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NUMERICAL TECHNIQUES FOR SOLVING PARTIAL DIFFERENTIAL EQUATIONS IN HETEROGENEOUS MEDIA

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Abstract. *This paper deals with numerical issues involved in the solution of partial differential equations in heterogeneous media. One important application in this class of problems is the simulation of petroleum reservoirs. For these simulations, three different methodologies are usually employed: finite element, classical finite volume and element-based finite volume methods. The main contribution of the paper is to perform a comparison among the results given by these methods in some reference test problems, considering the accuracy of the fluxes evaluation and the techniques for averaging the physical properties at the control volume interfaces, since in these problems large heterogeneities are common. It is shown that the methods that do not require an average of the physical properties at the interfaces produce more accurate solutions. It is also proposed a new local grid refinement scheme that uses higher order interpolation functions.*

Keywords: *reservoir simulation, numerical methods, heterogeneities, porous media.*

1. INTRODUCTION

The numerical simulation is undoubtedly a valuable tool in the petroleum industry. The information provided by numerical simulators can be a significant contribution on the evaluation process of a petroleum reservoir and, even more important, on the decision making process. The increasing importance of this kind of analysis tools has promoted an intense study of the different methodologies involved, especially in the academic community.

There are many numerical methods that are commonly used in the development of commercial and academic simulators, and the differences among them are not always obvious. Thus, this paper begins presenting a general view about the principal numerical methods used in the reservoir simulation field, pointing out the conceptual similarities or differences among them. However, the aim of this work is not to conclude or express an opinion about which the better method is, because certainly there is no method that is efficient in all aspects.

Some simple study cases are presented and the performance of different numerical methods is analyzed. The results obtained allow drawing some important conclusions about the influence of different aspects such boundary conditions, heterogeneities treatment, interpolation practices, etc. Finally, this work ends presenting a proposal about a local grid refinement technique, having as special feature the use of elements defined by a variable number of nodes.

2. COMPARISON OF DIFFERENT NUMERICAL SCHEMES IN SOLVING THE DISCRETE LAPLACE EQUATION

In this section we discuss the numerical solution of simple problems involving the Laplace's equation by different methods, trying to have indications about the accuracy of them. In fact, it is very difficult to compare methods developed in different areas of knowledge (Maliska 2003). For example, the Finite Differences Method (FDM) was always used in fluid flow, whereas the Finite Element Method (FEM) has been used, mainly, in structural problems. Physically, these problems are completely different. The Finite Volume Method (FVM), on the other hand, is a numerical method that results in equations where the conservation principle is assured. This is the reason why it has been successfully used for heat transfer and mass flow problems. Nevertheless, the Element-based Finite Volume Method (EbFVM) has recently appeared as a good option in the numerical simulation. It employs the ideas of Raw (1985) when developing the FIELD method for solving the Navier-Stokes equations. EbFVM is a better denomination for the method (Maliska, 2003), also known in the literature as Control Volume Finite Element Method (CVFEM) since it is a finite volume methodology which borrows from the finite element technique the concept of elements. CVFEM would erroneously suggest a finite element formulation that obeys the conservation principles at discrete level. It is important to stress again that we do not want to show here which of these methods is the best, since we believe that there is no method able to solve with the highest accuracy and flexibility all the physical situations in practical problems. So, this paper presents the results of applying different methods to solve simple problems in order to discuss some particular details involved in each method, like grid type used, averaging procedures, and so on, and finally how these can impact the results.

Figure 1 shows that all methods cited before can be considered as weighted residual methods. This figure summarizes the task of any numerical technique, namely, to transform a partial differential equation in a system of n linear algebraic equation with n unknowns, one for each node. A weighted residual formulation can be written as

$$\int_V L(f)WdV = 0 \tag{1}$$

where V is the volume, W is the weighting function and f the approximation for the unknown variables. If W is the unit in a control volume and zero elsewhere, and the equation is in its conservative form, the resulting methods are FVM or EbFVM, depending on the type of interpolation function. If the weighting function is assumed as the Dirac delta function in a point, the resulting method is FDM, whereas if the W is assumed as the element shape functions, one obtains the FEM (of Galerkin type). Other observations and comparisons among these methods can be found in Banaszek (1995) and Maliska (2003).

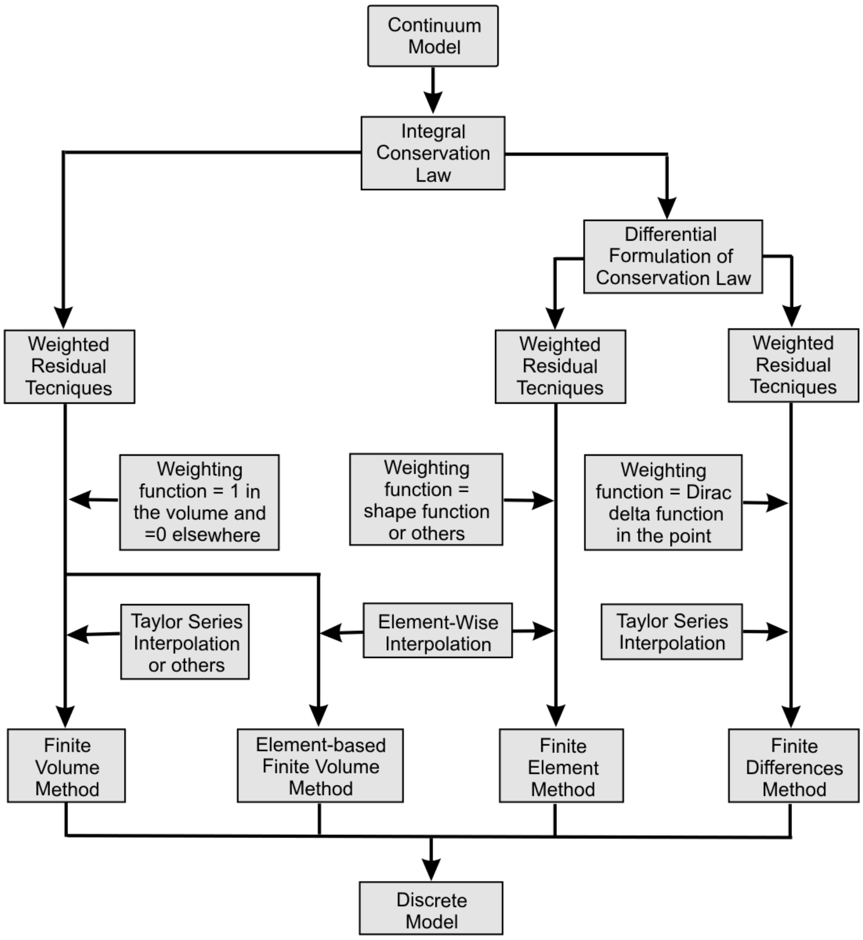


Figure 1- Differences among numerical methods (adapted from Banaszek, 1995)

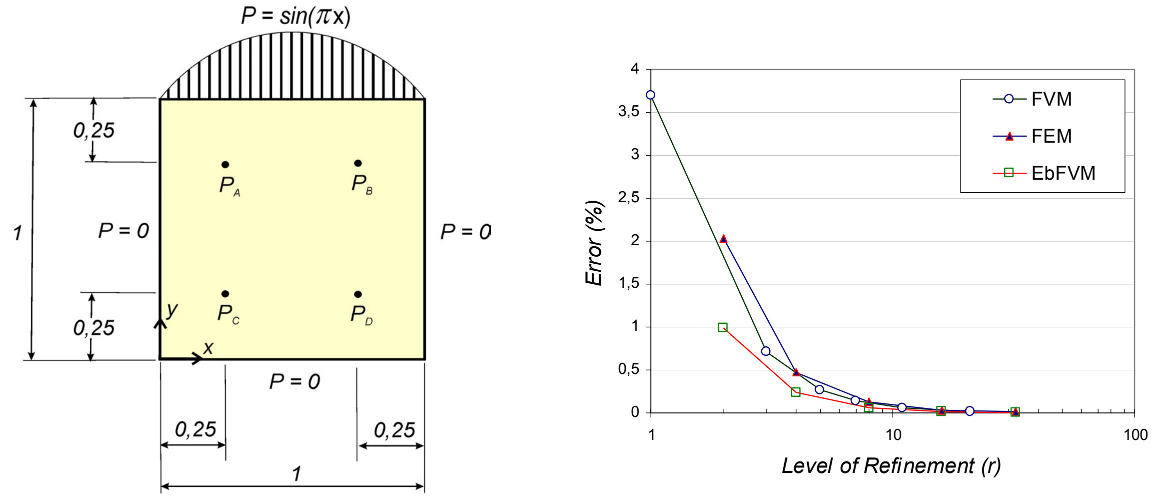
As already stated, it is difficult to find the most efficient and flexible numerical method for use in reservoir simulation because its performance depends on many features of the problem being considered. Nevertheless, we present in the next section some cases to study the differences among the methods in simple problems, showing the strengths and weaknesses of each one. Initially, problems with Dirichlet boundary conditions are presented, and the differences among the numerical methods are analyzed in homogeneous and heterogeneous cases. Following, simple problems of upscaling, involving Neumann boundary conditions are solved in two different cases of heterogeneities in the domain. This section ends with the comparison among results of different types of shape function in the EbFVM, for the heterogeneous case. Other details about these methods, like basic ideas and the main steps, can be found, for example, in Patankar (1980), Raw (1985), Cook *et al.* (1989) and Maliska(2003).

2.1 Test cases with Dirichlet boundary conditions

Homogeneous case. The problem analyzed is presented in Fig. 2*a*, where a square domain with sides length of 1 has pressure P=0 prescribed for all boundary surfaces, except for the top surface where P assumes a senoidal variation. In some points, which are called P_A, P_B, P_C, and P_D, are computed the values that are compared with the analytical solution given by

$$P(x,y) = sin(\pi x)\frac{sinh(\pi y)}{sinh(\pi)} \tag{2}$$

Even though some points analyzed in this figure are symmetrical and, therefore, they present symmetrical errors, we maintain them because they will be used in the next example, which is asymmetrical.



(a) *(b)*

Figure 2- *(a)* Dirichlet boundary conditions problem in a homogeneous case, and *(b)* values of absolute perceptual errors vs. level of refinement for different methods.

Figure 2*b* presents the values of absolute perceptual errors vs. level of refinement for different methods. Numerical grid refinement is represented by the parameter r. The level of refinement for 2x2 grids, for example, is r=1, for 4x4 is r=2, and so on. We can see in Fig. 2*b* that the results of EbFVM are better than the other methods (FEM and FVM). In the homogeneous Dirichlet problems, the EbFVM presents the same accuracy (2nd order) throughout the domain. Results from other authors have shown that the EbFVM has truncation error smaller than the Galerkin FEM and FVM for Laplace's equation in homogeneous case (Rozon, 1989; Banaszek, 1989).

Heterogeneous case. In this paper it is considered heterogeneous the domain that presents spatial variation of permeability and/or porosity. However, before presenting the problem itself, it is important to mention that in the EbFVM, the physical properties, like absolute permeability and porosity, are stored in the centre of the elements, unlike the other methods, even other CVFE methods, that store the physical properties in the control volumes centre (Verma & Aziz, 1997). Even though using this storage scheme for the properties, the principal variables calculated in the numerical model, like pressure and saturation, are still stored in the grid-nodes. Figure 3 compares the usual scheme of commercial simulators with the one proposed in Cordazzo (2002).

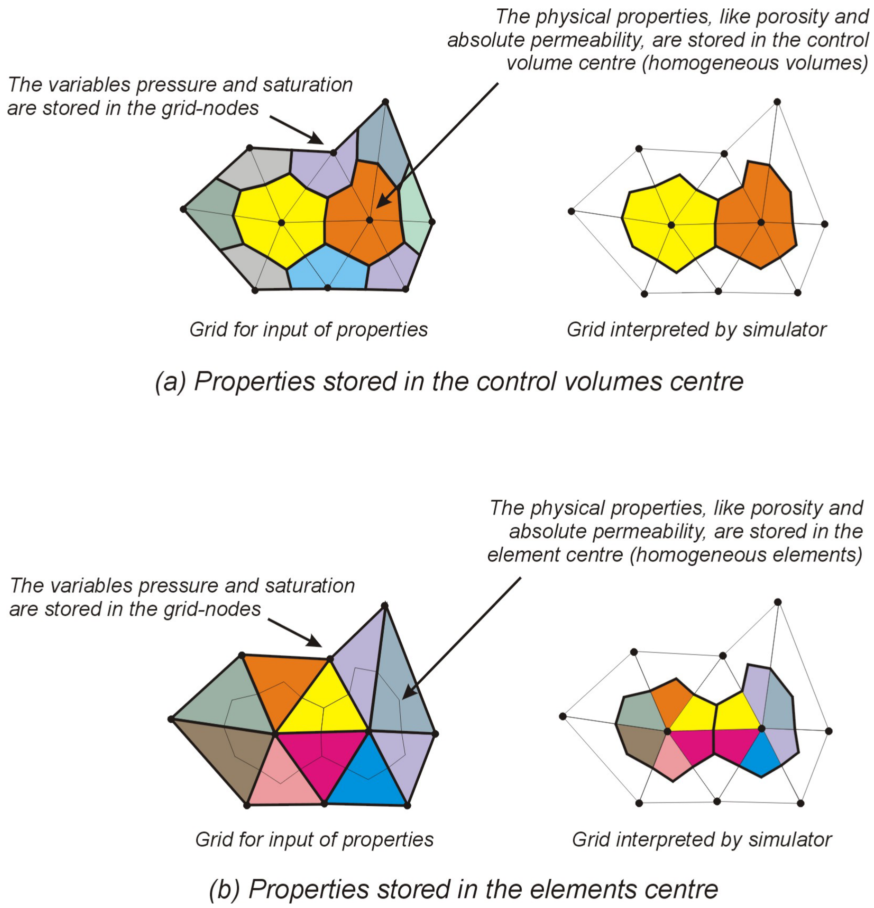
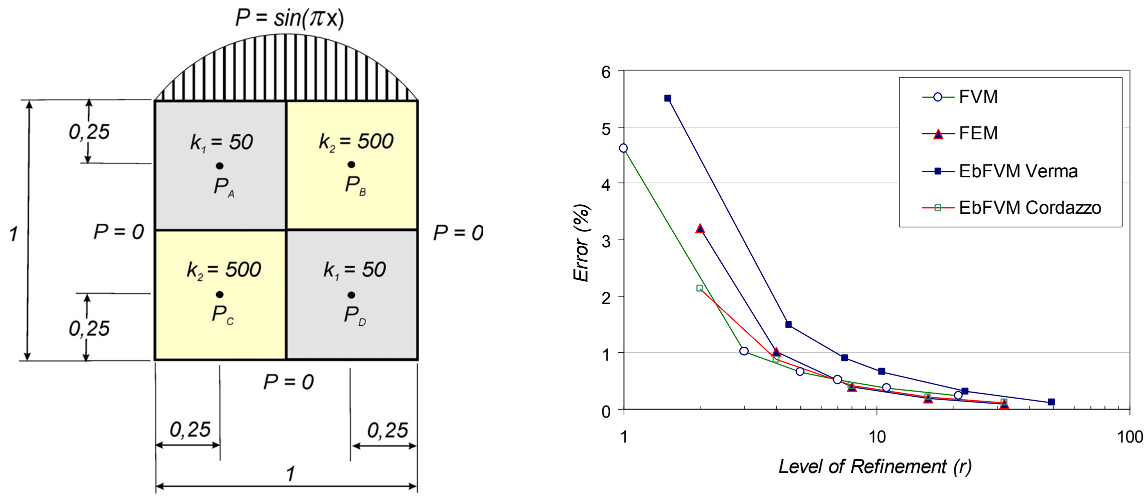


Figure 3- Different ways to store the physical properties: *(a)* in the control volume centre (proposed by Verma & Aziz, 1997), and *(b)* in the elements centre (proposed by Cordazzo, 2002)

The main advantage of the EbFVM is the fact that is only needed to deal with one grid (the elements), which is built using triangles and/or quadrilaterals. In the center of the elements it is stored the physical properties like absolute permeabilities, porosity, etc. It results in an easy procedure to build grids that represent the heterogeneities with more fidelity. From a practical point of view of the simulator users, this method only demands to "see" a grid of elements instead of dealing also with a grid of control volumes, as is needed with other methods. Moreover, due to the harmonic average process done in commercial simulators in order to estimate the internodal permeabilities, some simulation results, sometimes can have been obtained with an erroneous heterogeneous map. In the EbFVM, on the other hand, as the integration points are inside the elements, there is no need to make any average to calculate the permeabilities at the control volume interfaces. Thus, this implies in a errors source that has vanished in the numerical model. Figure 3*b* shows that in EbFVM, the control volumes are heterogeneous, instead of the elements as in other methods.

In the homogeneous elements approach, however, the transient term of the partial differential equation should be rewritten. More details can be obtained in Cordazzo *et al.* (2003). There are at least two reasons why we are be able to say that employing a mean value of porosity is not so troublesome than using a mean value of permeability. First, the range of variation of permeabilities values is often greater than the range variation of porosity values in a field. Second, the permeability is a term appearing in Darcy law, while porosity is not. We should remember that the Darcy law is the momentum equation for a porous media. These reasons justify the use of a numerical method that employs an average porosity value instead of an average permeability value.

Having done those considerations, we can present now a second example. The geometry and Dirichlet boundary conditions are the same as in the previous problem, while is used a new permeability map that is shown in Figure 4*a*. We intend to investigate the influence of heterogeneities on the results given by different methods for same grids and Dirichlet boundary conditions.



(a) *(b)*

Figure 4- Figure 1- *(a)* Dirichlet boundary conditions problem in a heterogeneous case, and *(b)* values of absolute perceptual errors vs. level of refinement for different methods

The reference solution was calculated by FEM for r = 216, i.e. refining the original 4x4 grid up to 512x512. Figure 4*b* presents the values of absolute perceptual errors vs. level of refinement for different methods. It is denoted by "EbFVM Cordazzo" the Element-based Finite Volume Method which stores the physical properties, like absolute permeability and porosity, in the centre of the elements, whereas "EbFVM Verma" is called the Element-based Finite Volume Method which stores the same physical properties in the centre of the control volumes (Verma & Aziz, 1997). According to this figure, the errors in the points analyzed are almost of the same order for all methods, except for EbFVM Verma, which has the greater errors for all levels of refinement.

2.2 Test cases with Neumann boundary conditions

In this section we investigate the influence, even though only qualitatively, that the Neumann boundary conditions have on results. The two cases chosen here are similar problems of upscaling with different heterogeneity levels. Several authors have examined the performance of different numerical methods on the computation of the effective permeability in coarse and refined grids for some examples of heterogeneous media (Romeu & Noetinger, 1995; Ribeiro & Romeu, 1997; Renard *et al.*, 2000). The most general and accurate technique is calculating numerically the equivalent conductivity of a heterogeneous media by solving the Laplace's equation. This solution is biased when the grid is not over-discretized due to truncation errors, errors in averaging the properties, among others. The simpler case analyzed is the 2D chess-board given in Fig. 5*a*, where the domain is subjected to no-flow boundary

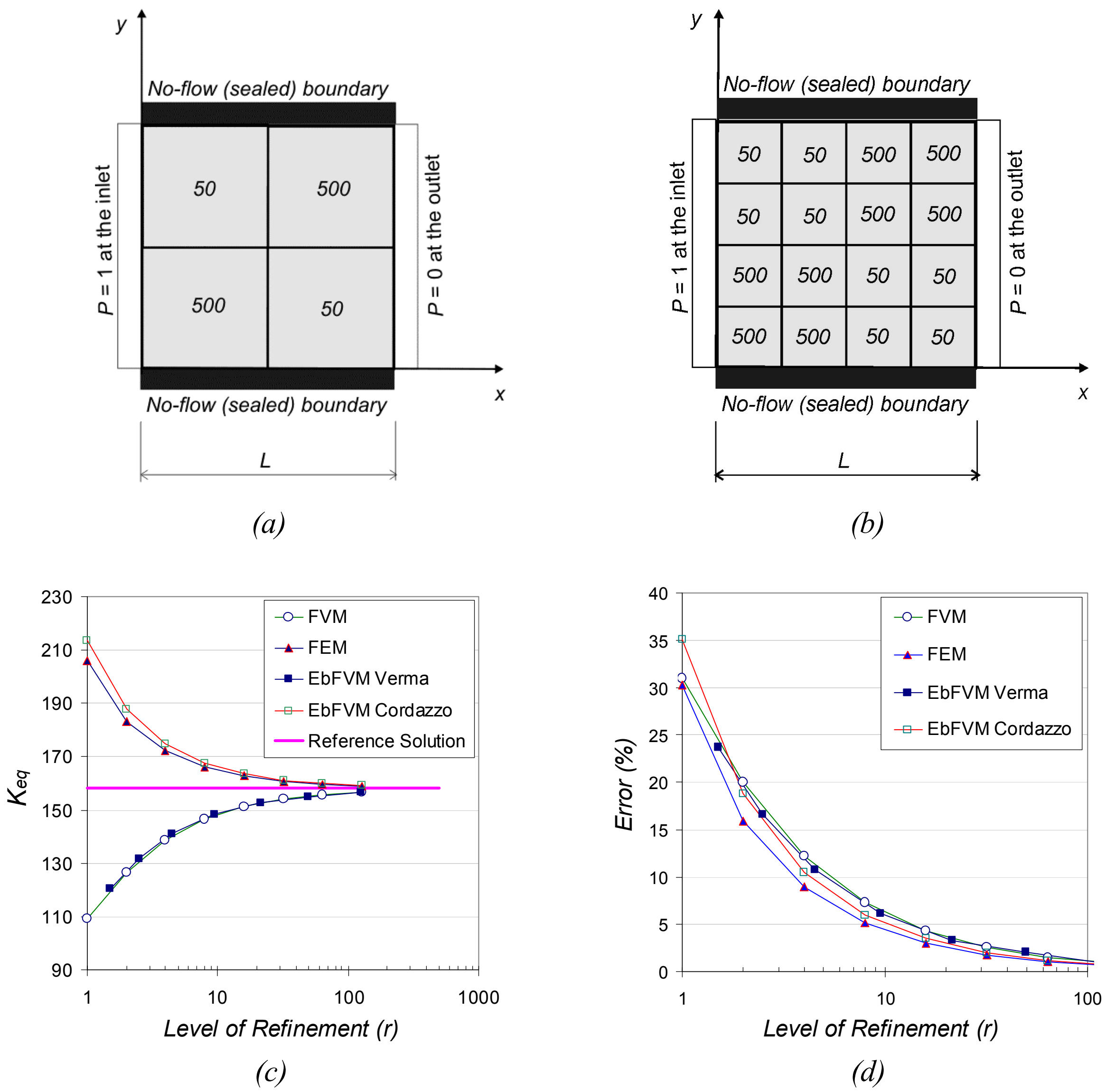


Figure 5- 2D chess-board problem: *(a)* boundary conditions and permeability map used to compute the effective permeability in a grid without refinement (r=1), and *(b)* in a grid with two levels of refinement (r=2); *(c)* values of k_{eq} computed by different methods as a function of refinement; *(d)* values of absolute perceptual errors vs. level of refinement for different methods

conditions along the perpendicular sides, P=1 at inlet, and P=0 at the outlet. The effective permeability in the x direction is given by QL/A, where Q is the total rate that enters or exits the system, A is the cross section area and L is the length shown in the Figure 5*a*. Therefore, if $L = A = 1$, the effective permeability is the total rate in the system that can be calculated from the numerical solution. The permeability map is shown also in the same figure.

The equivalent permeability of a 2D infinite chess-board is the geometric mean of the local permeabilities (Matheron, 1967), that we will call the reference solution. Here the numerical grid refinement is still represented by the paramenter r. In Fig. 5*a*, for instance, the refinement level, r, is 1, whereas in Fig. 5*b* this parameter assumes value 2, and so on. Figure 5*c* presents the results obtained by different numerical methods. We can conclude that both FEM and "EbFVM Cordazzo" overestimate the solution for k_{eq}, and both FVM and "EbFVM Verma" underestimate the solution for k_{eq}. However, all of these methods converge to the reference solution when the grid is sufficiently refined. Figure 5*c* shows how the three methods converge when the refinement ratio, r, increases. We can note that the methods that, besides having truncation errors, have the need to use harmonic average for calculating the permeabilities at the control volume interfaces, like FVM and "EbFVM Verma", the solutions are always underestimated. The other methods, FEM and "EbFVM Cordazzo", showed solutions overestimated, but according to Fig. 5*d* with smaller errors.

Ribeiro & Romeu (1997) have examined the performance of some numerical methods on the computation of the effective permeability in coarse and refined grids for another example of heterogeneous media. They solved the problem depicted in Figure 6*a*, where the domain is subjected to the same boundary conditions as the previous problem, but with a new permeability map presented in that figure.

The reference solution (k_{eq} = 37.71) was calculated by Ribeiro & Romeu (1997) refining the original 4x4 grid up to 700x700. The results obtained here are shown in Fig. 6*c*, where we can note the same tendency as the previous problem, which is both FE and "EbFVM Cordazzo" overestimating the solution for k_{eq}, and both FVM and "EbFVM Verma" underestimating the solution for k_{eq}. But now, the "EbFVM Verma" has presented much worse results, as we can see in Fig. 6*d*.

Therefore, the greater accuracy of the EbFVM solution in steady-state Dirichlet problems is not achieved in steady-state Neumann problems. Actually, for the problems considered here with specified boundary fluxes, the performances of the EbFVM that stores the physical properties in the centre of the elements and the Galerkin FEM formulations are comparable. Other examples corroborating this feature have already been showed in the literature (Banaszek, 1989). On the other hand, both the EbFVM that stores the physical properties in the centre of the control-volumes, and the FVM have not presented so good results. The main reason seems to be the averaging done in the internodal permeabilities. Although, as they are only preliminary results, it is important to study even more the influence of averaging properties in the simulation results, mainly in problems involving saturation.

2.3 Comparison among different shape functions in the EbFVM

In this section, the solutions of the EbFVM, which stores the physical properties in the centre of the elements, using different shape functions in the upscaling problem depicted in Fig. 5 are compared. The comparison is done among cases involving triangular elements with linear shape functions, Fig. 7*a*, quadrilateral elements with bi-linear shape functions, Fig. 7*b*, and quadrilateral elements with quadratic shape functions, Fig. 7*c*, for cases where the number of nodes is identical.

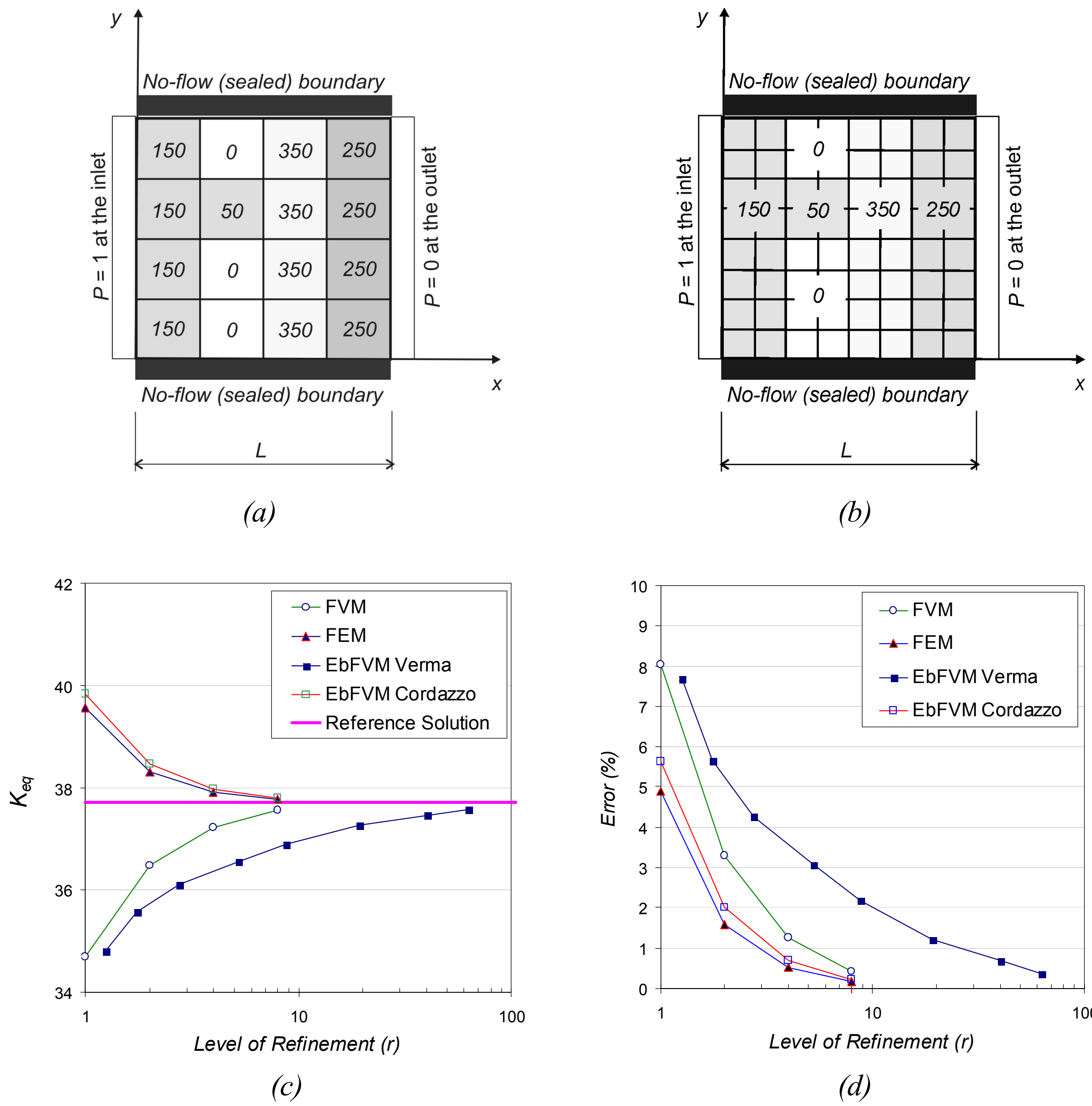


Figure 6- Second upscaling problem analyzed: *(a)* boundary conditions and permeability map used to compute the effective permeability in a grid without refinement (r=1), and *(b)* in a grid with two levels of refinement (r=2); *(c)* values of k_{eq} computed by different methods as a function of refinement; *(d)* values of absolute perceptual errors vs. level of refinement for different methods

The elements presented in Fig. 7*c* are called higher-order elements, and they often give more accurate representations than the linear elements considered in Fig. 7*a* e 7*b*. At the same time, however, they are generally more expensive in terms of computational effort than the basic linear elements. Thus, the cost-effectiveness of various elements is often in dispute. Nevertheless, due to our purpose of using quadratic shape functions in a new local mesh refinement technique for EbFVM in the next section of this paper, the comparison done here is justified. The linear, bi-linear and quadratic shape functions used in the simulations can be obtained in Cook *et al*. (1989).

It is possible to show that for single-phase incompressible flow problems using linear triangles, Galerkin FEM and EbFVM formulations give the same discretized equations (Fung *et al*., 1991), but it does not occur when one deals with quadrilateral elements. Thus in Fig.

7*d*, the results for FEM and EbFVM, for the grids presented in Fig. 7*a*, are identical and have been called here "Triangles FEM/EbFVM". Note in the same figure that the results with greater accuracy are given by the EbFVM quadratic, as expected. This characteristic can be utilized with advantage in regions where we would desire to refine, because in these regions, very often, there is required a more accurate solution. The using of a higher order shape function can be a good choice.

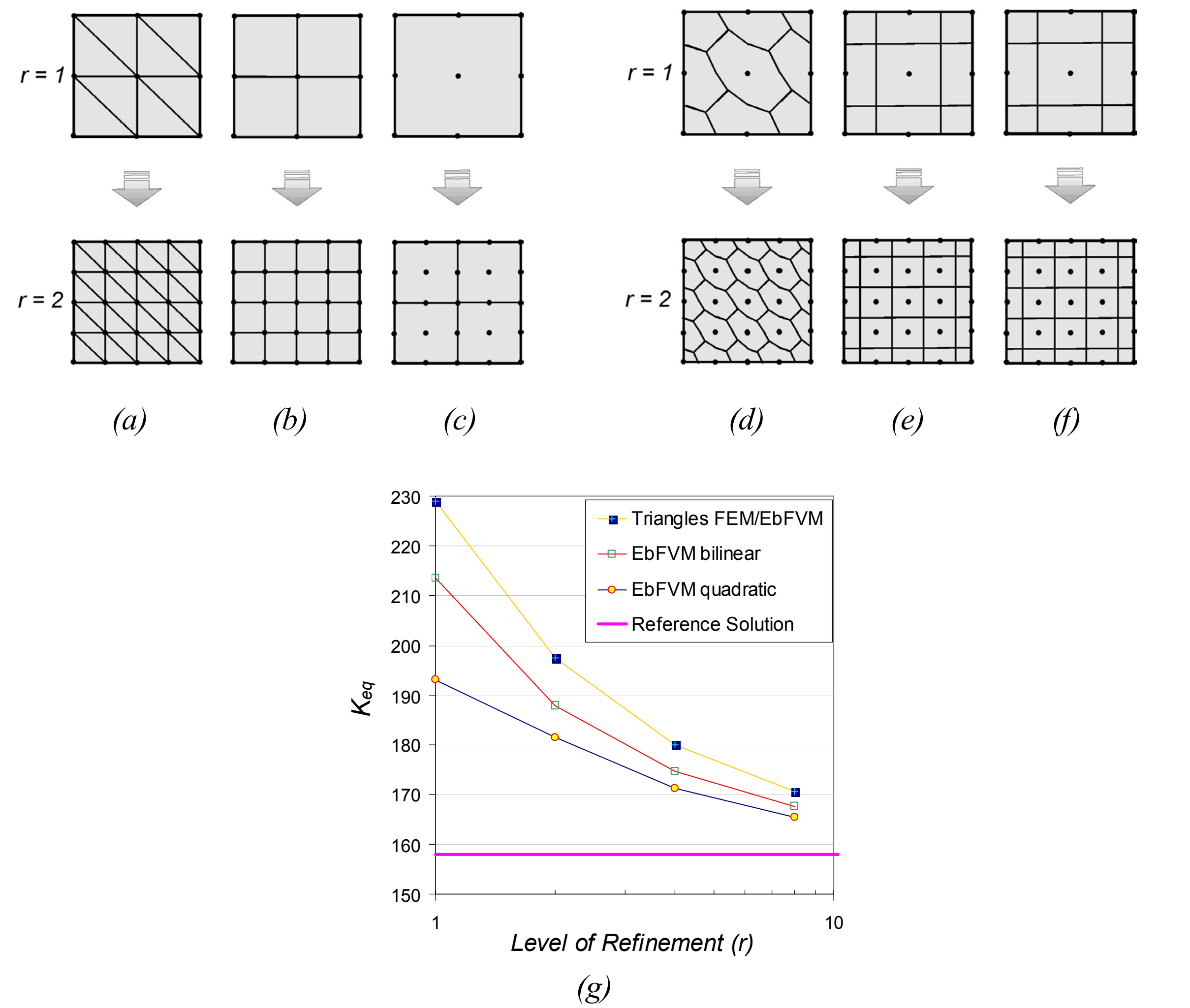


Figure 7- Comparison among the solutions of EbFVM with different shape functions: *(a)* linear (triangular elements), *(b)* bi-linear (quadrilateral elements), and *(c)* quadratic (quadrilateral elements). The control volumes are shown in *(d)*, *(e)* and *(f)*. The values of k_{eq} computed by different methods as a function of refinement are presented in *(g)*.

3. A LOCAL MESH REFINEMENT TECHNIQUE FOR EbFVM

The local mesh refinement aims to save computational effort, since a simple grid is often not sufficient for supplying a good description of particularly areas, e.g. in the vicinity of the wells, boundaries and discontinuities. In this section, the basic ideas of a new local mesh refinement technique for EbFVM are presented.

This technique is based on the using of elements with variable numbers of nodes, which possess four through eight nodes. Figure 8*a* presents a grid composed by elements with 3 to 8 nodes, and its related control-volumes. Note that in this approach, even though the global grid is still unstructured with triangular and quadrilateral elements, the refined elements are locally structured, because they are always quadrilateral elements divided uniformly in four elements. Besides, it is easy to understand that this solution is applicable only if the refinement is 1:2 for each direction, i.e. at any element face, one element may only have one or two neighboring elements on each side. This feature is found in other works also (Zeeuw, 1993; Heinemann & Brand, 1989).

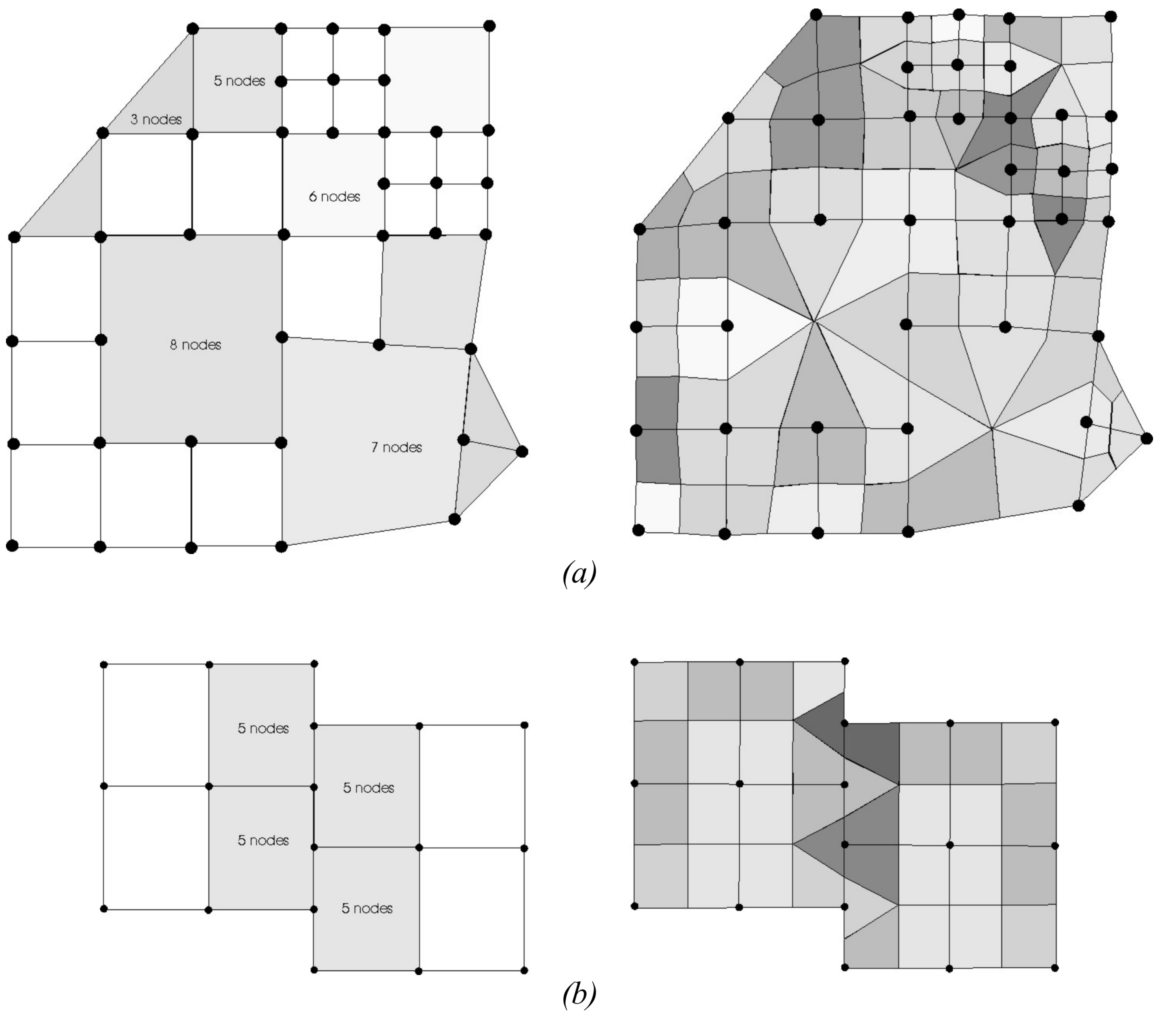


Figure 8- Grid composed by elements with variable numbers of nodes (left), and its control-volumes related (right) in *(a)* a general case and *(b)* a vertical fault case.

In Fig. 8*b* is presented a vertical fault that is discretized using elements with variable numbers of nodes. Therefore, the same technique presented before for local refinement can be used successfully in the fault discretization.

Figure 9 shows an example of an eight-node element. When all eight nodes are present, the element is a Lagrange element, except for the central node presented in the previous section. When only four nodes are present, the element degenerates to the basic bilinear quadrilateral. Any of nodes 5 through 8, according to Figure 9, may be added or omitted.

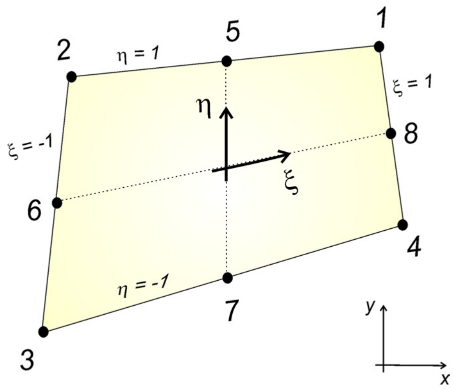


Figure 9- Eight-node element

The shape functions for midside-nodes 5 to 8 can be constructed as (Hughes, 1987)

$$N_a = \frac{1}{2}\left(1 - \xi^2\right)\left(1 + \eta_a \eta\right), \qquad a = 5 \text{ and } 7 \tag{3}$$

$$N_b = \frac{1}{2}\left(1 + \xi_b \xi\right)\left(1 - \eta^2\right), \qquad b = 6 \text{ and } 8 \tag{4}$$

We can construct the other four shape functions (N_1 to N_4) in a much appropriated form as

$$N_1 = N_1^* - \frac{1}{2}\left(N_8 + N_5\right) \tag{5}$$

$$N_2 = N_2^* - \frac{1}{2}\left(N_5 + N_6\right) \tag{6}$$

$$N_3 = N_3^* - \frac{1}{2}\left(N_6 + N_7\right) \tag{7}$$

$$N_4 = N_4^* - \frac{1}{2}\left(N_7 + N_8\right) \tag{8}$$

where N_a^* is the unmodified bilinear shape functions of the four-node quadrilateral elements given as

$$N_a^* = \frac{1}{4}\left(1 + \xi_a \xi\right)\left(1 + \eta_a \eta\right), \qquad a = 1, 2, 3, 4 \tag{9}$$

We can note if any of nodes 5, 6, 7 and 8 are absent, one may formally define N_5, N_6, N_7 and N_8 to be identically zero, respectively. About the control volumes construction, we use the same rule employed in elements of four nodes, i. e. the control volumes are created joining the center of the elements to its medians. In this case, all fluxes at one specified integration point can be calculated using data from the element where the integration point lies.

The procedure to calculate the shape functions to contemplate the local mesh refinement technique for EbFVM, as explained before, can be summarized as follows:

1. Determine the shape functions (N_i^*) for nodes 1, 2, 3 and 4 by Eq. (9). This step is done for all quadrilateral elements in the domain.
2. Determine the shape functions (N_i) for nodes 5, 6, 7 and 8 by Eq. (3) and (4) in the neighbor elements to the refined region and faults.
3. Determine the new shape functions (N_i) for for nodes 1, 2, 3 and 4 by Eq. (5) to (8) in the neighbor elements to the refined region and/or faults.

The algorithm to solve the EbFVM using this technique is still under development, but we can see previously that this implementation facilitates also the further using of multigrid techniques.

4. CONCLUSIONS

This work has initially presented a brief review of the most used numerical methods for the solution of partial differential equations, aiming their application in the petroleum reservoir simulation area. It was pointed out that all of them belong to the weighted residual approach methods. The differences among them are in the definition of the weighting and interpolation functions used. The special features of each method are consequence of the choice of those functions.

Through the solution of the Laplace's equation for the flow in a homogeneous porous media with Dirichlet boundary conditions, was possible to compare results obtained with the finite volume method (FVM), the finite element method (FEM), and the element based finite volume method (EbFVM). It was demonstrated the superiority of the EbFVM results, based on the discretization errors, for all levels of grid refinement. However, this tendency was not maintained for the same problem solved for a heterogeneous media, in which all methods show errors of the same order.

It was also analyzed some typical upscaling problems with Neumann boundary conditions. Those problems were also solved with different numerical methods and the results compared. It was shown that the least accurate results are given by the methods in which an averaging of the properties at the control volume interfaces is used. The solution of a problem with a different level of heterogeneity showed that the higher this level, the worse the results with those methods. However, because the results presented are still preliminary, is recommended a deeper study, especially with problems involving multi-phase flows.

Finally, it was presented a comparison among solutions obtained with EbFVM for a simple upscaling problem (2D chess-board problem), using different interpolation functions. Solutions with triangular, bilinear quadrangular and quadratic quadrangular elements were compared, maintaining the same number of grid-nodes in each case. As was expected, the results with quadratic quadrangular elements were the best. It was also shown that it is very promising the use of those higher order interpolation functions in a new local grid refinement scheme, as was proposed in the final part of this work. The algorithm that would use this local refinement scheme has some features that would facilitate the implementation of multigrid solution techniques.

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