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Numerical modeling of single-phase flows in heterogeneous and anisotropic porous media using the *MPFA-H* method satisfying the *Discrete Maximum Principle (DMP)* through a flux correction technique

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Abstract. The numerical simulation of fluid flow in porous media is a technical tool of fundamental importance in the oil industry. It represents a significant challenge for the design of efficient algorithms. Standard reservoir simulators use the classic *Two-Point Flow Approximation (TPFA)* technique to discretize diffusive flows. However, this technique does not provide adequate results for complex reservoirs with highly anisotropic (full tensor) and heterogeneous media and does not provide convergent results whenever using unstructured and non-k-orthogonal meshes. It is, therefore, essential to adopt efficient numerical methods and computational strategies to overcome these limitations and provide proper solutions. In this context, the cell-centered *Multipoint Flux Approximation with Harmonic Points (MPFA-H)* method is a robust and accurate alternative, capable of dealing with unstructured and non-k-orthogonal general meshes. In addition, applying the *Discrete Maximum Principle (DMP)* is essential to avoid spurious unphysical pressure oscillations, particularly for multiphase flows. In the present work, we have developed a non-linear flux-limiting procedure to avoid unphysical oscillatory pressures using the *Flux Corrected Transport (FCT)* philosophy. Our strategy guarantees that the MPFA-H method formally satisfies the DMP, even for very extreme cases involving highly anisotropic permeability tensors and extremely distorted meshes. We have solved some benchmark problems from the literature to evaluate our formulation, and our results are promising.

Keywords: Single-phase flow, Heterogeneous and anisotropic media, MPFA-H, FCT, DMP.

1 Introduction

In the context of porous media simulators, a classic approach is the segregated formulation, with the diffusion operator discretized using the Two-Point Flux Approximation (TPFA) scheme. However, this scheme fails to produce consistent solutions for non-k-orthogonal grids and for media with full permeability tensors [1, 2]. To this end, consistent Multi-Point Flux Approximation (MPFA) schemes have been developed. However, they can generate spurious oscillatory pressures fields, violating the Discrete Maximum Principle (DMP) [3]. This article uses a cell-centered MPFA using harmonic point (MPFA-H) developed by [4] to design the non-linear algebraic system satisfying the DMP constraint by a limitation process via conventional FCT [5, 6], and method of fixed-point defect correction [2, 6].

2 Mathematical Model

This section describes the mathematical model that describes the single-phase flow in heterogeneous and anisotropic media. This model is derived from the mass consarvation equation and from the generalized Darcy's law [7], considering the following simplifying assumptions: The fluid and rock are incompressible, the flow is isothermal, and total mobility is unitary. We also neglected the effects of capillarity, gravity, and chemical reactions.

2.1 Pressure equation

Let Ω be a bounded computational domain, such that $\Omega \subset \mathbb{R}^2$, with a smooth Γ boundary. Thus, in our 2D model, the elliptic pressure equation is written as [8]:

$$\nabla \cdot \vec{v} = Q, \quad \text{with} \quad \vec{v} = -\underset{\sim}{K} \nabla p \tag{1}$$

where $\vec{v}$ and Q are the total fluid velocity and the total volumetric flow rate. $\underset{\sim}{K}$ represents the absolute permeability tensor of the porous medium and p the phase pressure field. From a mathematical point of view, this tensor must be a positive-definite symmetric matrix in $\vec{x} \in \Omega$ satisfying the ellipticity condition [9].

Equation (1) is completely defined by the following boundary conditions:

$$p(\vec{x}) = p_{_D}, \quad \text{in} \quad \Gamma_D; \qquad \vec{v} \cdot \vec{n} = g_{_N}, \quad \text{in} \quad \Gamma_N \tag{2}$$

where $\vec{n}$ is a normal area vector. Furthermore, $p_{_D}$ and $g_{_N}$ represent prescribed pressure on the Dirichlet boundary (Γ_D) and prescribed flow on the Neumann boundary (Γ_N), respectively.

3 Numerical method: linear MPFA-H

The finite volume method used in this work to approximate the elliptic operator in eq. (1) is a cell-centered scheme based on the work of [1, 4, 10–12], known as MPFA-H. This method is robust for heterogeneous and anisotropic media on general polygonal meshes [12].

4 Satisfaction of the DMP: Correction of the MPFA-H via FCT

In the context of transport algorithms, the seminal work by Boris and Book [13] proposed a classic flux-limiting algorithm. Subsequently, Zalesak [5] expanded the construction of the flux limiter to a truly multidimensional approach consisting of selecting the optimal correction factors. The FCT algorithm consists of adding compensating anti-diffusion to a monotone low-order solution to obtain high-order accuracy on smooth portions of the solutions and preclude the occurrence of nonphysical oscillations in vicinity of shocks and discontinuities [14]. In the case of flux-limiting to ensure that the diffusion operators satisfy the DMP, the algebraic flux correction may provide a general framework for the design of monotone formulations on flexible unstructured meshes [3].

4.1 Discrete Maximum Principle

By discretizing the physical domain Ω with boundary Γ into a mesh $\mathcal{M}$ with a finite number of control volumes (CVs) denoted by $\Omega_{\hat{L}}$, we write the mass balance given in eq. (1) for a generic control volume $\hat{L}$ as follows:

$$\sum_{IJ \in \Gamma_{\hat{L}}} \vec{v}_{_{IJ}} \cdot \vec{N}_{_{IJ}} = \bar{Q}_{\hat{L}} V_{\hat{L}}, \quad \forall \hat{L} \in \mathcal{M}. \tag{3}$$

The global system of equations can be represented in matrix form as below:

$$M^{hi} \mathbf{p} = \mathbf{q} \tag{4}$$

where the matrix M^{hi} is the transmissibility matrix or discrete matrix obtained by a high-order operator, $\mathbf{p}$ is the pressure field vector, and $\mathbf{q}$ includes source term and the boundary conditions.

The DMP refers to the discrete analogous of the continuous maximum and minimum principles valid in second-order elliptic problems with Dirichlet or mixed boundary conditions. The global system of equations given in eq. (5) holds the DMP if $\mathbf{q} \geq 0 \rightarrow \mathbf{p} \geq 0$ [3]. If there are no sources or sinks, then the cell-centered values are limited by discrete maximum principle at steady state [15]:

$$\min_{\forall \hat{R} \in \mathcal{S}_{\hat{L}}} \left\{ p_{\hat{L}}, p_{\hat{R}} \right\} \leq p_{\hat{L}} \leq \max_{\forall \hat{R} \in \mathcal{S}_{\hat{L}}} \left\{ p_{\hat{L}}, p_{\hat{R}} \right\}, \quad \forall \hat{L} \in \mathcal{M} \tag{5}$$

where $\mathcal{S}_{\hat{L}}$ is the stencil of the control volume $\hat{L}$, which is composed of all neighboring control volumes of $\hat{R}$ that shares at least a node with it. More details can be found in [3].

4.2 Conservative algebraic splitting of fluxes

On the way to rendering this discrete scheme into one that ensures DMP, the discrete transport operator M^{hi} is modified by subtracting an appropriate amount of anti-diffusion [3, 6, 14]. To this end, we define an anti-diffusion discrete matrix M^{ad} as a symmetric matrix, with the sum of each row and each column equals to zero, designed to eliminate all positive off-diagonal entries from the higher-order operator, keeping the conservation of mass.

$$m_{ii}^{ad} = -\sum_{j\neq i} m_{ij}^{ad}, \quad m_{ij}^{ad} = m_{ji}^{ad} = \max\left\{0,\ m_{ij}^{hi},\ m_{ji}^{hi}\right\} \tag{6}$$

By subtracting the discrete anti-diffusion matrix from the higher-order diffusion operator, we get its lower-order counterpart $M^{lo} = M^{hi} - M^{ad}$. In this way, we can rewrite the higher-order operator as:

$$M^{hi} = M^{lo} + M^{ad} \tag{7}$$

Therefore, our algebraic splitting consists of obtaining a lower-order operator and an anti-diffusive operator. The lower-order counterpart must satisfy the necessary conditions of an M-matrix [14, 16]; this is important for the satisfaction of the local DMP and for the convergence of non-linear solvers[2, 14]. In addition, it is essential to note that M-matrices are also monotone [2, 3].

Finally, from eq. (6), the i-th element of the vector $M^{ad}\mathbf{p}$ is given by:

$$\left(M^{ad}\mathbf{p}\right)_i = \sum_{j} m_{ij}^{ad}(p_i - p_j), \ \ \forall\, i = 1,\ 2,\ \ldots, \mathcal{N} \tag{8}$$

Equation (8) is written again in terms of the anti-diffusive numerical fluxes as follows:

$$\left(M^{ad}\mathbf{p}\right)_i = \sum_{j\neq i} f_{ij}^{ad}, \ \ f_{ij}^{ad} = m_{ij}^{ad}(p_i - p_j) \tag{9}$$

We can also observe that, due to the symmetry of the M^{ad} matrix, we have $f_{ij}^{ad} = -f_{ji}^{ad}$. As seen in the next section, this property is essential for defining the limitation process via conventional FCT.

4.3 Linearity-preserving limiters

From eq. (7) and eq. (5), we can rewrite the global system of the discrete equations as:

$$\left(M^{lo} + M^{ad}\right)\mathbf{p} = \mathbf{q} \tag{10}$$

Equation (10) can be manipulated to obtain the semi-implicit scheme for pressure equation, leading to the following iterative recurrence law:

$$\mathbf{p}^{m+1} = \overline{\mathbf{p}} - \left(M^{lo}\right)^{-1} M^{ad}\mathbf{p}^{m}, \quad \text{with} \quad \overline{\mathbf{p}} = \left(M^{lo}\right)^{-1}\mathbf{q} \tag{11}$$

where $\overline{\mathbf{p}}$ corresponds to a low-order intermediate solution of the conventional FCT method. Next, we can represent the right-hand side of our semi-implicit scheme as follows:

$$\text{RHS} = \overline{\mathbf{p}} - \left(M^{lo}\right)^{-1} \sum_{j\neq i} \alpha_{ij} f_{ij}^{ad}\left(\overline{\mathbf{p}},\ \mathbf{p}^{m}\right) \tag{12}$$

where α_{ij} corresponds to the correction factors that will multiply the anti-diffusive numerical fluxes.

Consider that the pressure values at the local extrema of a generic cell i are given by $\overline{p}_{\mathcal{S}_i}^{max}$ and $\overline{p}_{\mathcal{S}_i}^{min}$, where the stencil $\mathcal{S}_i$ is composed of all the neighboring control volumes k that share at least a vertex with the cell i. Thus, from the Local Extremum Diminishing (LED) [17] property of the anti-diffusive term, it becomes possible to rewrite eq. (12) as:

$$\gamma_i \left|\overline{p}_{\mathcal{S}_i}^{\min} - \overline{p}_i\right| \leq \sum_{k \in \mathcal{S}_i} \alpha_{kj} f_{kj}^{ad}\left(\overline{\mathbf{p}}, \mathbf{p}^m\right) \leq \gamma_i \left|\overline{p}_{\mathcal{S}_i}^{\max} - \overline{p}_i\right|, \quad \text{with} \quad \gamma_i = \sum_{k \in \mathcal{S}_i} \frac{\theta_k}{\Omega_k} \left|\mathbf{w}_{ik} \cdot (\mathbf{x}_k - \mathbf{x}_i)\right| m_{ik}^{lo} \tag{13}$$

where γ_i is a non-negative coefficient defined in the context of the SLIP (Slope-Limited Positive) technique for the recovery of $\overline{p}_i$ [14, 18], $\mathbf{w}_{ik}$ is the vector of weights obtained by evaluating the gradients using the least squares approach [19], and $\theta_k = 1/\left|\mathbf{x}_k - \mathbf{x}_i\right|^2$ is a geometrical weighting term to be applied to unstructured meshes in order to maintain the locality of the reconstruction [20]. Furthermore, we defined γ_i using the transmissibility coefficient of the low-order operator m_{ik}^{lo} to calculate the pressure values at the local extremes. As far as the authors know, this definition was attempted for the first time in the literature and is of fundamental importance for the stability of the limitation process, which we will describe in the next section.

4.4 Limiting anti-diffusion fluxes via the FCT

In order to limit the anti-diffusion fluxes via the FCT method, we first consider a stencil $\mathcal{S}_{\hat{L}}$ made up of all the neighboring control volumes $\hat{R}$ that share at least a vertex with $\hat{L}$. Without loss of generality, we consider the anti-diffusive fluxes of a generic control volume $\hat{L}$ as follows:

$$f_{\hat{L}\hat{R}}^{ad} = m_{\hat{L}\hat{R}}^{ad}\left(p_{\hat{L}} - p_{\hat{R}}\right) \tag{14}$$

where $m_{\hat{L}\hat{R}}^{ad}$ is the transmissibility coefficient of the symmetric matrix M^{ad} obtained by algebraically splitting.

For limiting anti-diffusion fluxes, we compute the coefficients for each control volume $\hat{L}$ according to the work of [5, 6]. We then calculate the coefficients $\mathcal{P}_{\hat{L}}^{\pm}$ that represent the sums of all anti-diffusive fluxes whose effect is to increase or decrease, respectively, the value of $p_{\hat{L}}$, as follows:

$$\mathcal{P}_{\hat{L}}^{\pm} = \sum_{\hat{R} \in \mathcal{S}_{\hat{L}}} \left| \begin{matrix}\max \\ \min\end{matrix} \left(0\,,\, f_{\hat{L}\hat{R}}^{ad}\right)\right| \tag{15}$$

We also calculate the coefficients $\mathcal{Q}_{\hat{L}}^{\pm}$ which represent the maximum and minimum allowable net fluxes into or out a control volume $\hat{L}$, as follows:

$$\mathcal{Q}_{\hat{L}}^{\pm} = \gamma_{\hat{L}}\left(p_{\mathcal{S}_{\hat{L}}}^{\substack{\max \\ \min}} - \overline{p}_{\hat{L}}\right), \quad \text{with} \quad \gamma_{\hat{L}} = \sum_{\hat{R} \in \mathcal{S}_{\hat{L}}} \frac{\theta_{\hat{R}}}{\Omega_{\hat{R}}} \left|\mathbf{w}_{\hat{L}\hat{R}} \cdot \left(\mathbf{x}_{\hat{R}} - \mathbf{x}_{\hat{L}}\right)\right| m_{\hat{L}\hat{R}}^{lo} \tag{16}$$

where $p_{\hat{L}}^{\max}$ and $p_{\hat{L}}^{\min}$ are the maximum and minimum values of the pressure in the stencil $\mathcal{S}_{\hat{L}}$.

Finally, we calculate the smoothing ratios of the anti-diffusive fluxes $\mathcal{R}_{\hat{L}}^{\pm}$ and the multidimensional correction factors $\left(\alpha_{\hat{L}\hat{R}} = \alpha_{\hat{R}\hat{L}}\right)$ given, respectively, as:

$$\mathcal{R}_{\hat{L}}^{\pm} = \min\left(1\,,\, \frac{\mathcal{Q}_{\hat{L}}^{\pm}}{\mathcal{P}_{\hat{L}}^{\pm}}\right) \;\text{ if }\; \mathcal{P}_{\hat{L}}^{\pm} > 0,\;\; 1 \;\text{ o/w}, \quad \alpha_{\hat{I}\hat{R}} = \begin{cases} \min\left(R_{\hat{L}}^{-}, R_{\hat{R}}^{+}\right) & \text{if } f_{\hat{L}\hat{R}}^{ad} \geq 0 \\ \min\left(R_{\hat{R}}^{-}, R_{\hat{L}}^{+}\right) & \text{if } f_{\hat{L}\hat{R}}^{ad} < 0 \end{cases} \tag{17}$$

4.5 Non-linear defect correction scheme

Algorithm 1 presents the defect correction scheme used in this work. Our algorithm is similar to the one presented by Kuzmin Kuzmin [6] which was developed in the context of the constrained Galerkin Finite Element method by a Slope Limiting strategy – GFEM/SL.

5 Computational Examples

For all problems, we have used the standard solver in Python's Scipy module to solve the linear system of equations and $tol_1 = 1e^{-9}$ and $tol_2 = 1e^{-4}$ to solve the defect correction scheme (see Algorithm 1). We have presented a convergence study for the L_2 norm of the error and the approximate numerical convergence rate R_{L_2}, given below:

Algorithm 1: Defect correction scheme.

Input : $M^{hi}, \ \mathbf{q}$
Output: $\mathbf{p}^n$

Initialize stopping criteria: $\varepsilon_1, \varepsilon_2 \leftarrow 1$;
Initialize outer iterative counter: $n \leftarrow 1$;
Initialize the intermediate solution: $\mathbf{p}^{n=1}$;
Splitting of M^{hi}: $M^{hi} = M^{lo} - M^{ad}$;
Set the relaxation parameter: $\omega \leftarrow 1$;
while $\varepsilon_1 > tol_1$ **do**
    Initialize inner iterative counter: $m \leftarrow 1$;
    Set: $\mathbf{p}^{m=1} \leftarrow \mathbf{p}^n$;
    while $\varepsilon_2 > tol_2$ **do**
        Calculate the limited antidiffusive flux: $\bar{\mathbf{f}}^{ad}\left(\mathbf{p}^n, \mathbf{p}^m, M^{ad}\right)$ ▷ see section 4.4 ;
        Calculate the residual vector: $r^m \leftarrow \mathbf{q} - \left(M^{lo}\mathbf{p}^m + \bar{\mathbf{f}}^{ad}\right)$;
        Solve the linear system: $M^{lo}\Delta\mathbf{p}^m = \mathbf{r}^m$:
        Update the solution: $\mathbf{p}^{m+1} \leftarrow \mathbf{p}^m + \omega\Delta\mathbf{p}^m$;
        Update the stopping criteria: $\varepsilon_2 \leftarrow \|\mathbf{p}^{m+1} - \mathbf{p}^m\|_2 / \|\mathbf{p}^m\|_2$;
        Update the inner iterative counter: $m \leftarrow m + 1$;
    end
    Update the intermediate solution: $\mathbf{p}^{n+1} \leftarrow \mathbf{p}^m$;
    Update the stopping criteria: $\varepsilon_1 \leftarrow \|\mathbf{p}^{n+1} - \mathbf{p}^n\|_2 / \|\mathbf{p}^n\|_2$;
    Update the outer iterative counter: $n \leftarrow n + 1$;
end

$$E_{L_2} = \left(\frac{\sum_{i=1}^{\mathcal{N}} |\left(p(x) - \bar{p}(x)\right)^2 |\Omega_i}{\sum_{i=1}^{\mathcal{N}} \Omega_i} \right)^{1/2}, \quad R_{L_2} = \frac{\log\left(E_{L_2}(h_2)/E_{L_2}(h_1)\right)}{\log\left(h_2/h_1\right)}, \tag{18}$$

where, $E_{L_2}(h)$ is the error computed with the cell spacing of h.

5.1 Single-Phase Flow with a Smooth Solution

This first example, with smooth solutions, is presented in [3]. The objective is to compare the accuracy and convergence rate of the non-linear MPF-H/FCT against the linear MPFA-H scheme. The domain is a unitary square with Dirichlet boundary conditions obtained from the exact solution. The diffusion tensor, the source term, and the exact solution are given, respectively, by:

$$\underset{\sim}{K} = \begin{bmatrix} 100 & 0 \\ 0 & 1 \end{bmatrix}, \quad q(x,y) = 50.5 \sin \pi x \sin \pi y, \quad p(x,y) = \frac{1}{2\pi^2} \sin \pi x \sin \pi y. \tag{19}$$

Finally, we solve the problem for a sequence of distorted quadrilateral meshes. For this purpose, given a structured mesh with spacing h, its distorted counterpart is generated by applying random perturbations to the Cartesian coordinates of the internal nodes, according to the following expression: $x = x + 0.4\xi_x h, \ y = y + 0.4\xi_y h$, where ξ_x and ξ_y are random numbers with values in the range of -0.5 to 0.5.

Table 1 presents the results obtained for the convergence test of the smooth problem. As we can see, the errors and rates of the MPFA-H/FCT scheme are equivalent to those of the MPFA-H scheme; i.e., there is no significant loss of accuracy for this specific case. Furthermore, the errors obtained for our non-linear MPFA-H/FCT scheme are slightly higher for refined meshes than the results of the GFEM/SL of Kuzmin et al. [3].

Table 1. Convergence study for the MPFA-H, the MPFA-H/FCT and the GFEM/SL schemes.

h	MPFA-H			MPFA-H/FCT			GFEM/SL		
	$E_{L_{inf}}$	E_{L_2}	R_{L_2}	$E_{L_{inf}}$	E_{L_2}	R_{L_2}	$E_{L_{inf}}$	E_{L_2}	R_{L_2}
1/16	3.76E-04	1.12E-04	-	3.75E-04	1.12E-04	-	1.03E-03	2.65E-04	-
1/32	1.54E-04	2.95E-05	1.92	1.53E-04	2.94E-05	1.93	3.37E-04	6.16E-05	2.10
1/64	3.42E-05	7.80E-06	1.92	3.42E-05	7.80E-06	1.91	8.47E-05	1.04E-05	2.57
1/128	1.29E-05	2.24E-06	1.80	1.27E-05	2.24E-06	1.80	2.11E-05	2.04E-06	2,35
1/256	3.58E-06	6.28E-07	1.83	3.58E-06	6.28E-07	1.83	6.42E-06	4.68E-07	2.12

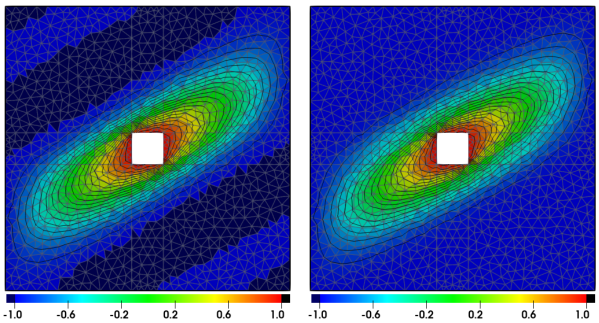
5.2 Highly Anisotropic Problem

In the second example, we consider a single-phase flow in a highly anisotropic media as described in the work of [3]. This problem aims to demonstrate that the MPFA-H scheme violates the DMP and that the limitation performs well through the non-linear MPFA-H/FCT scheme. The computational domain is a unitary square with a central hole of dimensions $[4/9, 5/9]^2$. The boundary conditions are purely Dirichlet, where the pressures at the outer and inner boundaries are given by $\bar{p}_{out} = -1$ and $\bar{p}_{inn} = 1$, respectively. The diffusion tensor is given by:

$$\underset{\sim}{K} = \underset{\sim}{R} \begin{bmatrix} 100 & 0 \\ 0 & 1 \end{bmatrix} \underset{\sim}{R}^T, \quad \underset{\sim}{R} = \begin{bmatrix} \cos(\pi/6) & -\sin(\pi/6) \\ \sin(\pi/6) & \cos(\pi/6) \end{bmatrix}. \tag{20}$$

The source term is considered zero ($Q = 0$), and the Dirichlet boundary values bound the problem's solution. We have solved this problem using an unstructured triangular mesh with 1970 CVs.

Figures 1 present the pressure field profiles obtained using the schemes described in this work. The first figure shows spurious pressures in about 34% of the mesh cells for the case analyzed with the linear MPFA-H scheme, which violates the DMP. On the other hand, our non-linear MPFA-H/FCT scheme obtains qualitatively similar results without violating the DMP (see Figure 1). Furthermore, we note that, in contrast to the results of Kuzmin et al. [3], the solution of our non-linear MPFA-H/FCT scheme is qualitatively good despite slightly more diffusion.



(a) (b)

Figure 1. Pressure field profile obtained using the unstructured triangular mesh with 1970 CVs: (a) linear MPFA-H scheme; (b) MPFA-H/FCT scheme.

6 Conclusions

In this work we have presented a non-linear MPFA-H/FCT scheme to solve single-phase flow problems in highly heterogeneous and anisotropic porous media. The scheme is based on the application of the Flux Corrected Transport formalism together with the MPFA-H method to produce accurate 2^{nd} order solutions that respect the Discrete Maximum principle even for non-orthogonal meshes and anisotropic permeability tensors. The results of our formulation are compatible with the non-linear GFEM/SL scheme. Regarding the computational cost, the inner loop presents good convergence due to the properties of the low-order operator. However, we are investigating strategies to accelerate convergence and reduce the computational cost of our non-linear defect correction scheme.

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