Evaluation of the accuracy of two edge-based finite volume formulations for the solution of elliptic problems in non-homogeneous and non-isotropic media

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Abstract: The numerical simulation of fluid flow problems in non-homogeneous and non-isotropic media poses a great challenge from mathematical and numerical point of views. The numerical simulation of oil recovery in petroleum reservoirs and the transport of contaminants in aquifers, may involve the solution of an elliptic type equation with highly discontinuous coefficients for the pressure field, and a non-linear hyperbolic type equation for saturation field. In this work, we compare two different vertex-centered control volume formulations for the numerical solution of the elliptic equation. Both methods use median dual control volumes with an edge-based data structure. These formulations are capable of handling non-homogeneous and non-isotropic media using unstructured meshes. The first algorithm consists in a modification of the two step Crumpton’s edge-based approach. The second algorithm is closely related to the linear finite element method. Both formulations include the cross-diffusion terms in a very elegant manner, guaranteeing local conservation. For sufficient smooth problems, both methods achieve second order accuracy for the scalar field on triangular meshes. To compare the accuracy of the two edge-based procedures, we present a numerical experiment involving a non-homogeneous and non-isotropic media. For the benchmark problem solved, both formulations compare well with others found in literature.

Keywords: Elliptic Problems, Finite Volume Methods, Edge-Based Data Structure, Non-homogeneous and Non-Isotropic Media.
globally, but not locally conservative (i.e. at the cell level), requires some kind of flux recovery in order to formally guarantee local conservation [6].

In this paper, we briefly compare two different vertex-centered finite volume formulations. Both methods use median dual control volumes (Donald’s dual) with an edge-based data structure in such a way that the geometrical coefficients are associated to the edges and nodes of the primal mesh. These formulations are capable of handling both, heterogeneous and anisotropic (full tensor) media using structured and unstructured meshes. The first algorithm consists in a modification of the two step Crumpton’s edge-based approach [2]. The second algorithm is analogous to an edge-based implementation of a linear control volume finite element method. Both formulations formally include the cross-diffusion terms in a very elegant manner guaranteeing local conservation even for non-orthogonal meshes and discontinuous coefficients, keeping second order accuracy for the pressure field and, at least, first order accuracy for fluxes on general triangular meshes and on orthogonal quadrilateral meshes.

The edge-based data structure has been chosen due to the fact that vertex-centered FV schemes are superior to cell centered schemes in terms of memory usage [8,9,10], and because edge-based data structures are known to be computationally more efficient than their element-based counterparts [7,8]. In the present paper we have concentrated on the study of the accuracy and the convergence behavior of the edge-based finite volume scheme for the solution of elliptic equations with full tensor discontinuous coefficients, comparing their solutions to other obtained by using other well established formulations through the solution of some benchmark problems.

Mathematical Formulation

In the two dimensional model, the equation which defines an elliptic problem in a heterogeneous and anisotropic medium can be written as

\[ \nabla \cdot ( -K(\vec{x})\nabla u) = f(\vec{x}), \text{ with } \vec{x} = (x, y) \in \Omega \subset \mathbb{R}^2 \] (1)

where

\[ K(\vec{x}) = \begin{pmatrix} K_{xx} & K_{xy} \\ K_{yx} & K_{yy} \end{pmatrix} \] (2)

is a symmetric matrix that is allowed to be discontinuous through the internal boundaries of the domain \( \Omega \). In order to formally define an elliptic problem [3], we further assume that

\[ K_{xx} K_{yy} \geq K_{xy}^2 \] (3)

Integrating Eq. (1) and applying the divergence theorem to its left side, yields

\[ \int_{\Gamma} (-K \nabla u) \cdot \vec{n} d\Gamma = \int_{\Omega} f d\Omega \] (4)

Equation (4), which is the integral form of Eq. (1), defines, for instance, the pressure field in the fluid flow of oil and water in heterogeneous and anisotropic petroleum reservoirs or in the transport of contaminants in aquifers [2,9].

Numerical Formulation

In this section, we will briefly describe the two edge-based median-dual control volume formulations. First, we will derive the variation of the two-step edge-based Crumpton’s approach which was adapted for the solution of diffusion problems in heterogeneous media [7], in sequence we will derive an edge-based implementation of a more traditional control volume finite element method.

Edge-Based Finite Volume 1 (EBFV1)

The present approach was originally devised by Crumpton [4] for the discretization of diffusion terms in the Navier-Stokes equations with the modifications proposed by Carvalho [2]. In this approach, we first compute nodal gradients as functions of the discrete scalar field and then, we use these gradients to compute the elliptic terms in a second step. The gradients computed in the first step in a finite volume fashion are used to calculate the cross diffusion terms which naturally arise when we are handling full tensor problems (i.e. \( K_{xx} = K_{yy} \neq 0.0 \)) or when we are using non-orthogonal meshes, as both problems can be seen as equivalent [1]. The major difference between the original Crumpton’s approach [4] and the formulation presented by Carvalho [2] is that, in the latter, gradients are recovered in a domain by domain approach in order to honor possible material discontinuity.

For a general node \( I \) of the mesh, using the edge-based finite volume, Eq. (4) can be approximated, as

\[ \sum_{I_e \in \Omega} F_{\Omega}^{I} \vec{c}_{I_e} + \sum_{I_e \in \Gamma} F_{\Gamma}^{I} \vec{d}_{I_e} = f_I V_I \] (5)

where \( F_{\Omega}^{I_e} = -K \nabla u_{I_e} \) is the flux function defined at the control surface, \( V_I \) is the volume of the CV surrounding node \( I \), the upper index \( \Omega \) represents approximations that are associated to every edge \( I_\iota \).
of the primary mesh which is connected to node \( I \), \( \Gamma \) refers only to boundary edges connected to that node, the summation \( \sum_{I \in \Omega} \) is performed over the internal edges connected to node \( I \) and \( \sum_{I \in \Gamma} \) is only performed over boundary edges. The geometrical coefficients \( \tilde{C}_{IJ} \) and \( \tilde{D}_{IJ} \) are defined as

\[
\begin{align*}
\tilde{C}_{IJ} &= A_x, \tilde{n}_{k+1} + A_x \tilde{n}_K \\
\tilde{D}_{IJ} &= A_x \tilde{n}_L
\end{align*}
\]  

(6)

In Equation (6), \( A_x, A_{x+1} \) and \( A_x \) are the areas of the control surfaces associated to the control surface normals \( \tilde{n}_K, \tilde{n}_{x+1} \) and \( \tilde{n}_x \). Further details can be found in [2].

In order to compute the nodal gradient, we use the divergence theorem to integrate the gradient of the scalar variable at node \( I \), obtaining

\[
\int_{\Omega} \nabla u_I \, d\Omega = \int_{\Gamma} u_I \tilde{n} \, d\Gamma
\]  

(7)

The average gradient \( \nabla u_I \) in the control volume can be computed as

\[
\nabla u_I = \left( \int_{\Omega} \nabla u_I \, d\Omega \right) / V_I
\]  

(8)

Similarly to Eq. (5), and by dropping out the over bar, we can write the discrete form of Eq. (7) as

\[
\nabla u_I V_I = \left( \sum_{I \in \Omega} u_{I_1} \tilde{C}_{IJ} + \sum_{I \in \Gamma} u_{I_1} \tilde{D}_{IJ} \right)
\]  

(9)

In the case of heterogeneous media, fluxes definitions over the control surfaces located at the interface between different materials can be ambiguous. If the nodal gradients computed as described in Eq. (9) are directly used for flux computations, an inconsistent flux would be obtained along control surfaces adjacent to material discontinuities. In order to circumvent this problem, gradients are recovered in a sub-domain by sub-domain approach. First, material properties (e.g. permeability) are associated to sub-domains. For each physical sub-domain, we store a list of edges and nodes and their associated geometrical coefficients. For the mesh considered in Fig. (1), it is necessary to include new geometrical coefficients and \( \tilde{D}_{IJ} = A_x \tilde{n}_L \), which are quantities related to internal boundary edges, in order to properly reconstruct gradients and fluxes in a particular sub-domain. These coefficients are used to properly recover gradients for each physical sub-domain of the problem, allowing for a continuous by parts gradient computation. Therefore, for heterogeneous media, we can rewrite Eq.(9) as

\[
\nabla u_I^{OL} = \frac{1}{V_I} \left[ \sum_{I \in \Omega} C_{IJ} \frac{(u_I + u_{I_1})}{2} + \sum_{I \in \Gamma} D_{IJ} \frac{(5u_I + u_{I_1})}{6} + \sum_{I \in \Gamma} D_{IJ} \frac{(5u_I + u_{I_1})}{6} \right]
\]  

(10)

In Equation (10), \( \nabla u_I^{OL} \) is the nodal gradient and \( V_I^{OL} \) is the control volume of a node \( I \) associated to the sub-domain \( \Omega_g \), and \( \tilde{C}_{IJ} \) and \( \tilde{D}_{IJ} \) refer to the geometrical coefficients of the edge \( IJ \) associated to the sub-domain \( \Omega_g \). Finally, it is worth noting that in the present sub-domain by sub-domain approach, \( \tilde{D}_{IJ} \) refers to both, external and internal boundary edges, and \( \Gamma_{RE} \) and \( \Gamma_{RI} \) refer, respectively, to loops over external boundary edges and internal edges between multiple sub-domains. In order to compute the fluxes of Eq. (5), we define a local frame of reference, in which one axis is placed along the edge direction (P), and another axis (N) is orthogonal to the direction (P), and split the gradients into two components

\[
\nabla u_I^{OL} = \nabla u_I^{OL}(N) + \nabla u_I^{OL}(P)
\]  

(11)

The component of the gradient parallel to the edge direction \( \nabla u_I^{OL}(P) \) is replaced by a local second order central difference approximation \( \nabla u_I^{OL}(P) \), while the normal component is computed using the arithmetic mean between the two nodal gradients computed by Eq.(9), and Eq. (11) may be rewritten as

\[
\nabla u_I^{OL} = \nabla u_I^{OL}(N) + \nabla u_I^{OL}(P)
\]  

(12)

Defining the continuous “hybrid” mid-edge flux function as

\[
F_{IJ}^{OL} = -K^{OL} \nabla u_I^{OL}
\]  

(13)

in which the term hybrid was used to indicate that one part of the mid-edge gradient is computed using the traditional edge-based finite volume approach by averaging the nodal recovered gradients, and the other part is computed using the compact two point finite
difference scheme. Using the new surface flux approximation given by Eq. (13), we can redefine Eq. (5) as

\[
\sum_{E \in \Omega} \left( \sum_{i=1}^{N_{\text{ele}}} \vec{F}_{i}^{\alpha_{i}} \cdot \vec{C}_{i}^{\alpha_{i}} + \sum_{i=1}^{N_{\text{ele}}} \vec{F}_{i}^{T} \cdot \vec{D}_{i}^{T} \right) = \sum_{E \in \Omega} \vec{f}_{E} \cdot V_{E}^{\alpha_{E}}
\] (14)

and \(N_{\text{dom}}\) refers to the number of domains that surrounds node \(I\), and the term \(f_{E}^{\alpha_{E}}\) stands for the distributed source term associated to the volume \(V_{E}^{\alpha_{E}}\) within the sub-domain \(\Omega_{h}\).

The expression above is built in a sub-domain by sub-domain basis (i.e. looping over sub-domains) in order to formally guarantee that nodal gradients and fluxes are correctly approximated for each material along interface edges. Further details can be found in [2]

**Edge-Based Finite Volume 2 (EBFV2)**

This approach can be obtained considering a simple linear variation of the scalar variable “\(u\)” throughout the edges of the primal mesh. In this case, gradients are constant over the elements of the primal mesh and fluxes can be readily computed through the dual mesh because the diffusion coefficient is constant throughout the edges of the primal mesh. In this case, the left hand side of Eq. (4) can be written as:

\[
- \frac{1}{V'} \left( K \nabla u \right) \cdot \vec{n} \partial \Omega_{E} = \sum_{i} \left(-K \nabla u^{e} \right) \cdot \vec{C}_{i}^{e} - \sum_{i} \vec{E}_{i}^{e} \cdot \vec{C}_{i}^{e}
\] (15)

In Eq (15) the superscript “\(e\)” refers to the flux contribution \(\vec{F}_{i}^{e} = -K \nabla u^{e}\) that comes from edge \(IJ\) and that is associated to element “\(e\)” adjacent to the edge \(IJ\). For a general element “\(e\)” of the primal mesh, the gradient can be computed as:

\[
\nabla u^{e} = \frac{1}{V'} \left( \frac{u_{i} + u_{j}}{2} \right) \left( 2 \vec{D}_{i}^{e} \right)
\] (16)

where \(V'\) is the volume (area in 2-D) of the element, \(\vec{D}_{i}^{e}\) are the outward edge/area vectors, and the summation is performed along the edges of the primal mesh that define this element. In the present paper, we have used only triangular elements.

Therefore, for a single triangular element defined by nodes 1, 2 and 3, we can write:

\[
\nabla u^{e} = \frac{1}{V'} \left[ \frac{u_{1} + u_{2}}{2} \right] \left( 2 \vec{D}_{12} \right) + \frac{u_{2} + u_{3}}{2} \left( 2 \vec{D}_{23} \right) + \frac{u_{3} + u_{1}}{2} \left( 2 \vec{D}_{31} \right)
\] (17)

This gradient is then placed in Eq. (15) in order to compute the fluxes through control surfaces. After some geometrical and algebraic manipulation (to be presented in a future paper) it is possible to write flux contributions in a pure edge-based fashion. Source terms are computed analogously to the EBFV1 as described in the previous section. This formulation produces a symmetric system of equations which is assembled in an edge-by-edge basis.

**Error Definition**

To evaluate the accuracy of both finite volume methods, we define the asymptotic truncation error as

\[
\|E_{\Omega}\| = Ch^{q} + O(h^{q+1})
\] (18)

where \(h\) is the mesh spacing, \(q\) is the order of the error, which represents the convergence rate and \(C\) is a constant that is independent of \(h\) and \(\|\cdot\|\) is some specified norm. In this case, the convergence rate \(q\) is estimated as:

\[
q = \log_{2} \frac{\|E_{h}\|}{\|E_{h/2}\|}
\] (19)

The convergence rates were estimated using the following discrete norm: the RMS (Root Mean Square) norm, \(\|E\|_{\text{RMS}}\), which is computed as

\[
\|E\|_{\text{RMS}} = \|\hat{u} - u\|_{\text{rms}} = \left( \sum_{i=1}^{NP} \left( \hat{u}_{i} - u_{i} \right)^{2} / NP \right)^{1/2}
\] (20)

where \(u\) is the exact solution, \(\hat{u}\) is the approximate solution and \(NP\) is the number of nodes of the computational mesh.

**Example: Non-Homogeneous and Non-Isotropic Media**

The following example consists in a unity square formed by two different materials. Numerical Dirichlet boundary conditions are obtained from the exact
solution. Crumpton [2] solved this problem using a FCFV with structured orthogonal quadrilateral meshes. The problem can be compactly defined by

\[ \nabla (K \nabla u) = f(x, y) \]  

where the discontinuous source term and the full tensor discontinuous diffusion coefficient are given, respectively, by

\[ f(x, y) = \begin{cases} 
-2\sin(y) - \cos(y) & \text{for } x \leq 0 \\
2\alpha x - \sin(y) & \text{for } x > 0 
\end{cases} \]

and

\[ K = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \text{ for } x < 0 \\
\alpha \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \text{ for } x > 0 \]  

with \( \alpha \) controls the strength of the discontinuity (i.e. the jump in the material property) between the two different regions. The exact solution for this problem, given in [2,3], is also presented in Eq. (24).

\[ u(x, y) = \begin{cases} 
2\sin(y) + \cos(y) & \text{for } x \leq 0 \\
\exp(x) \cos(y) & \text{for } x > 0 
\end{cases} \]

We have solved this problem using a sequence of uniform structured triangular meshes with \( N = (9 \times 9), (17 \times 17), (33 \times 33) \) and \( (65 \times 65) \) nodes.

Tables (1) to (6) present the root mean square errors, \( \|E\|_{\text{RMS}} = \|\bar{u} - u\|_{\text{RMS}} = \left( \sum_{N=1}^{N} (\bar{u}_j - u_j)^2 / NP \right)^{1/2} \), where \( \bar{u} \) is the exact solution, \( \bar{u} \) is the approximate solution and \( NP \) is the number of nodes of the computational mesh, and the convergence rates \( q \approx \log_{10}(\|E_1\|_{\text{RMS}} / \|E_{10}^2\|_{\text{RMS}}) \), for \( \alpha = 1.0 \) and \( \alpha = 1000.0 \), obtained with the FCFV method of Crumpton [3] using orthogonal quadrilateral meshes, and the EBFV1 and the EBFV2 schemes using structured triangular meshes. As it can be clearly observed in Tables (1) to (6), for this particular benchmark problem, despite the fact that the increase of the strength of the discontinuity also increases the magnitude of the error for the three methods, the EBFV1, the EBFV2 and the FCFV methods show second order spatial accuracy for both values of \( \alpha \). It can also be noted that for all tested cases, that the results obtained with the EBFV1 and EBFV2 schemes are quite similar to the results obtained with the FCFV method.

**Table 1. Errors and convergence rates for the FCFV (with \( \alpha = 1.0 \).)**

<table>
<thead>
<tr>
<th>N</th>
<th>( |E|_{\text{RMS}} )</th>
<th>( q_{\text{RMS}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>3.33e-003</td>
<td>1.8294</td>
</tr>
<tr>
<td>17</td>
<td>9.37e-004</td>
<td>1.9533</td>
</tr>
<tr>
<td>33</td>
<td>2.45e-004</td>
<td>1.9709</td>
</tr>
<tr>
<td>65</td>
<td>6.25e-005</td>
<td></td>
</tr>
</tbody>
</table>

**Table 2. Errors and convergence rates for the EBFV1 (with \( \alpha = 1.0 \).)**

<table>
<thead>
<tr>
<th>N</th>
<th>( |E|_{\text{RMS}} )</th>
<th>( q_{\text{RMS}} )</th>
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<tr>
<td>9</td>
<td>6.02e-003</td>
<td>1.9989</td>
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<tr>
<td>17</td>
<td>1.50e-003</td>
<td>1.9999</td>
</tr>
<tr>
<td>33</td>
<td>3.77e-004</td>
<td>2.0012</td>
</tr>
<tr>
<td>65</td>
<td>9.40e-005</td>
<td>2.0014</td>
</tr>
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</table>

**Table 3. Errors and convergence rates for the EBFV2 (with \( \alpha = 1.0 \).)**

<table>
<thead>
<tr>
<th>N</th>
<th>( |E|_{\text{RMS}} )</th>
<th>( q_{\text{RMS}} )</th>
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</thead>
<tbody>
<tr>
<td>9</td>
<td>1.49e-003</td>
<td>1.9536</td>
</tr>
<tr>
<td>17</td>
<td>3.92e-004</td>
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<tr>
<td>33</td>
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<td>65</td>
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<td>1.9915</td>
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</table>

**Table 4. Errors and convergence rates for the FCFV (with \( \alpha = 1000.0 \).)**

<table>
<thead>
<tr>
<th>N</th>
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<th>( q_{\text{RMS}} )</th>
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</thead>
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<tr>
<td>9</td>
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<td>17</td>
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<td>33</td>
<td>1.21e-002</td>
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<tr>
<td>65</td>
<td>3.04e-003</td>
<td>1.9929</td>
</tr>
</tbody>
</table>

**Table 5. Errors and convergence rates for the EBFV1 (with \( \alpha = 1000.0 \).)**

<table>
<thead>
<tr>
<th>N</th>
<th>( |E|_{\text{RMS}} )</th>
<th>( q_{\text{RMS}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>4.39e-000</td>
<td>1.9536</td>
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<td>1.13e-000</td>
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<td>65</td>
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<td>1.9915</td>
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</tbody>
</table>

**Table 6. Errors and convergence rates for the EBFV2 (with \( \alpha = 1000.0 \).)**

<table>
<thead>
<tr>
<th>N</th>
<th>( |E|_{\text{RMS}} )</th>
<th>( q_{\text{RMS}} )</th>
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<td>1.14E-001</td>
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<td>33</td>
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<tr>
<td>65</td>
<td>8.04E-003</td>
<td>1.9760</td>
</tr>
</tbody>
</table>
Conclusions

In this paper we have briefly presented two edge-based node centered finite volume formulations (EBFV1 and EBFV2) which can be used to solve elliptic type equations with highly discontinuous coefficients using edge-based data structures. These elliptic equations naturally arise in the modeling of heat conduction problems and flux flow through porous media, such as the two-phase flow of oil and water in petroleum reservoirs and the transport of contaminants in aquifers. Full tensors (non-diagonal diffusion coefficients) and unstructured non-orthogonal meshes are naturally handled by both EBFV formulations and the cross diffusion terms are properly computed. To show the relative accuracy of the two presented finite volume procedures, we have solved a benchmark problem that involves a non-diagonal and discontinuous diffusion coefficient and a discontinuous distributed source term. Both methods have shown second order accuracy for the scalar variable (e.g. pressure). Computational efficiency and mononicity in the presence of highly non-isotropic solutions of the two EBFV methods will be investigated in the near future. For the example analyzed our results compare quite well with other results found in literature.

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