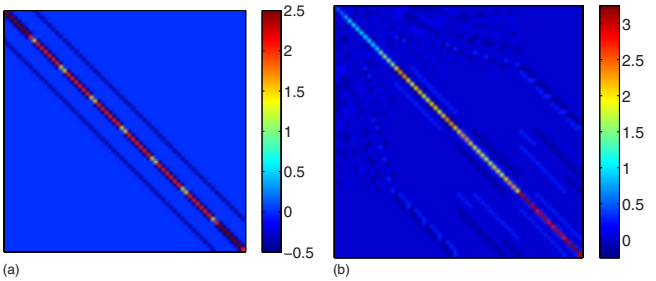

FIG. 4. (Color online) (a) The fine-scale transmissibility matrix for an 8×8 system of homogeneous unit permeability **T**. (b) The transformed transmissibility matrix $\mathbf{T}' = \mathbf{HTH}^{\mathbf{T}}$. Notice the interesting structure of the non-zero elements off the main diagonal (more clearly visible in the online version).

on the fine scale. To this purpose, we apply the hierarchical transform to Eq. (1):

$$\mathbf{TP} = \mathbf{R} \Leftrightarrow \mathbf{TH}^{\mathbf{T}}\mathbf{HP} = \mathbf{R}. \tag{2}$$

To complete the equation transformation, we multiply by **H** on both sides to obtain a new transmissibility matrix and a new boundary condition vector applied to the transformed pressure:

$$(\mathbf{HTH}^{\mathbf{T}})\mathbf{HP} = \mathbf{HR}. \tag{3}$$

Defining the transformed variables

$$\mathbf{T}' = \mathbf{HTH}^{\mathbf{T}}, \tag{4a}$$

$$\mathbf{P}' = \mathbf{HP}, \tag{4b}$$

$$\mathbf{R}' = \mathbf{HR}, \tag{4c}$$

we obtain

$$\mathbf{T}'\mathbf{P}' = \mathbf{R}'. \tag{5}$$

The transformed pressure vector $\mathbf{P}'$ has as its elements the pressure average followed by the differences of pressure in the different directions and at different levels. For example, for a 2×2 system with the previously described numbering scheme, $\mathbf{P}' = 1/4[p_1+p_2+p_3+p_4, p_1+p_2-p_3-p_4, p_1+p_3-p_2-p_4, p_1+p_4-p_2-p_3]^T$, where only level 0 and level 1 can be obtained because level 1 is already the fine-scale system. For larger systems, truncating the transforms of the transmissibility matrix and the boundary condition, we can obtain an estimate of pressure including details up to a specific level, corresponding to the scale we are interested in. The original and transformed transmissibility matrices are shown for an 8×8 system in Fig. 4.

In Pancaldi *et al.* [13] the same approach was carried out using a one-step Haar wavelet transform instead of the hierarchical matrix transform described above. In that case, the structure of the transformed matrix allowed us to develop a simple upscaling rule to coarsen the system progressively. The appearance of blocks within the transformed matrix having the same structure as the original matrix enabled the elements of the two matrices to be related. This stemmed from the fact that both the fine- and coarse-scale solutions obey Eq. (1). In this case, such a procedure is not possible,

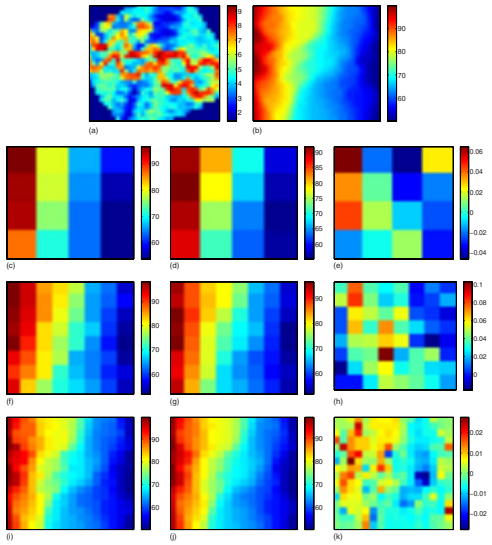

FIG. 5. (Color online) Comparison between pressure estimates and averages at a specific level (levels 2, 3, and 4). (a) Logarithm of the permeability map, 32×32 subset of the SPE10 data set [17]. (b) Fine-scale pressure solution, flow from left to right. (c) Estimated pressures at the specified resolution from inversion of the corresponding portion of the $\mathbf{T}'$ matrix. (d) Average of the fine-scale pressure solutions. (e) Relative difference between the average and the estimate.

because the nonzero difference terms change the equation relating flux to pressure. What we will do instead is to concentrate on Eq. (5) to study ways of extracting approximate estimates of pressure with the least computational effort.

III. PRESSURE SOLUTIONS: SOLVING FOR PRESSURE AT DIFFERENT SCALES

While the effect of $\mathbf{H}$ on the transmissibility is not obvious, its effect on the pressure is very clear and can be exploited. As we intended, we now have a hierarchical description of the pressure solution. We are at freedom to recover the original pressure including the desired level of detail. This is achieved simply by taking as our new transmissibility matrix the portion of $\mathbf{T}'$ that corresponds to the finest level of detail that we want to keep in the pressure. If all we are interested in is an estimate of the pressure average over the whole system, we just need to divide the first element of the boundary condition vector by the top left element of $\mathbf{T}'$ (level 0). The estimate will be accurate only if the pressure is approximately constant, because at level 0 we consider the pressure fluctuations to be negligible. This might not be of great use, but we should remember that this can be achieved without ever calculating the pressure on the fine scale.

More likely we are interested in some coarse but not single-valued representation of pressure. Assume that we start with a fine-scale system of size $N\times N$. In this case we could take the inverse of the 4×4 upper left corner of $\mathbf{T}'$ and the first four elements of the boundary condition vector. What we obtain is the transformed pressure on a 2×2 grid. To obtain the actual pressure values, we need to apply the inverse of the hierarchical transform for a system of the

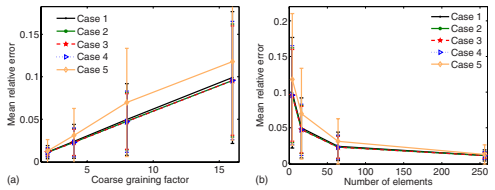

FIG. 6. (Color online) Discrepancy in pressure estimate for different levels of coarse graining. (a) Mean relative error vs coarse graining factor. Notice how the linear relationship does not have a strong dependence on the details of the permeability maps, which differ in each case. An overall linear fit to the data gives the equation $y=0.006x-0.001$. The only curve that does not fall on this line is the one where we have halved the correlation length and where the σ/μ ratio was consequently increased (case 5). (b) Mean relative error vs the number of elements kept. Again, case 5 is the only one not overlapping with the other curves.

original size to a vector containing the filtered transformed pressure values and zeros in all the other elements. This is easily done using the transpose of $\mathbf{H}$. The result will be an $N\times N$ pressure map with only four different values of pressure as in a 2×2 system (level 1). How does this approximation relate to the fine-scale pressure? It can be shown, and it is also expected given our experience with the $\mathbf{W}$ transform in Pancaldi *et al.* [13], that this 2×2 coarse pressure is an estimate of the average of the $N\times N$ fine-scale one, averaged $N/2\times N/2$ cells at a time.

As shown in Fig. 5, there is a correspondence between the approximations that can be obtained by inverting larger and larger portions of the transformed transmissibility matrices and the pressure averages that can be obtained averaging fewer and fewer cells at a time.

An interesting comparison can be made between the estimates of pressure at different scales and the fine-scale solution. To assess the relationship between the error in the estimates and the level of the representation, an ensemble of 30 log-normally correlated permeability realizations was generated for 5 separate cases. The permeability distribution is characterized by mean μ, standard deviation σ, and correlation length ξ. Starting from case 1, cases 2 and 3 were obtained by increasing the average permeability keeping the σ/μ ratio and the correlation length constant. Cases 4 and 5 are obtained by, respectively, decreasing and increasing the average permeability as the correlation length is, respectively, doubled or halved. Figure 6 shows an analysis of the error in the estimate of pressure as a function of the coarse-graining factor. Since our estimates of pressure at all scales are expressed on a fine grid, we can compare them directly to the fine-scale solution (see Fig. 7). We define the coarse-graining factor N_{CG} as the initial linear system size divided

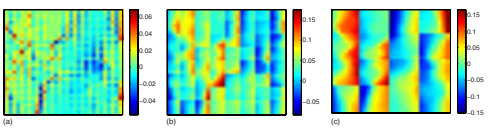

FIG. 7. (Color online) Differences between estimates of pressure at different scales and the fine-scale solution. (a) $N_{\mathrm{CG}}=2$ (level 4). (b) $N_{\mathrm{CG}}=4$ (level 3). (c) $N_{\mathrm{CG}}=8$ (level 2).

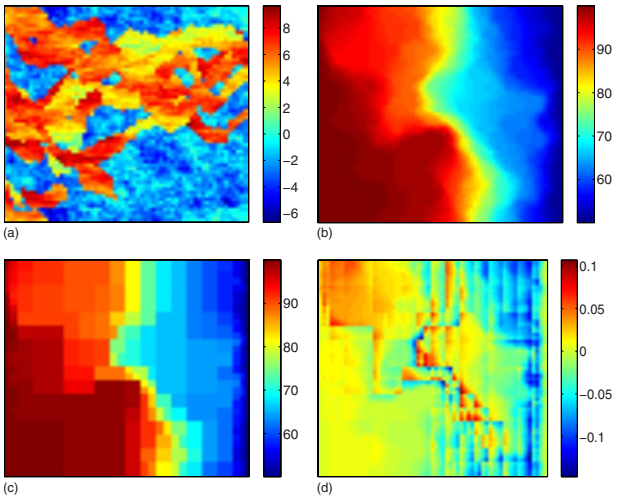

FIG. 8. (Color online) Nonuniform coarse graining based on keeping only the largest elements in the transform of pressure $\mathbf{P}'$. (a) Logarithm of the fine-scale permeability, 64×64 subset of SPE10 [17]. (b) The fine-scale pressure solution. (c) An estimate of pressure keeping only 442 out of the 4096 elements of $\mathbf{P}'$. (d) Relative error between fine-scale solution and estimate in (c).

by the linear size at the specific level i: $N_{\mathrm{CG}}=N/2^i$.

In conclusion, the pressure can be calculated with any degree of detail, depending on the computational power available or the specific requirements.

IV. NONUNIFORM COARSE GRAINING

So far, the coarse graining of the pressure profile has been uniform in space. In heterogeneous systems it is expected that different areas will require different levels of details to achieve a satisfactory approximation of the pressure field. Ultimately, we would like to be able to reduce the size of the matrix to be inverted not simply by eliminating fine-scale detail everywhere, but being able to keep different scale coefficients in different locations.

In the context of a full-field reservoir simulation, the obvious regions where a high level of detail should be kept are around the wells, or at the location of geological features of considerable importance. However, on a smaller scale, we might not have anything but the permeability map to decide where to keep the details.

One possibility to provide a criterion for which areas should be preserved in more detail is to perform a coarse pressure and flow calculation. Once the main flow paths have been identified, the nonuniform pressure solution can be calculated. Although this is a fairly common technique in the adaptive mesh refinement literature [7], an attempt will be made to avoid any flow simulations prior to the nonuniform pressure solution.

To gain some insight, we can look at the size of the elements in the hierarchical transform of the pressure, $\mathbf{P}'=\mathbf{HP}$. Clearly this can only be done in the developing stage of the method, where we are allowed to know the pressure on the fine scale and hence its transform. Keeping only the elements in $\mathbf{P}'$ above a certain arbitrary threshold, we notice how,

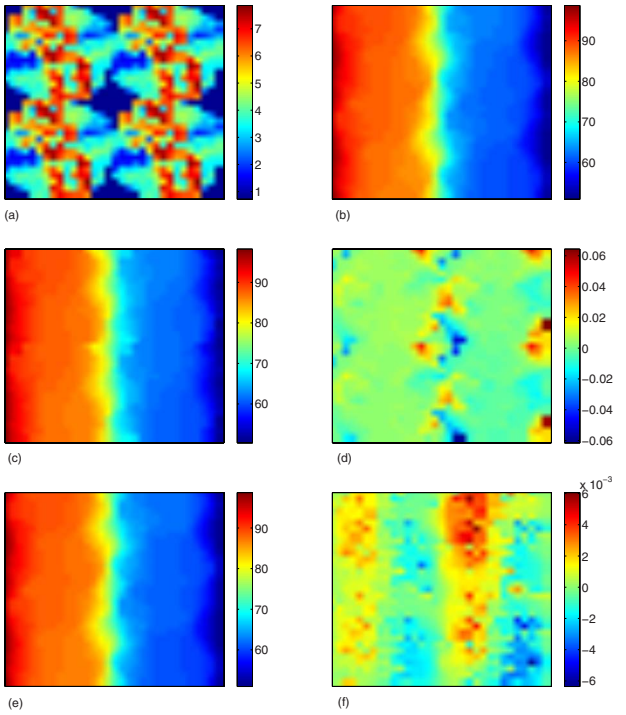

FIG. 9. (Color online) Analysis of the importance of diagonal differences. (a) Fine-scale permeability map, 32×32, modified subset of the SPE10 data set [17]. (b) Fine-scale pressure solution. (c) Estimate of pressure by eliminating coefficients referring to diagonal differences (keeping 683/1024 elements). (d) Relative error between the pressure estimate in (c) and the fine-scale solution. (e) Estimate of pressure by eliminating coefficients below a certain threshold in the pressure transform (keeping 683/1024 elements). (f) Relative error between the pressure estimate in (e) and the fine-scale solutions. In this case the diagonal differences can be neglected without compromising the quality of the pressure estimate.

even with very few elements, we can reproduce the pressure fairly accurately (see Fig. 8). The issue is identifying which elements should be kept to preserve the important pressure features.

Assuming that we are allowed to perform the fine-scale inversion or the inversion of the transformed fine-scale problem, which requires the same computational effort, we can check up to what point our system can be coarse grained without losing important features.

As it is rather idealistic to assume that we have access to the fine-scale pressure solution, we wish to find some criterion to relate the size of the elements in $\mathbf{P}'$ directly to the permeability field.

If we know which elements of $\mathbf{P}'$ were negligible, we can "compress" the $\mathbf{T}'$ matrix by eliminating rows and columns corresponding to those elements. The solution obtained for this smaller system can be inserted into a full size vector padded with zeros. Taking the inverse $\mathbf{H}$ transform of this vector will give us a pressure map with resolution varying across the system [see Fig. 8(c)].

A. Importance of different types of difference

Having decomposed the pressure into differences in the three directions (horizontal, vertical, and diagonal), in some

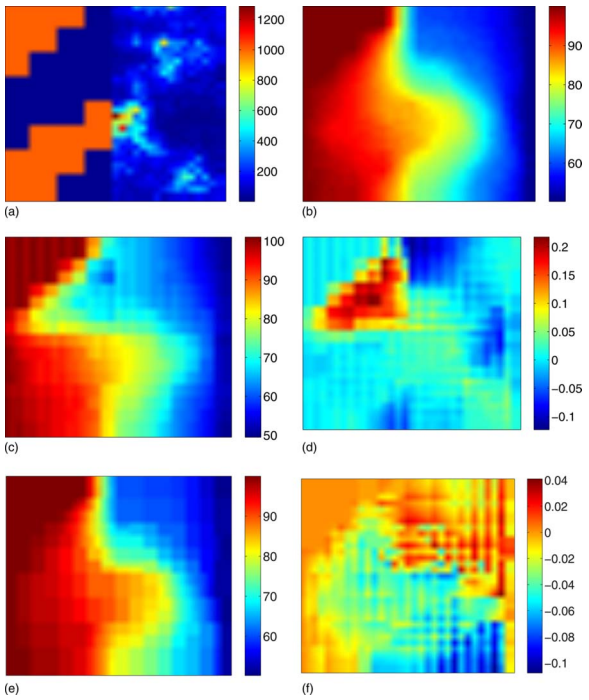

FIG. 10. (Color online) Analysis of the importance of diagonal differences. (a) Fine-scale synthetic permeability map, 32×32. (b) Fine-scale pressure solution. (c) Estimate of pressure by eliminating coefficients referring to diagonal differences and all details at level 4 (keeping 171/1024 elements). (d) Relative error between the pressure estimate in (c) and the fine-scale solution. (e) Estimate of pressure by eliminating coefficients below a certain threshold in the pressure transform (keeping 171/1024 elements). (f) Relative error between the pressure estimate in (e) and the fine-scale solution. In this case diagonal differences are important.

cases the size of these differences can be inferred from the permeability itself. For example, for a homogeneous or layered system we know that imposing flow from left to right will generate no vertical variations in pressure. This means that the vertical and diagonal differences will be almost zero at all scales. Also, in regions where there are no diagonal features in the pressure, we can ask what happens if we assume that diagonal differences will not have importance (see Fig. 9). In Fig. 10 we see a case where keeping diagonal differences is important. The problem, once again, is that, while we can identify these cases by looking at the pressure, we wish to be able to do this only using the permeability map.

B. Selecting the coefficients to be retained

A possible strategy focuses on identifying the areas in the permeability field where the pressure will differ considerably from the linear profile obtained with uniform permeability. One ideal property of an adaptive grid is that it can resolve areas of pressure with nontrivial profiles with a finer resolution than areas where pressure is simply linear. There is a clear relationship between localized permeability heterogeneity and interesting features in the pressure profile, but the pressure field is by definition not locally determined and the effects of a small region of heterogeneous permeability can be seen on the whole pressure profile. Nevertheless, if the region of heterogeneity is sufficiently small compared to the entire system, the pressure features induced should be localized.

Let us consider the transformed pressure vector $\mathbf{P}'$ that we would obtain for a homogeneous permeability map and a specific set of boundary conditions. These values will be our "default" values for the transformed pressure vector of a heterogeneous case with localized heterogeneity and those same boundary conditions. If we allow the assumption that the pressure field will be mostly affected where the heterogeneities are located, we can calculate the appropriate values of $\mathbf{P}'$ in that region by solving a small subset of the transformed Darcy's equation.

Thanks to the linearity of the $\mathbf{H}$ transform, we can split the pressure into a homogeneous contribution and one due to the heterogeneity. Define $\mathbf{P}=\mathbf{P}_{\text{hom}}+\mathbf{P}_{\text{het}}$, where $\mathbf{P}_{\text{hom}}$ is the pressure for a homogeneous system and $\mathbf{P}_{\text{het}}$ is the effect on pressure of the heterogeneity. Using the transformed version of Darcy's law and the notation previously introduced in Eq. (5), we can find an expression for the transform of $\mathbf{P}_{\text{het}}$ and hence the values of $\mathbf{P}_{\text{het}}$:

$$\mathbf{T}'\mathbf{P}' = \mathbf{R}', \tag{6a}$$

$$\mathbf{T}'\mathbf{H}\mathbf{P}_{\text{hom}} + \mathbf{T}'\mathbf{H}\mathbf{P}_{\text{het}} = \mathbf{R}', \tag{6b}$$

$$\mathbf{P}_{\text{het}} = \mathbf{H}^{\mathbf{T}}\mathbf{T}'^{-1}(\mathbf{R}' - \mathbf{T}'\mathbf{H}\mathbf{P}_{\text{hom}}). \tag{6c}$$

If the equations are solved on the entire system, this is just as expensive as calculating the entire fine-scale pressure solution. However, in the case where we can predict where or at what scales the deviation of pressure from the homogeneous case will be more severe, we can arbitrarily choose to keep only the corresponding elements in the calculation of $\mathbf{P}_{\text{het}}$, leading to savings in computational time. The linear size of the matrix $\mathbf{T}'$ that we need to invert is reduced as we delete the rows and columns corresponding to elements in $\mathbf{P}_{\text{het}}$ that we do not wish to calculate. This solution is then integrated with the previously determined "default" values to give an $N\times N$ system that is nonuniformly coarse grained.

On the other hand, if we have the resources to calculate $\mathbf{P}$ and $\mathbf{P}_{\text{het}}$ at every location, we can can compare them to automatically detect the regions where heterogeneity is strongly affecting the pressure profile.

In Fig. 11 an example can be seen. The permeability map was constructed by taking a 16×16 section of SPE10 data [17] and substituting it in the upper left quarter of a 32×32 unit permeability system. One way of producing the nonuniform coarse graining is by only keeping the coefficients in the regions where the transform of $\mathbf{P}_{\text{het}}$ is large. This leads to a correct pressure solution where details are only kept at the locations and scales needed.

More realistically, we do not know the fine-scale pressure solution *a priori* and we require a criterion to select the elements to keep. Figure 12 shows the elements kept in the thresholding of $\mathbf{P}_{\text{het}}$. We notice how most of the elements kept at the high levels (3 and 4) correspond to the location of the heterogeneities. Moreover, the diagonal coefficients are

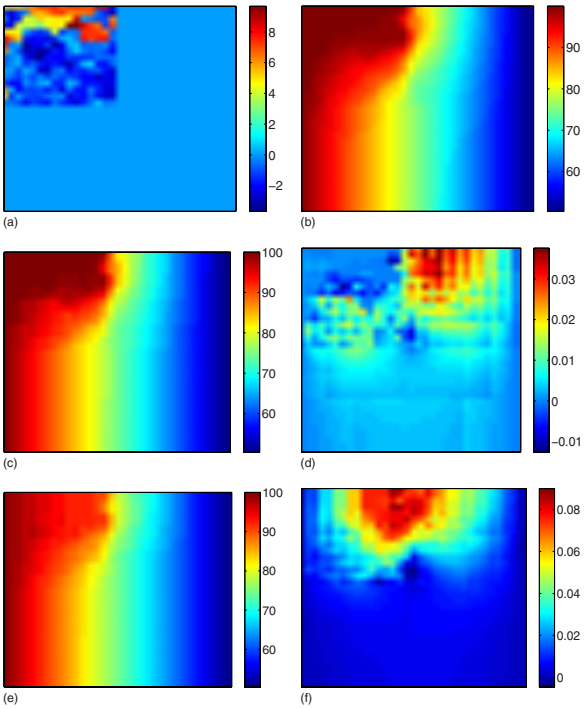

FIG. 11. (Color online) Example of a permeability map with localized heterogeneity. The permeability map was constructed by taking a 16×16 section of SPE10 data and substituting it in the upper left quarter of a 32×32 unit permeability system. (a) Logarithm of permeability. (b) Fine-scale pressure solution, flow from left to right. (c) Estimate of pressure obtained by keeping the 150 largest elements in the transform of $\mathbf{P}_{\text{het}}$. (d) Relative error between fine-scale solution and estimate in (c). (e) Estimate of pressure obtained by keeping the 95 largest elements in the transform of $\mathbf{P}_{\text{het}}$. (f) Relative error between fine-scale solution and estimate in (e).

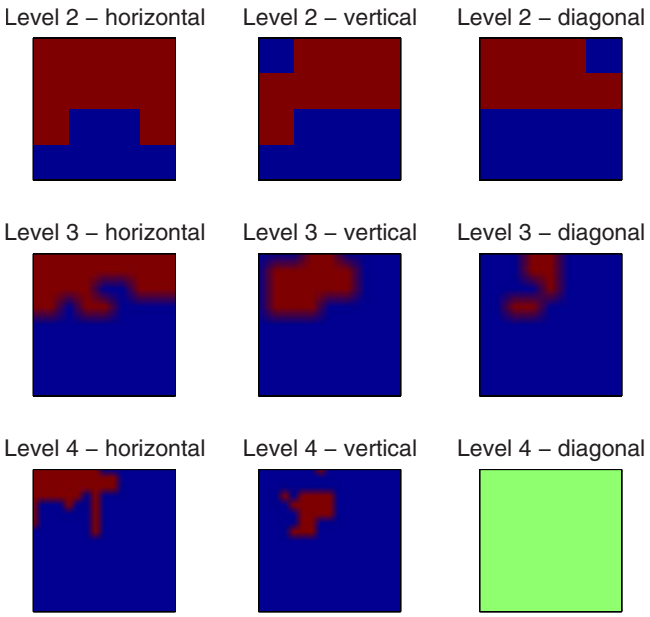

FIG. 12. (Color online) A visualization of the elements kept at different scales in the estimate of Fig. 11(c). At levels 3 and 4 most of the elements kept are located in the same location as the heterogeneous permeability.

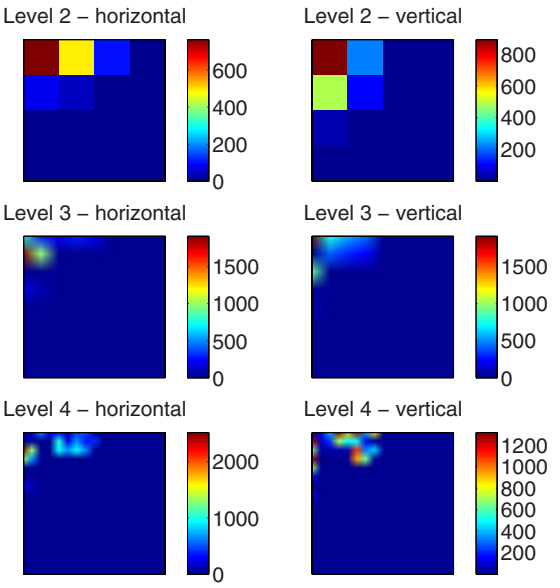

FIG. 13. (Color online) A plot of the horizontal and vertical gradients of permeability at different levels for the map shown in Fig. 11. Notice a correspondence between high gradients in the heterogeneous regions and the locations of the coefficients kept in Fig. 12.

only kept in levels 2 and 3. For the automatization of this method, we need to detect the location of the heterogeneities. One indicator of heterogeneity is the permeability gradient. In Fig. 13 we can see the horizontal and vertical gradients of permeability at the different levels.

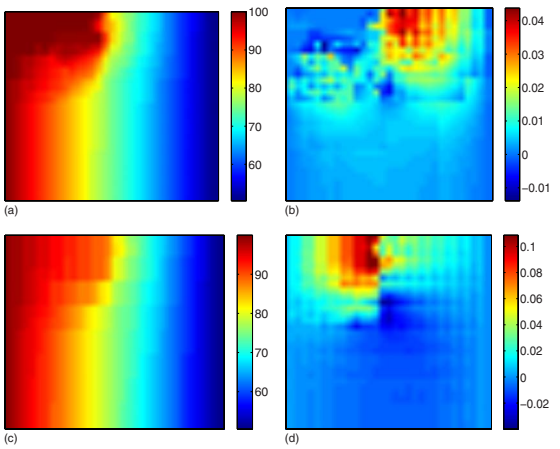

FIG. 14. (Color online) An estimate of pressure based on keeping elements where the gradients of permeability are high. (a) Estimate of pressure obtained by keeping the 137 largest elements in the transform of $\mathbf{P}_{\text{het}}$. (b) Relative error between fine-scale solution and estimate in (c). (c) Pressure estimate having kept 137 out of 1024 coefficients where the permeability gradients are higher. (d) Relative error between fine-scale solution and estimate in (c). The error for case (c), where the coefficients are chosen based on the gradient, is approximately twice as large as in (a) for the same number of coefficients kept. The reason for this is that in case (c) only coefficients for horizontal and vertical differences were allowed and only at scale 4.

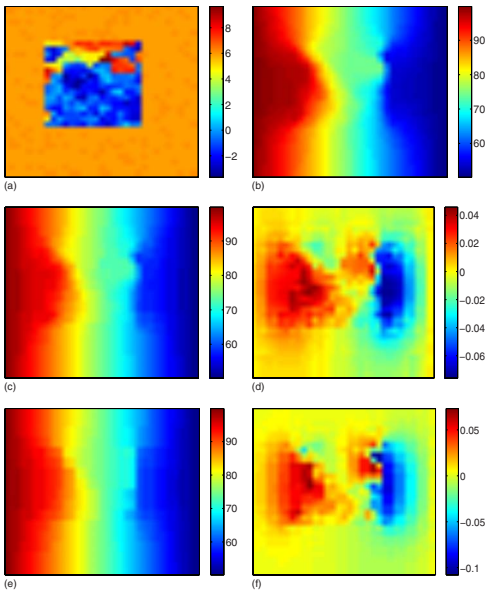

FIG. 15. (Color online) A normally distributed permeability with a more heterogeneous inclusion, a 16×16 subset of SPE10 at its center. (a) Logarithm of permeability. (b) Fine-scale pressure solution, flow from left to right. (c) Estimate of pressure obtained by keeping the 192 largest elements in the transform of $\mathbf{P}_{\text{het}}$. (d) Relative error between fine-scale solution and estimate in (c). (e) Estimate of pressure obtained by keeping only 192 coefficients referring to the locations of high permeability gradients, as in Fig. 14. (f) Relative error between fine-scale solution and estimate in (e).

We can arbitrarily decide to keep all elements up to level 3 and elements at levels 4 only where the permeability gradient of the corresponding direction is high (see Fig. 14). This is a criterion that we can use to generate pressure solutions that are nonuniformly coarse grained starting only with a fine-scale permeability map. It could be argued that the example chosen is not representative as the heterogeneity is only present in a small part of the system and, more importantly, this part is conveniently situated in one of the blocks that we can recognize even at level 1.

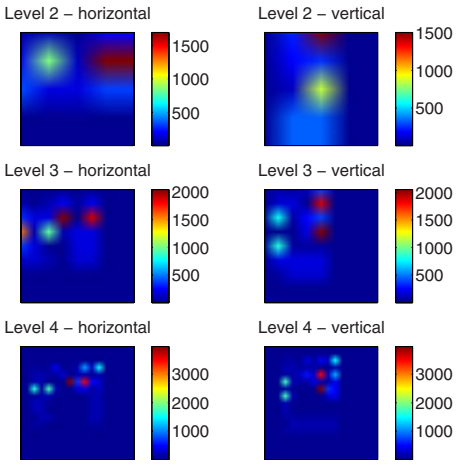

FIG. 16. (Color online) A plot of the horizontal and vertical gradients of permeability at different levels for the map shown in Fig. 15. Notice a correspondence between high gradients and the heterogeneous regions and the locations of the coefficients kept in Fig. 15.

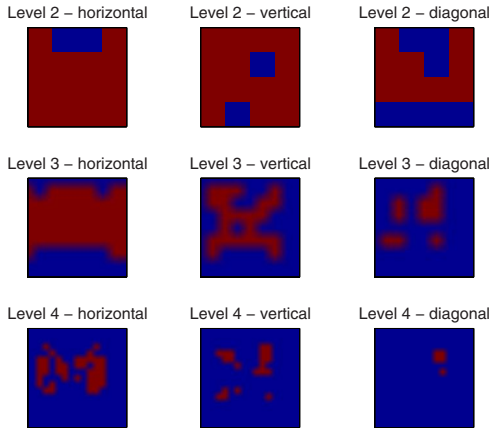

FIG. 17. (Color online) A visualization of the elements kept at different scales for the permeability of Fig. 15.

Figure 15 refers to a less idealised case: the 16×16 heterogeneous SPE block has been set at the center of a system with permeability normally distributed around the mean of the SPE block.

The corresponding map of permeability gradients and coefficients kept can be found in Figs. 16 and 17.

Finally, the new algorithm was applied to the previously mentioned sample of 30 permeability realizations. Plots of the mean relative error versus the thresholding parameter and the number of elements kept can be seen in Fig. 18. Consider the gradient $\Delta_x^i k$ of permeability in the horizontal direction at level i: the corresponding element is retained in the transform if

$$\Delta_x^i k > \max(\Delta_x^i k) - q\sigma(\Delta_x^i k).$$

The higher the filtering parameter q, the more elements will be kept and the better the pressure estimate. Notice that this method preserves areas of high gradient, where the pressure is not "linear" (as would be given by uniform permeability with the specified boundary conditions).

The error is only around 3.5% if keeping fewer than 100 of the 1024 elements More analysis for different kinds of systems would be needed to draw a definite estimate of the likely error in performing this approximate solution.

To summarize, one way of obtaining a nonuniformly coarse grained pressure solution is to express the pressure as a sum of a component due to a uniform permeability under the specified boundary conditions and an extra term due to the heterogeneity. By storing the solution for the homogeneous permeability and adding terms explicitly calculated only in regions where the permeability gradients are high, we can obtain an estimate of the pressure with limited computational cost.

C. Discussion

A method was suggested to achieve an automatic nonuniform coarse graining of the pressure profile. The focus is on the location of particularly heterogeneous permeability re-

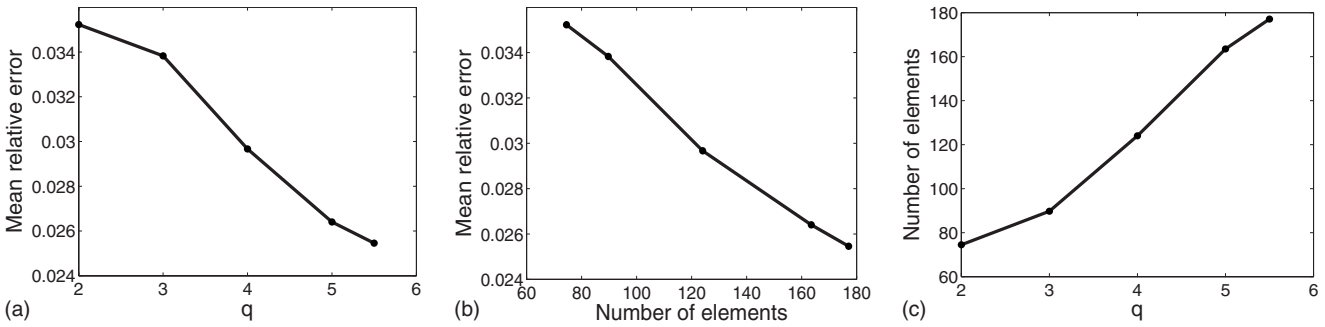

FIG. 18. Plots of relationship between mean relative error in the estimate of pressure compared to the fine-scale pressure as a function of the filtering parameter q, and the number of elements kept. Notice the criterion for thresholding: Consider the gradient of permeability in the horizontal direction at level i, $\Delta_x^i k$: the corresponding element is retained in the transform if $\Delta_x^i k > \max(\Delta_x^i k) - q\sigma(\Delta_x^i k)$. (a) Mean relative error vs q. (b) Mean relative error vs the number of elements kept. (c) Number of elements kept vs q.

gions. The underlying pressure solution is taken to be a linear pressure gradient or, more in general, the pressure solution that would be obtained with uniform permeability and the specified boundary conditions. The correct pressure solution can be expressed as the sum of this linear pressure and a contribution due to the heterogeneity. Using the formalism described in Eq. (6c), we find an expression for the transform of $\mathbf{P}_{\text{het}}$, the contribution to the pressure given by the heterogeneity. We now select the coefficients in $\mathbf{P}_{\text{het}}$ that we want to calculate, based on high-permeability gradients. These are related to the regions where the pressure is not linear. By combining these coefficients with the linear solution, we obtain a nonuniform pressure solution.

In the case where we start by knowing $\mathbf{P}$ and $\mathbf{P}_{\text{het}}$, this method can be reversed to locate regions of linear pressure (in the sense imposed by the boundary conditions). For each specific case we would need to apply the known boundary conditions to a homogeneous system to calculate the homogeneous pressure component. Once this is known, we could proceed to find the correct entire pressure solution at the level of detail required.

An improvement could be achieved by including also diagonal differences at some scales, and it is likely that tuning the thresholding parameters for the various types of differences at each scale would lead to a better and more optimized pressure estimate.

An advantage of this approach is that although the calculation of pressure is done with a reduced number of elements, the final upscaled pressure is on the same grid as the fine one. This eliminates problems to do with the change of coordination number of the permeability map on coarse regions that border finer ones. The errors encountered with the first method over 30 realizations of heterogeneous permeability suggest that, unless there are specific requirements in the accuracy of the estimate, this method can guarantee a satisfactory estimate of the pressure on an adaptive grid to within 10% or less of the original fine-scale solution. It could also be argued that possible inaccuracies in this stage of upscaling are a smaller source of error than the inherent uncertainty of the fine-scale model. In Sec. V this issue will be considered further.

V. ENSEMBLE UPSCALING

Given the great uncertainty present in the permeability data available, it is often better to upscale the statistics of permeability rather than permeability itself. So the solution to an upscaling problem does not necessarily have to be a single coarse permeability map or pressure profile; it could well be an ensemble of them, which should in some way preserve the statistics of the fine-scale permeability. A probabilistic approach to choosing the elements to be kept in the $\mathbf{T}'$ matrix might be a way to achieve this kind of upscaling. We could assign to each element in $\mathbf{P}'$ a probability of being eliminated depending on whether the element is present or not in the $\mathbf{P}'$ for one of the special cases.

From a single fine-scale permeability map, multiple pressure solutions could be obtained. Unfortunately it is unlikely that such a way of proceeding could be proved to ensure preservation of the underlying permeability statistics. Nevertheless, generating an ensemble of pressure solutions would probably mitigate both the uncertainty in the fine-scale permeability and upscaling errors.

VI. SUMMARY

A hierarchical transform was introduced to represent pressure solutions as an average value plus some fluctuations at different scales and locations. With the formalism introduced in Pancaldi *et al.* [13], applying this transform to Darcy's law, a transformed transmissibility matrix was obtained. A method was suggested to select which parts of this matrix is to be retained to produce a nonuniformly coarse grained pressure solution.

Looking at ensemble statistics, it can be said that nonuniform coarse graining can produce more faithful estimates of the pressure solution compared to the uniform case for the same number of elements kept, and hence the same computational cost.

In the literature, many criteria have been used to guide the adaptivity of nonuniform grids [3,6,7]. Mostly these methods are based on flow calculations performed to identify the areas of high flow rate. The method suggested does not require any such prior information. A more advanced localization of areas to be preserved in detail would certainly improve the performance of the method, although at some computational efficiency cost.

Finally, the possibility of generating an ensemble of pressure solutions from a single fine-scale permeability was discussed.

APPENDIX A: THE HIERARCHICAL TRANSFORM—WRITING THE H MATRIX

A useful property of the **H** matrix is that its elements can be determined based on the binary representation of the number of the cell to which they refer. In the following, **H** for a 4×4 system will be written starting from the cell indices.

By identifying each cell with its row and column indices and expressing these in binary format, different digits determine to which subgroup it belongs to at the different levels. The subgroup will be associated with value 1 or −1 depending on what type of difference is being considered.

For example, let us consider the indices for a 4×4 system (starting the indexing from 0):

$$\begin{bmatrix} 1(0,0) & 5(0,1) & 9(0,2) & 13(0,3) \\ 2(1,0) & 6(1,1) & 10(1,2) & 14(1,3) \\ 3(2,0) & 7(2,1) & 11(2,2) & 15(2,3) \\ 4(3,0) & 8(3,1) & 12(3,2) & 16(3,3) \end{bmatrix}. \tag{7}$$

If we express the i and j indices in binary format, we get

$$\begin{bmatrix} (00,00) & (00,01) & (00,10) & (00,11) \\ (01,00) & (01,01) & (01,10) & (01,11) \\ (10,00) & (10,01) & (10,10) & (10,11) \\ (11,00) & (11,01) & (11,10) & (11,11) \end{bmatrix}. \tag{8}$$

Looking at the digits in different positions of these indices, we recover the different levels of description. At each level the values of these digits can be used to determine which elements should be 1, −1, or 0 to recover the desired difference (horizontal, vertical, or diagonal). The algorithm was implemented to generate **H** matrices for systems of the desired size, always a power of 2.

If we look at the system at level 1, we need to concentrate on the left most digits in the i and j indices, which are

$$\begin{bmatrix} (0,0) & (0,0) & (0,1) & (0,1) \\ (0,0) & (0,0) & (0,1) & (0,1) \\ (1,0) & (1,0) & (1,1) & (1,1) \\ (1,0) & (1,0) & (1,1) & (1,1) \end{bmatrix}. \tag{9}$$

Elements which belong to the same level 1 subgroups have equal i and j indices, clearly showing the four corners.

Using these indices in binary format, we can write the rows of the **H** matrix one by one to reproduce the correct differences (horizontal, vertical, and diagonal) at the right levels.

Labeling the rows and columns of **H** with k and l, rows $k=2,3,4$ refer to the level 1 description. The horizontal differences at this level are on row 2, row 3 is for vertical, and row 4 is for diagonal ones. All elements are either 1 or −1 according to the following rule [see Eq. (9)]:

For row $k=2$, the upper and lower left corners are 1 and the rest −1:

```
if i(l)=0
   element=1
else
   element=-1
```

For row $k=3$, right and left upper corners are 1 and the rest −1:

```
if j(l)=0
   element=1
else
   element=-1
```

For row $k=4$, right upper and left lower corners are 1 and the rest −1:

```
if j(l)=i(l)
   element=1
else
   element=-1
```

To obtain the elements for level 2, we need to consider the second digits of the indices in Eq. (8):

$$\begin{bmatrix} (0,0) & (0,1) & (0,0) & (0,1) \\ (1,0) & (1,1) & (1,0) & (1,1) \\ (0,0) & (0,1) & (0,0) & (0,1) \\ (1,0) & (1,1) & (1,0) & (1,1) \end{bmatrix}. \tag{10}$$

Now the system is subdivided into 16 blocks (level 2), which we can combine into 4 groups, each of which we can describe with the three types of differences.

In **H** rows 5–8 are reserved for horizontal differences in the four subgroups (numbered down and then right), 9–12 are for vertical, and finally 13–16 are for diagonal differences. The elements which refer to subgroups which are not being considered are simply 0.

The normalization is performed ensuring that that the sum of the squares of the elements in each row sum to 1.

APPENDIX B: FIGURE 1, THE SCHEME UNDERLYING H

The following explains Fig. 1 in more detail. Consider a single row in **H**:

row $1=[c_1\,c_2\,c_3\,c_4\,c_5\,c_6\,c_7\,c_8\,c_9\,c_{10}\,c_{11}\,c_{12}\,c_{13}\,c_{14}\,c_{15}\,c_{16}]$. If we consider each row as independent, each element in the above vector multiplies a single corresponding pressure value. The coefficients c_i can be therefore seen as "weights" in a weighted sum of all the pressure values. Figure 1 shows a matrix representation of the weights for each column. Representing row 1 as a matrix (columns first), we get the level-0 weights as

$$\begin{bmatrix} c_1 & c_5 & c_9 & c_{13} \\ c_2 & c_6 & c_{10} & c_{14} \\ c_3 & c_7 & c_{11} & c_{15} \\ c_4 & c_8 & c_{12} & c_{16} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}.$$

This square is the square in the top left corner of Fig. 1. This multiplies element by element the pressure map:

$$\begin{bmatrix} p_1 & p_5 & p_9 & p_{13} \\ p_2 & p_6 & p_{10} & p_{14} \\ p_3 & p_7 & p_{11} & p_{15} \\ p_4 & p_8 & p_{12} & p_{16} \end{bmatrix},$$

which gives a sum of all pressures.

For level 1, vertical differences (row 2) are given by

$$\begin{bmatrix} c_1 & c_5 & c_9 & c_{13} \\ c_2 & c_6 & c_{10} & c_{14} \\ c_3 & c_7 & c_{11} & c_{15} \\ c_4 & c_8 & c_{12} & c_{16} \end{bmatrix} = \begin{bmatrix} 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \end{bmatrix}.$$

For level 2, vertical differences for subgroup 1 (row 5) are given by

$$\begin{bmatrix} c_1 & c_5 & c_9 & c_{13} \\ c_2 & c_6 & c_{10} & c_{14} \\ c_3 & c_7 & c_{11} & c_{15} \\ c_4 & c_8 & c_{12} & c_{16} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 \end{bmatrix},$$

and so on, as shown pictorially in Fig. 1.

[1] P. Zhang, G. E. Pickup, and M. A. Christie, Pet. Geosci. **13**, 17 (2007).
[2] M. Gerritsen and L. Durlofsky, Annu. Rev. Fluid Mech. **37**, 211 (2005).
[3] J. Aarnes and Y. Efendiev, Multiscale Model. Simul. **5**, 918 (2006).
[4] M. G. Gerritsen and J. V. Lambers, Comput. Geosci. **12**, 193 (2008).
[5] J. Nilson, M. Gerritsen, and R. Younis (unpublished).
[6] R. M. Younis and J. Caers (unpublished).
[7] L. J. Durlovsky, R. C. Jones, and W. J. Milliken, Adv. Water Resour. **20**, 335 (1997).
[8] J. E. Aarnes, S. Krogstad, and K. A. Lie, Comput. Geosci. **12**, 297 (2008).
[9] J. V. Lambers, M. G. Gerritsen, and B. T. Mallison, Comput. Geosci. **12**, 399 (2008).
[10] S. S. Berg and E. Øian, Pet. Geosci. **13**, 25 (2007).
[11] H. Gotovac, R. Andricevic, and B. Gotovac, Adv. Water Resour. **30**, 1105 (2007).
[12] I. Daubechies, *Ten Lectures on Wavelets*, CBMS-NSF Regional Conference Series in Applied Mathematics (SIAM, Philadelphia, 1992).
[13] V. Pancaldi, K. Christensen, and P. King, Transp. Porous Media **67**(3), 395 (2007).
[14] K. J. Hersvik and M. S. Espedal, Comput. Geosci. **2**, 311 (1998).
[15] K. Aziz and A. Settari, *Petroleum Reservoir Simulation* (Kluwer Academic, Dordrecht, 1979).
[16] P. R. King, Transp. Porous Media **23**, 337 (1996).
[17] M. Christie and M. J. Blunt, SPE Reservoir Eval. Eng. **4**(4), 308 (2001).