Finite Volume Methods with Multi-Point Flux Approximation with Unstructured Grids for Diffusion Problems

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Abstract. This paper addresses the key issue of calculating fluxes at the control-volume interfaces when finite-volumes are employed for the solution of partial differential equations. This calculation becomes even more significant when unstructured grids are used, since the flux approximation involving only two grid points is no longer correct. Two finite volume methods with the ability in dealing with unstructured grids, the *EbFVM-Element-based Finite Volume Method* and the *MPFA-Multi-Point Flux Approximation* are presented, pointing out the way the fluxes are numerically evaluated. The methods are applied to a porous media flow with a full permeability tensors and non-orthogonal grids and the results compared with analytical solutions. The results can be extended to any diffusion operator, like heat and mass diffusion, in anisotropic media.

Introduction

Finite Volume Methods have the important characteristic of being conservative at control volume level, ensuring that the discrete equations tend to the exact partial differential equations when the grid is refined at the point level. This is strongly recommended, since it guarantees that all physical quantities, like mass, momentum, energy, mass components etc, are conserved, and no sinks and/or sources of the property are numerically generated [1][2][3]. In those methods, to obtain the approximate equations, it is required the calculation of the diffusion fluxes at the interfaces of the control volumes. This calculation is of utmost importance since it influences the monotonicity and stability of the numerical scheme. For low degrees of anisotropy (of the media and of the grid) it may be attractive to keep a two-point approximation, for the sake of simplicity and stability, and to cope with the errors in the flux calculation. However, for developing more general algorithms, the two-point approximation does not suffice, and more grid points (multiple points) need to be involved to obtain a correct flux determination.

Problem Formulation. Single Phase Flow in Porous Media

The analysis of the EbFVM and MPFA methods is realized by solving a single phase flow in porous media. This problem contains all the ingredients for the analysis, especially the calculation of the normal gradient at the integration points, the key question under consideration in this paper. Considering a single phase flow of an incompressible fluid in a porous media, the governing equations are the mass conservation equation,

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0 \tag{1}$$

and the Darcy's equation

$$\vec{V} = -\overline{\overline{K}} \cdot \vec{\nabla} p \tag{2}$$

resulting in the following elliptic equation for pressure

$$\nabla \cdot \left(-\overline{\overline{K}} \cdot \vec{\nabla} p \right) = q \tag{3}$$

The mass flux calculation at each integration point, (see Fig.1), the key issue in a finite volume method, can be calculated by

$$f_i = \left(-\overline{\overline{K}} \cdot \vec{\nabla} p \right)_i \cdot \vec{\Delta} S_i \tag{4}$$

where $\vec{\Delta} S_i$ is the normal vector at the integration point. How to calculate the pressure gradient in Eq. (4) with the EbFVM and MPFA methods is now addressed. It should be recalled that there are methods which uses the two grid points approach to calculate the principal flux adding a correction to account for anisotropy and grid nonorthogonality. These are not considered here.

Finite Volume Methods

EbFVM. The Element-based Finite Volume Method was introduced in the field of fluid mechanics and heat transfer in the 80's [4] using triangular meshes. Improvements were made on co-located grids in order to avoid the pressure coupling of this arrangement [5]. Nowadays, EbFVM is largely employed for fluid flow simulations using Navier-Stokes equation and is gaining attention for simulating petroleum reservoir flows [6,7,8]. Fig. 1 depicts the elements and the control-volume constructed with the sub-elements.

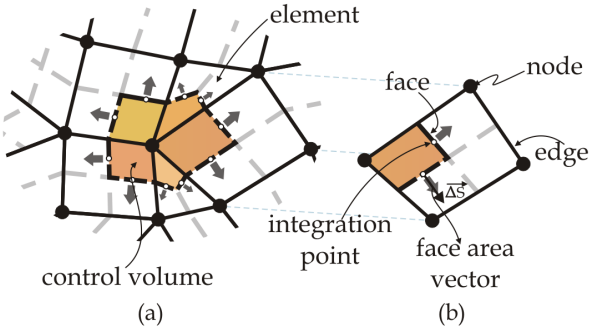

Fig. 1 EbFVM- Element and control volume (CV)

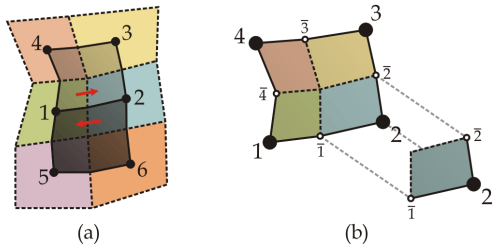

Fig. 2 MPFA–Interaction region and CV

EbFVM is a cell-vertex method which borrows from the FEM all the geometrical identities and the way to interpolate inside the domain. The approximate equations, in the other hand, are obtained via a finite volume balance of the property. The assemble procedure is also very much like as done in FEM, sweeping element-by-element, since all required information is calculated for the element. The discretized conservation equation for a control volume is obtained by summing up all fluxes at the interfaces of the sub-elements which forms the control volume, as seen in Fig.1. Considering a quadrilateral control volume, it can be seen that there are eight fluxes entering the approximate equation, against four in the case of quadrilateral grids for a cell-center method. The shape functions for a quadrilateral element are given by

$$[N]=\frac{1}{4}\begin{bmatrix}(1+\xi)(1+\eta)\\(1-\xi)(1+\eta)\\(1-\xi)(1-\eta)\\(1+\xi)(1-\eta)\end{bmatrix} \tag{5}$$

Since in our problem the variable of interest is the pressure p, it can be interpolated inside the element using shape functions as

$$p(\xi,\eta)=\sum_j N_j p_j=[N]^T[p]_e \tag{6}$$

with the corresponding gradient calculated by

$$\vec{\nabla}p\,|_{\xi,\eta}\equiv\begin{bmatrix}\partial_x p\\ \partial_y p\end{bmatrix}=\sum_j\begin{bmatrix}\partial_x N_j\\ \partial_y N_j\end{bmatrix}p_j \tag{7}$$

Defining the derivative matrix as

$$[D]=\begin{bmatrix}\partial_\xi N_1 & \partial_\xi N_2 & \partial_\xi N_3 & \partial_\xi N_4\\ \partial_\eta N_1 & \partial_\eta N_2 & \partial_\eta N_3 & \partial_\eta N_4\end{bmatrix} \tag{8}$$

and the jacobian matrix by

$$[J]=\sum_j\begin{bmatrix}\partial_\xi N_j\\ \partial_\eta N_j\end{bmatrix}\begin{bmatrix}x_j & y_j\end{bmatrix} \tag{9}$$

one obtains

$$\vec{\nabla}p=[J]^{-1}[D][p]_e \tag{10}$$

where the subscript "e" indicates that the gradient is evaluated at the element. Using now Eq. (4) the fluxes can be calculated. The four fluxes belonging to an element are determined solely as a function of the four node points which defines the element. The option of storing all media properties at the element, instead of at the control volume, avoids a discontinuity in the media properties at the location where the flux needed to be calculated. In 2D, when the eight fluxes are summed-up, to construct the approximation equation, nine grid points will be involved, being the EbFVM a multi-point flux approximation scheme too.

MPFA. This cell-center method also uses two entities, the control volume and an interaction region for calculating the fluxes, as depicted in Fig. 2. While in the EbFVM the pressure distribution inside the element is represented by a bi-linear function, given by Eq. (6), in the MPFA it is constructed an expression for the pressure gradient using linear approximations inside the interaction region. Consider Fig. 2(b), where an interaction region is shown. The pressure at point $\overline{1}$ and $\overline{2}$ can be written as

$$\overline{p_1}=p_2+[r_1]\cdot\vec{\nabla}p \tag{11}$$

$$\overline{p_2}=p_2+[r_2]\cdot\vec{\nabla}p \tag{12}$$

It is possible to combine the above expressions resulting in

$$\vec{\nabla} p = \frac{1}{V} \sum_{k=1}^{2} [\nu]_k \left(\overline{p_k} - p_0 \right) \tag{13}$$

in which

$$\begin{aligned} [\nu_1] &= [R][r_2] \\ [\nu_2] &= -[R][r_1] \end{aligned} \tag{14}$$

This pressure gradient holds for the triangular bottom right corner of the interaction region, but it is extrapolated for calculating the flux at the surface which joins point $\overline{1}$ and the center of the region, as

$$f_i = -[\Delta S]_i^T [K]_j \frac{1}{V_j} \sum_{k=1}^{2} [\nu]_k \left(\overline{p_{jk}} - p_j \right) \tag{15}$$

Defining

$$\omega_{ijk} = -\frac{[\Delta S]_i^T [K]_j [\nu]_{jk}}{V_j} \tag{16}$$

the flow rate can be calculated by

$$f_i = \sum_{k=1}^{2} \omega_{ijk} \left(\overline{p_{jk}} - p_j \right) \tag{17}$$

It must be noted that the variables $\overline{p_{jk}}$ are not known. They can be determined by applying the mass flow continuity between regions. Observe in Fig. 2(a) that it is possible to compute the mass flux at each interface using the two different gradients from the neighboring triangular regions which shares the same interface. Equating two-by-two, one obtains

$$\begin{aligned} \left(\omega_{111} \left(\overline{p_1} - p_1 \right) + \omega_{112} \left(\overline{p_4} - p_1 \right) \right) &= \left(\omega_{121} \left(\overline{p_2} - p_2 \right) + \omega_{122} \left(\overline{p_1} - p_2 \right) \right) \\ \left(\omega_{221} \left(\overline{p_2} - p_2 \right) + \omega_{222} \left(\overline{p_1} - p_2 \right) \right) &= \left(\omega_{231} \left(\overline{p_3} - p_3 \right) + \omega_{232} \left(\overline{p_2} - p_3 \right) \right) \\ \left(\omega_{331} \left(\overline{p_3} - p_3 \right) + \omega_{332} \left(\overline{p_2} - p_3 \right) \right) &= \left(\omega_{341} \left(\overline{p_4} - p_4 \right) + \omega_{342} \left(\overline{p_3} - p_4 \right) \right) \\ \left(\omega_{441} \left(\overline{p_4} - p_4 \right) + \omega_{442} \left(\overline{p_3} - p_4 \right) \right) &= \left(\omega_{411} \left(\overline{p_1} - p_1 \right) + \omega_{412} \left(\overline{p_4} - p_1 \right) \right) \end{aligned} \tag{18}$$

Solving the above system of equations one obtain the $\overline{p_{jk}}$ pressures and the four fluxes can be calculated. The original paper on the MPFA method calculates transmissibility for this system too. The relation between transmissibility and the coefficients involving geometrical and physical properties is discussed in details in [9,10].

Results.

Several comparisons were made [11] among these two versatile methods, but due to the lack of space only few will be presented here. To evaluate the accuracy in calculating the pressure gradients, two single phase flow problems in a porous media are solved for two anisotropic

situations, homogeneous and heterogeneous, using analytical solutions for comparison. The equation for both problems is

$$\nabla \cdot \left(-\overline{\overline{K}} \cdot \nabla p \right) = q \tag{19}$$

For the first problem, solved in the grid shown in Fig. 3, with a permeability tensor given by $k_{xx} = k_{yy} = 2$ and $k_{xy} = k_{yx} = 1$, and the source term by $q = 2(1 + x^2 + y^2 + xy)e^{xy}$, the solution is

$$p(x, y) = e^{xy} \tag{20}$$

It can be seen in Fig. 4 that both methods show a convergence behavior of the second order when the grid is refined (2nd order reference curve), with the MPFA presenting slightly better results. For the second problem (heterogeneous media) one has, for a square domain, $k_{xx} = k_{yy} = 1$, $k_{xy} = k_{yx} = 0$ for the left part of the domain, and $k_{xx} = k_{yy} = 20$, $k_{xy} = k_{yx} = 10$ for the right part. The source term and the solution are

$$q = \begin{cases} 10x[2sen(y) + cos(y)] + sen(y) & x < 0 \\ -20e^{x} cos(y) & x > 0 \end{cases} \qquad p(x, y) = \begin{cases} 10x[2sen(y) + cos(y)] + sen(y) & x < 0 \\ e^{x} sen(y) & x > 0 \end{cases} \tag{21}$$

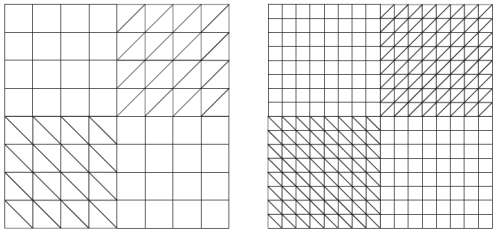

Fig. 3 Grid for the homogeneous problem

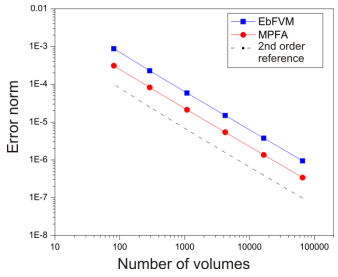

Fig. 4 Error: Homogeneous problem

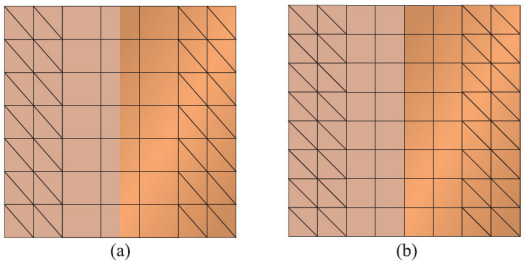

Fig. 5 Grid for the heterogeneous problem

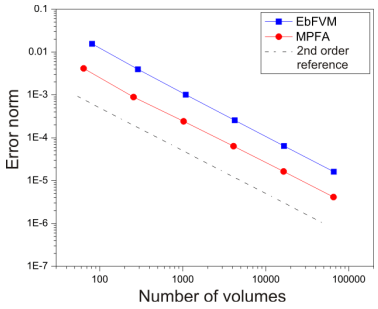

Fig. 6 Error: Heterogeneous problem

The final problem considers briefly the monotonicity of the solution. The same problem, now with a punctual source term in the center of the domain with $k_{xx} = 250.75$, $k_{yy} = 750.25$ and $k_{yx} = 432,58$ is solved. Figs. 7 and 8 show, respectively, the graphical solution for the MPFA and EbFVM methods. The pictures on the right paint in blue the elements where at least there is one of its four nodes with a value below zero, what demonstrates that monotonicity was not obeyed in both methods. The EbFVM presented smaller maximum values, but a solution with a higher degree of smoothness, compared with the oscillations presented by the MPFA method.

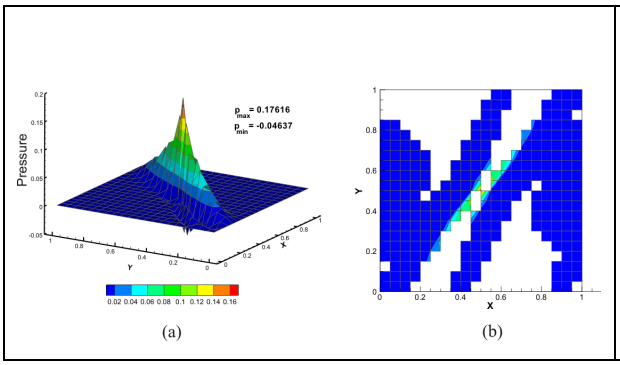

Fig. 7 Monotonicity - MPFA solution

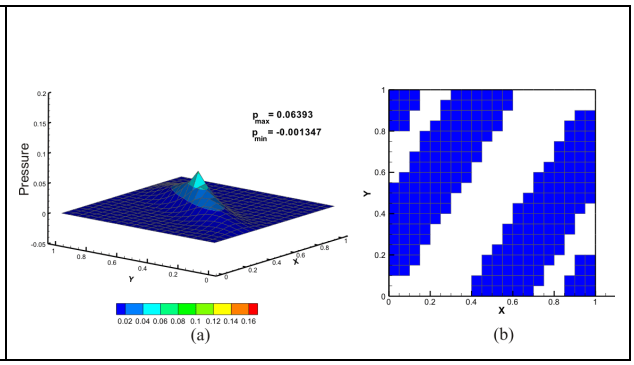

Fig. 8 Monotonicity - EbFVM Solution

Summary

The outcome of this study shows that EbFVM and MPFA are two multi-point flux approximation methods with strong capabilities for dealing with unstructured grids, but both are not unconditionally monotonic when dealing with very large gradients, a common problem for numerical schemes. Further comparisons among these methods can be found in [11].

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