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METHODS FOR CALCULATING THE THERMAL CONDUCTIVITY AT THE CONTROL-VOLUME SURFACES

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Abstract. *The solution for equations which contains problems of convection-diffusion using the methods of finite volumes, the thermal conductivity value is required at the faces of the control volumes. The primary role of this study is to assess the performance of some standard numerical schemes and introduce new schemes for the interpolation of the thermal conductivity at the faces of the control volumes being them a function of temperature and the medium (solid or fluid). Results are obtained for five one-dimensional problems related to conduction and advection-diffusion of heat, with or without a source of heat generation which involves uniform and non-uniform thermal conductivity. In addition, different meshes are used to assess the reliance of the results of the meshing. The performance of the schemes to interpolate the thermal conductivity takes into account the accuracy of the results and the computational costs for obtaining the solution. Two of the proposed schemes presented higher accuracy and consistency in the results.*

Keywords: *finite volumes method; thermal conductivity; discretization errors; effective order*

1. INTRODUCTION

The use of numerical techniques in order to solve problems in engineering and physics is nowadays a reality, thanks to the development of high-speed computers and large storage capacity (Maliska (2004)). The aim of the numerical method is to solve one or more differential equations, replacing the existing derived ones by algebraic expressions which involve the unknown function. When the analytic solution is not an option the choice is made by the numerical one. The solution is reached through a discrete number of points with a specific error, it is expected that the greater the number of points, the closer to the exact solution the numerical solution will be.

Regardless the numerical methodology used, the results must be checked in order to ensure their relevance. Verification is the process which quantifies the numerical error by comparing the results of the numerical solution with the existing analytical solution (AIAA (1998); Roache (1998)).

The solution for problems of advection-diffusion via numerical methods can be obtained by the Finite Volume Method (FVM). The FVM is widely used for the solution of problems with fluid and heat flow (Maliska (2004); Patankar (1980)). One of the challenges which arises in the situations of problems involving heat or mass is about the treatment of the thermal conductivity when it is highly dependable on the temperature or discontinuities in the thermal conductivity are present due to different media (Chang and Payne (1990, 1992); Tao (1989)).

One very common example in which the thermal conductivity is highly dependent on the temperature is when phase changes are present (Voller (2001); Voller and Swaminathan (1993)). Other examples can be found in composite materials in which the structure is made from several layers of materials which have different thermal conductivities. Also, it is very common in engineering problems to occur walls composed of two or more materials. In all these cases it is necessary to build a numerical scheme in order to determine the coefficient of thermal conductivity of the faces of the control volumes (Maliska (2004); Patankar (1980); Versteeg and Malalasekera (1995)).

Figure 1 ilustrates the situation described above and shows the Control Volumes (CV) with uniform discretization for a one-dimensional case. The volumes are numbered from 1 to N (real volumes) for the calculation domain. Two other volumes, called virtual volumes, are placed beyond the left and right edges. Both are used to prescribe boundary conditions. According to Maliska (2004), the boundary conditions imposed when using the volume technique provides an easy implementation of orthogonal meshes.

Being the faces of CVs (faces "w" and "e") placed in an intermediate position between two nodes of the mesh, the temperature values are not known even after the completion of the solution process. Unless the thermal conductivity is

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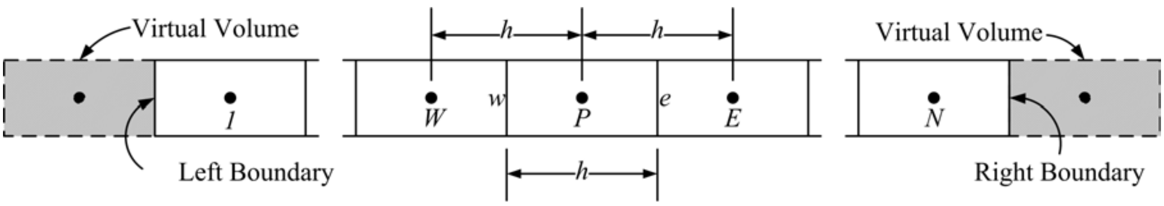

Figure 1. Control Volumes with uniform discretization.

not dependent on the temperature and also uniformly distributed throughout the calculation domain, a scheme must be built to determine the values of the thermal conductivity at the faces of CV (Patankar (1980)).

One of the most common schemes used to calculate the thermal conductivity at the faces of CVs is the arithmetic average which considers a linear distribution of the thermal conductivity (k) between two neighboring nodes at the face of the CV Patankar (1980). In this paper the arithmetic average scheme is named MAk.

Patankar (1980) presented the outline of the harmonic average of the thermal conductivity (MHk) scheme as an alternative to the arithmetic average. The scheme of the harmonic average gives good results without requiring large computational effort for the problems with changing media in which the thermal conductivity varies at the face of the CV.

Liu and MA (2005) presented an arithmetic average of the nodal temperatures between two neighboring nodes of a face of the VC (MAT). With this temperature it is possible to calculate the thermal conductivity in one face of the VC. The authors demonstrated that the scheme is effective and low computational cost in those problems with medium change in the meshing, the change in thermal conductivity occurs in the node.

The schemes KG2P and KG3P analyzed in this paper were presented by Voller (2001). In these schemes in order to assess the thermal conductivity at the faces of the CV, it is used the approach of Kirchhoff local processing. Kirchhoff's transformation (Crank (1984)) provokes a change of the variable by a numerical integration and consequently many problems such as the generation of discrete non-linear equations, the need for treatment of the term source and the boundary conditions are totally eliminated (Voller (2001)).

It has been observed contradictory results when choosing the best scheme to calculate the thermal conductivity, and which situations it might be applied. For instance, problems involving phase change, MAk does not provide the accuracy required and therefore the same with MHk which provides good results only when the phase change coincides with the face of CV (Voller and Swaminathan (1993)).

Some of the schemes widely known in the literature to calculate the thermal conductivity at the face of CV have special characteristics and thus are made dependent on the type of problem to which is being applied. Obviously, the accuracy and convergence of the scheme are key factors to the numerical solution of the problem (Schneider (2007)).

This study presents seven new schemes to calculate the thermal conductivity at the faces of CVs and also an assessment with five schemes frequently used in the literature. This assessment takes into account the discretization error, the effective order of approximation and computational cost to reach the solution. Further details are presented in Carvalho (2011).

2. DEFINITION OF TEST PROBLEMS

For the purpose of introducing various schemes to calculate the thermal conductivity at the face of the CV of a one-dimensional problem, it will be considered a permanent condition pre-arranged by the following main equation:

$$F\frac{dT}{dx} = \frac{d}{dx}\left(k\frac{dT}{dx}\right) + S \;, \tag{1a}$$

$$T\,|_{x=0} = T_0 \;, \tag{1b}$$

$$T\,|_{x=1} = 1 \;, \tag{1c}$$

T is temperature, x is the spatial coordinate of the calculation domain, k is the thermal conductivity, and S is a source term. A constant value other than zero for the term F allows the evaluation schemes to calculate the thermal conductivity in the existence of the advection term, whether or not this term is zero.

Based upon a uniform mesh, as Fig. 1, Eq. (1) is discretized by FVM, which provides for a generic node P, the following equation:

$$a_P T_P = a_e T_E + a_w T_W + b_P \tag{2}$$

where,

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$$a_w = \frac{k_w}{h} + \frac{F}{2}\ , \qquad a_e = \frac{k_e}{h} - \frac{F}{2}\ , \qquad a_P = a_w + a_e\ , \qquad b_P = \int_{x_w}^{x_e} S dx. \tag{3}$$

Equation (2) is the discretized algebraic equation for one-dimensional problems, where a_P, a_e and a_w are coefficients, and T_P, T_E and T_W are the temperatures in the central (P), east (E) and west (W) nodes. The independent term of algebraic equation is represented by b_P obtained analytically. The uppercase subscripts indicate the assessment in control nodes and the lower-case subscripts indicate the face on the CV assessment. The terms of Eq. (2), shown in Eq. (3) are obtained when using the CDS scheme (Central Differencing Scheme) (Maliska (2004); Patankar (1980); Ferziger and Peric (2002)).

Table 1. Test Problem

Problem	Thermal Condutivicty - k		T_0	F	S
A	$k = \exp(T)$	$0 \le x \le 1$	0	0	0
B	$k = T^3$	$0 \le x \le 1$	0.2	0	0
C	$k = \begin{cases} k_1 = 1 \\ k_2 = 10 \end{cases}$	$0 \le x < 0.5$ $0.5 \le x \le 1$	0	0	0
D	$k = \begin{cases} k_1 = 100\ \exp(T) \\ k_2 = \exp(T) \end{cases}$	$0 \le x < 0.5$ $0.5 \le x \le 1$	0	0	0
E	$k = 0.01 + T^2$	$0 \le x \le 1$	0	1	S^*

Table 1 presents the one-dimensional problems in constant use as a test problem in this study. All problems have analytical solution for T, so it is possible to identify the errors and work out the effective order of approximation (Marchi (2001)). The problem B is based on the study of Liu and MA (2005). The analytical solutions of Problems A, B, C and D are not revealed in order to save space.

And for problem E, the term source S^* is obtained in order to assign the analytical solution of Eq. (1) for the variable T is given by:

$$T(x) = \frac{\exp(10x) - 1}{\exp(10) - 1}\ . \tag{4}$$

The system of linear equations resulted from Eq.(2) is solved using the direct TDMA method (Tridiagonal Matrix Algorithm) (Maliska (2004); Patankar (1980)).

The computer program for the numerical solution of the problems was implemented in FORTRAN/95 language with settings to quadruple precision.

3. DEFINITION OF NEW SCHEMES TO CALCULATE THE THERMAL CONDUCTIVITY IN THE FACES OF CONTROL VOLUMES

The following is the description of schemes to calculate the conductivity of the faces of the CV proposed in this study. The definitions are made for the face of control volume "e".

3.1 Harmonic Average of k based on linear distribution of nodal temperature - LTMH

In this scheme, the face value of k is obtained using the harmonic average of the thermal conductivities of two intermediate points "a" and "b" located between consecutive nodes of a face of the CV, as shown in Fig. 2.

In LTMH, having as an example the consecutive nodes P and E, whose face is the control volume "e" (east face), point "a" is in an intermediate position between the generic node P and face "e", and the point "b" is located in an intermediate position between the face "e" and node E.

In points "a" and "b" temperatures T_a and T_b are calculated by:

$$T_a = T_P + \frac{T_E - T_P}{4} = \frac{3T_P + T_E}{4}\ , \tag{5}$$

$$T_b = T_P + 3\frac{T_E - T_P}{4} = \frac{T_P + 3T_E}{4}\ . \tag{6}$$

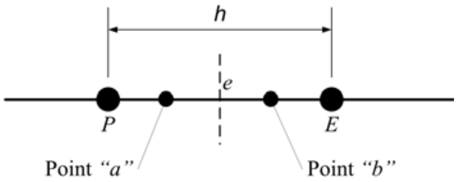

Figure 2. Auxiliary points "a" and "b" to the east face of the CV

Thus the conductivity at the face "e" (k_e) is obtained from $k_a = k(T_a)$ and $k_b = k(T_b)$, resulting:

$$k_e = \frac{2\,k_a\,k_b}{k_a + k_b}\ , \tag{7}$$

being Eq. (7) a equivalent scheme to MHk for the thermal conductivities calculated in points "a" and "b".

3.2 Harmonic average of k based on linear distribution of temperature in each control volume - TkMH

This scheme is planned considering the change in thermal conductivity at the face of CV. So between nodes P and E (adjacent nodes to face "e"), it is the thermal conductivity of the medium connecting node P and the face "e" as constant and equal to k_P (thermal conductivity value measured in node P). Towards the middle of the face "e" node E and the value of thermal conductivity is considered constant and equal to k_E (thermal conductivity value measured at node E).

The most important goal of this scheme is to achieve a high-quality representation for the heat flow. If the interface "e" is in an intermediary point among the mesh nodes, the heat flow q_e can be written , based on the CDS approximation (Patankar (1980)):

$$q_e = \frac{k_P\,(T_P - T_e)}{h/2} = \frac{k_E\,(T_e - T_E)}{h/2}\ . \tag{8}$$

With the heat flow q_e at the face "e" it is possible to calculate the temperature T_e which proves this condition :

$$T_e = \frac{k_P}{k_P + k_E} T_P + \frac{k_E}{k_P + k_E} T_E\ . \tag{9}$$

Therefore, it is possible to get an approximation of the temperature for a linear profile with different inclinations between the node P and the face "e", "e" and the node E. Thus, it is estimated temperature for two intermediate points "a" and "b" located between consecutive nodes. Figure 2 shows the location of the points "a" and "b". The thermal conductivity of the face "e" (k_e) is obtained from Eq. (7) where k_a and k_b thermal conductivities are calculated by:

$$k_a = k\left(\frac{T_P + T_e}{2}\right)\ , \tag{10}$$

$$k_b = k\left(\frac{T_e + T_E}{2}\right)\ . \tag{11}$$

3.3 Analytical solution of k at the face of the volume control for two differents materials - Lk2M

This scheme is planned to approximate the thermal conductivity of the face CV in the situation of two dissimilar materials. According to Fig. 3, the sudden change in the thermal conductivity occurs in the face of the control volume.

The value of the thermal conductivity at face "e" is specified by:

$$k_e = \frac{\displaystyle\int_{T_P}^{T_e} k_1(T)dT + \int_{T_e}^{T_E} k_2(T)dT}{T_E - T_P}\ . \tag{12}$$

In which k_1 and k_2 characterize the thermal conductivity functions in each of the volume controls adjacent to face "e". A fairly accurate solution to the Eq. (12) can be obtained by numerical integration, by rule of the rectangle

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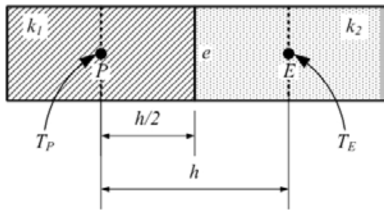

Figure 3. Adjacent CV with differents materials.

$$k_e = \frac{k_a\,(T_e - T_P) + k_b\,(T_E - T_e)}{T_E - T_P}\ . \tag{13}$$

In a situation when the thermal conductivity is independent of the temperature, it is feasible to substitute $k_a = k_P$ and $k_b = k_E$ in Eq. (13). With the temperature T_e of Eq. (9), the following is reached :

$$k_e = 2\,\frac{k_E\,k_P}{k_P + k_E}\ , \tag{14}$$

which is equal to MHk scheme.

3.4 Kirchhoff Transformation for two differents materials using numerical integration by the Gaussian quadrature

The schemes KG4P and KG6P were planned and based on the scheme Lk2M, making the integration of the numerator of the Eq. (12) by the Gaussian quadrature. The KG4P scheme is obtained once the sum given by the subscript i in the Eq. (15) is equivalent to 2 (see Table 2). The KG6P scheme, provided by the sum of the subscript i in Eq. (15) is equivalent to 3 (see Table 2).

$$\int_{T_P}^{T_e} k_1(T)dT + \int_{T_e}^{T_E} k_2(T)dT \approx [T_e - T_P]\sum w_i\,k(g_i) + [T_E - T_e]\sum w_i\,k(z_i)\ . \tag{15}$$

Table 2. Gaussian Integration - points and weights

Scheme	Integration Points			Weights
KG4P	$g_1 = \frac{T_e+T_P}{2} - \frac{1}{\sqrt{3}}\frac{T_e-T_P}{2}$	$g_2 = \frac{T_e+T_P}{2} + \frac{1}{\sqrt{3}}\frac{T_e-T_P}{2}$		$w_1 = \frac{1}{2} \quad w_2 = \frac{1}{2}$
	$z_1 = \frac{T_E+T_e}{2} - \frac{1}{\sqrt{3}}\frac{T_E-T_e}{2}$	$z_2 = \frac{T_E+T_e}{2} + \frac{1}{\sqrt{3}}\frac{T_E-T_e}{2}$		
KG6P	$g_1 = \frac{T_e+T_P}{2} - \frac{\sqrt{3}}{\sqrt{5}}\frac{T_e-T_P}{2}$	$g_2 = \frac{T_e+T_P}{2}$	$g_3 = \frac{T_e+T_P}{2} + \frac{\sqrt{3}}{\sqrt{5}}\frac{T_e-T_P}{2}$	$w_1 = \frac{5}{18} \quad w_2 = \frac{8}{18} \quad w_3 = \frac{5}{18}$
	$z_1 = \frac{T_E+T_e}{2} - \frac{\sqrt{3}}{\sqrt{5}}\frac{T_E-T_e}{2}$	$z_2 = \frac{T_E+T_e}{2}$	$z_3 = \frac{T_E+T_e}{2} + \frac{\sqrt{3}}{\sqrt{5}}\frac{T_E-T_e}{2}$	

3.5 Analytical solution of k based on the advection-diffusion problem - AD1D

The AD1D scheme is intended to calculate the thermal conductivity of the CV in the face of advection-diffusion problems using the exact solution as an approximation for temperature T_e in the interface between two CV. This scheme will be used only in order to solve the Problem E that is described in Tab. 1.

The exact solution to the problem of advection-diffusion, specified by Eq. (16), considering F constant and S null is stated in Patankar (1980):

$$T = T_P + \frac{\exp(P_e\,x/h) - 1}{\exp(P_e) - 1}(T_E - T_P)\ , \tag{16}$$

In the situation above P_e is the Peclet number. The solution presented in Eq. (16) to the advection-diffusion problem is valid for the range between the nodes P and E. Thus, x should range between x_E and x_P.

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At face "e" it is considered to be $k = k(Te)$ and $x = h/2$. Once with these values in Eq. (16), it is possible to achieve the value of the temperature T_e as follows:

$$T_e = T_P + \frac{\exp\left(\dfrac{F\,h}{2\,k(T_e)}\right) - 1}{\exp\left(\dfrac{F\,h}{k(T_e)}\right) - 1}(T_E - T_P)\,. \tag{17}$$

The temperature T_e to be obtained in Eq. (17) is dependent on $k(T_e)$. A satisfactory approximation to $k(T_e)$ is to consider the value of T_e of Eq. (9). After calculating T_e in Eq. (17) it is possible to calculate the conductivities k_a and k_b, Eqs (10) and (11) respectively for the intermediate points "a" and "b". The thermal conductivity of the face "e", k_e, is calculated based on Eq. (13).

3.6 Analytical solution of k based on the diffusion problem for two media - DK1D

In this scheme, the calculation of the thermal conductivity at the face of the CV is made based on the analytical solution for two media with different thermal conductivities and dependent on the temperature. The formulation of the problem is given by:

$$\begin{cases} \dfrac{d}{dx}\left(k_1(T_1)\dfrac{dT_1}{dx}\right) = 0 & x_P \le x \le x_e \\ \dfrac{d}{dx}\left(k_2(T_2)\dfrac{dT_2}{dx}\right) = 0 & x_e \le x \le x_E \\ T_1(x_e) = T_2(x_e) & \\ k_1(T_1)\left(\dfrac{dT_1}{dx}\right)\Big|_{x=x_e} = k_2(T_2)\left(\dfrac{dT_2}{dx}\right)\Big|_{x=x_e} & \end{cases} \tag{18}$$

The solution of Eq. (18) reached is based on the Kirchhoff's Transformation. Being the analytic solution available , it is possible to calculate the heat flow $q|_{x=x_e}$. Then,

$$q|_{x=x_e} = -\frac{2}{h\,\left(k_{1_{ref}} + k_{2_{ref}}\right)}\left[-k_{2_{ref}}\int_{T_{ref}}^{T_P} k_1(T_1)\,dT_1 \,+\, k_{1_{ref}}\int_{T_{ref}}^{T_E} k_2(T_2)\,dT_2\right]. \tag{19}$$

For the DK1D scheme is required an approximation for the heat flow. In this specifc case, the approximation using the interpolation function CDS the flow is written by:

$$q|_{x=x_e} \approx -k_e\,\frac{T_E - T_P}{h}. \tag{20}$$

By using Eq (19) in Eq (20) it is possible to reach the calculation of thermal conductivity k, as follows :

$$k_e = \frac{2}{(T_E - T_P)\,\left(k_{1_{ref}} + k_{2_{ref}}\right)}\left[-k_{2_{ref}}\int_{T_{ref}}^{T_P} k_1(T_1)\,dT_1 \,+\, k_{1_{ref}}\int_{T_{ref}}^{T_E} k_2(T_2)\,dT_2\right]. \tag{21}$$

In Eq (21), the values for $k_{1_{ref}}$, $k_{2_{ref}}$ and T_{ref} ought to use as reference temperature T_e. The value for T_e, if necessary can be obtained from Eq. (9).

4. RESULTS

4.1 Definition of the variable of interest

The variable of interest intended for calculating the numerical error considers all the nodes of the mesh. Thus it will be used to determine the numerical error, the average of norm l_1 of the discretization error which is obtained with the sum of the modules of numerical errors in the temperature of all nodes, divided by the number of volumes being defined mathematically by:

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$$L = \frac{\sum_{P=1}^{N} |E_P|}{N} \ , \tag{22}$$

L is the average of norm l_1 of the error discretization, N is the total number of volumes in the mesh and $|E_P|$ is the module of the numerical error. The module of the numerical error is given by

$$|E_P| = |T^{ex}(P) - T(P)| \ , \tag{23}$$

considering $T^{ex}(P)$ is the analytical solution of the temperature calculated in each volume and $T(P)$ is the numerical solution.

When the numerical error is known, it is possible to determine the effective order of the discretization error p_E. Thus, p_E is defined as the slope of the curve L versus the mesh size h on a logarithmic graph. The effective order measures the rate at which the numerical solution converges to the exact solution.

According to Marchi (2001), when the analytic solution of the problem is known, it is possible to determine p_E based on two numerical solutions. For two different meshes, h_1 (fine mesh) and h_2 (coarse mesh), the effective order of discretization error is given by:

$$p_{_E} = \frac{\log\left[\dfrac{L(\phi_2)}{L(\phi_1)}\right]}{\log(r)} \ . \tag{24}$$

Considering ϕ_1 and ϕ_2 are the numerical solutions obtained with the fine and coarse meshes, respectively, and r is the ratio of mesh refinement, $r = h_2/h_1$.

4.2 Discretization of the calculation domain

In order to solve the five problems of Tab. 1, it is used the discretization of uniform mesh with centered nodes. The size h was obtained by dividing the length of the field calculation H by the number of control volumes N:

$$h = \frac{H}{N} \ . \tag{25}$$

Being the rates for mesh refining defined as: $r = 2$ and $r = 3$. For $r = 2$ the change in the thermal conductivity occurs at the face of CV and $r = 3$ the change occurs at the node of the mesh. For $r = 2$ a number of analyzes were performed in 20 meshes with different initial number of nodes $N = 2$ and $r = 3$ in only 13 meshes with initial number of nodes $N = 3$.

4.3 Problems A and B

The Problems A and B were proposed to assess the various schemes for calculating the thermal conductivity in a single material with thermal conductivity variable with temperature, and consequently the spatial coordinate x. The difference between the two problems is in the class of the continuous functions of the thermal conductivity.

The analysis of the discretization error of the Problem A has been performed considering eleven calculation schemes of k at the face of the CV. Figure 4(a) shows the average of l_1 norm of discretization error as a function of h at a rate of refining mesh equal to two. In this figure are shown only the scheme with most significant discretization error, MHk, and the scheme with the least significant discretization error, MAk. For the convergent interval (Marchi (2001)) for this problem is amongst meshes with $N = 64$ to $N = 1,048,576$, it is possible to calculate the average difference discretization error between the best and worst scheme to be approximately 1.5%. The other schemes have their results with intermediate values in the MAk and MHk.

For Problem B, the calculation scheme of k which has presented the most significant discretization error was the MHk and the scheme with the the least significant error was the MAk. Figure 4(b) shows the curves of the $log(L)$ versus $log(h)$ for these two schemes, the ratio of the mesh refining equals two. The average difference involving the best and worst results of the calculation scheme for k is approximately 5.6%. The average difference is calculated for the convergent interval of the meshes with $N = 64$ to $N = 1,048,576$.

For Problems A and B, the results of effective order tend to two when h tends to zero, as expected when approximation is used with the CDS scheme for the discretization.

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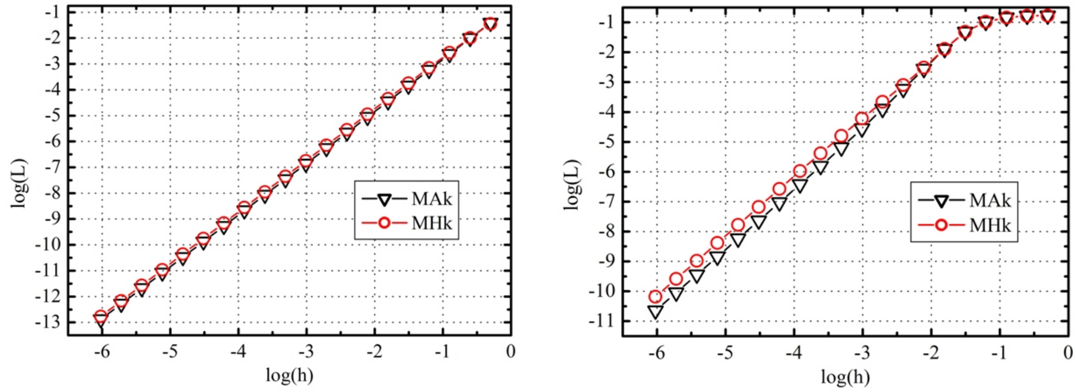
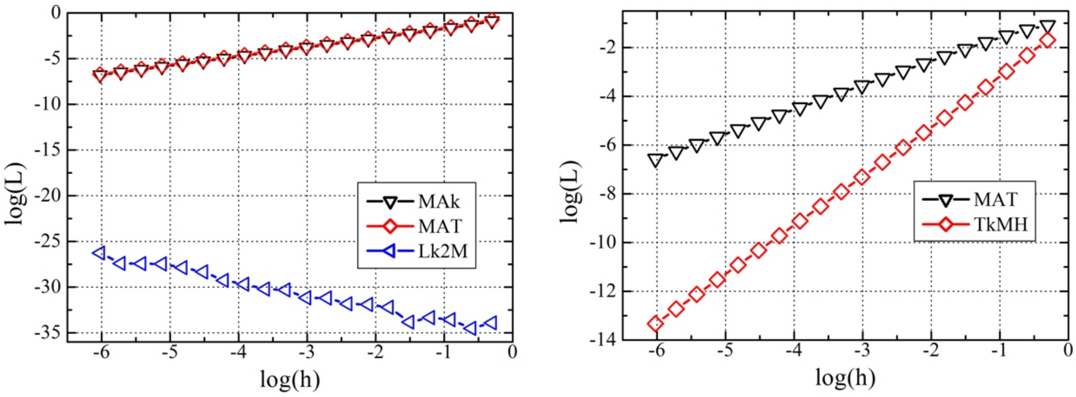


(a) Results for Problem A. (b) Results for problem B.

Figure 4. Average of norm l_1 of the true errors (E) for Problems A and B



(a) Results for Problem C. (b) Results for problem D.

Figure 5. Average of norm l_1 of the true errors (E) for Problems C and D

4.4 Problems C and D with material change in a face

The analyzes for C and D Problems take into account the position of change of thermal conductivity with respect to the mesh and assess calculation schemes of k on the face of CV where there are two materials with different thermal conductivities. In this case, the spatial position chosen for the changing conductivity is $x = 0.5$. The ratio for mesh refining in these problems is equal to two.

The results for the discretization error of Problem C are placed into two distinctive groups. The first is composed of the schemes MHk, LTMH, TkMH, KG4P, KG6P, DK1D and Lk2M do not contain discretization errors and the the second group for schemes with discretization errors. The schemes with discretization errors are: MAk, MAT, and KG2P KG3P. Among these four schemes which present discretization errors, MAk has the best results and MAT has the worst. The average difference between the MAk and MAT is roughly 2.4%. Figure 5(a) shows the curves of these two schemes which have discretization errors, and also the curve for Lk2M as representative of the schemes without discretization errors.

For Problem C, the calculation scheme of k without discretization errors, the solution obtained is exact. For schemas MAk, MAT, KG2P and KG3P, the effective order of the approximation converges to the unit when h tends to zero.

For Problem D, the thermal conductivities of the two media are temperature dependent, and therefore the spatial coordinate x. Figure 5(b) shows the results of discretization errors for the scheme with higher error MAT and less error TkMH. The results with respect to discretization error can be divided into two distinct groups. This division is made taking into account the proximity between the results of the numerical errors associated with the schemes for the calculation of k on the faces of the VC. The first group consists of schemes MAk, MAT, KG2P and KG3P whose order effective approach converges to the unit when h tends to zero. The second group, with approximately equal discretization errors, the results of effective order converges to two when h tends to zero is given by the schems MHk, LTMH, TkMH, Lk2M, KG4P, KG6P and DK1D. The average difference in performance of the two schemes, MAT and TkMH, representatives of the two groups of performance with respect to discretization error is quite large, being approximately 105%. This mean difference is obtained for the mesh with $N = 64$ to $N = 524,288$.

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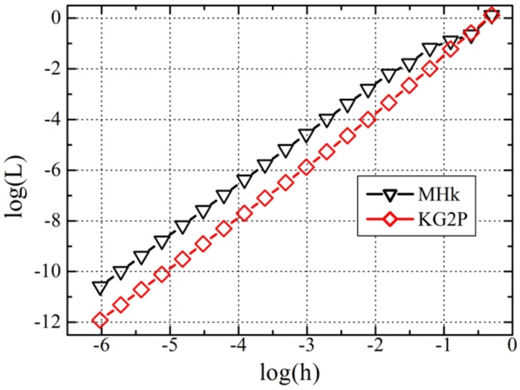
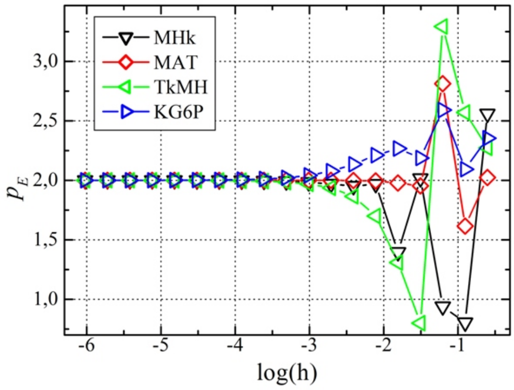
4.5 Problema E

The results obtained for Problem E take into account the effect of advection. For this problem were tested twelve different schemes to calculate the thermal conductivity in the face of VC. Figure 6(a) shows the discretization errors as a function of h at a rate of mesh refining equal to two. This figure shows the results for the scheme MHk presented the highest discretization errors and also the scheme KG2P as one of the representatives of schemes with less discretization error.

The schemes KG2P, KG3P, KG4P, KG6P and DK1D have presented results with the same discretization errors. Schemes KG2P, KG3P, KG4P KG6P have identical results because the process of numerical integration is performed identically in each of them.



(a) Average of norm l_1 of the true errors (E).



(b) Effective order of the discretization error.

Figure 6. Results for Problem E.

The average percentage difference between the best and worst scheme in comparison to the discretization error is approximately 25.5%. This average is obtained based on the results of the schemes MHk from KG2P from the meshes with $N = 64$ to $N = 524,288$, in the convergent interval.

Scheme AD1D, especially designed for advection-diffusion problems, presents results in average 2.6% higher than those obtained with the KG2P scheme.

Figure 6(b) illustrates the effective order of discretization for four schemes analyzed in Problem E. It is observed that all schemes converge to the effective order equal to two when h tends to zero.

4.6 Computational Cost

The analysis of the computational cost is made as a function of the time spent in the data processing phase for each of the calculation schemes of k evaluated. The assessment of the computational cost was made for the same convergence criterion of 10^{-10} in all meshes and problems analyzed. The convergence criterion is based on the norm l_∞, is specified by:

$$l_\infty = \max_{1 \leq i \leq n} \left| T(P)^i - T(P)^{i-1} \right| < 10^{-10} \tag{26}$$

note that $T(P)^i$ is the vector in the current iteration, $T(P)^{i-1}$ is the vector from the previous iteration and n is the specified maximum number of iterations.

Table 3 shows the ratio between the CPU time (in seconds) spent in solving the problems listed in Tab. 1 for each of the schemes with respect to scheme MAk used as reference, considering the mesh $N = 1,024$ and $N = 1,048,576$. A comparison of the schemes is based on the parameter R:

$$R = \frac{T_{cpu_n}}{T_{cpu_{MAk}}} , \tag{27}$$

where T_{cpu_n} is the CPU time for the scheme which is being evaluated and $T_{cpu_{MAk}}$ is the CPU time for the MAk scheme used as reference.

In order to obtain the CPU time in each analysis the procedure is to multiply the reference time (in seconds)by the ratio of the CPU times found in Tab. 3.

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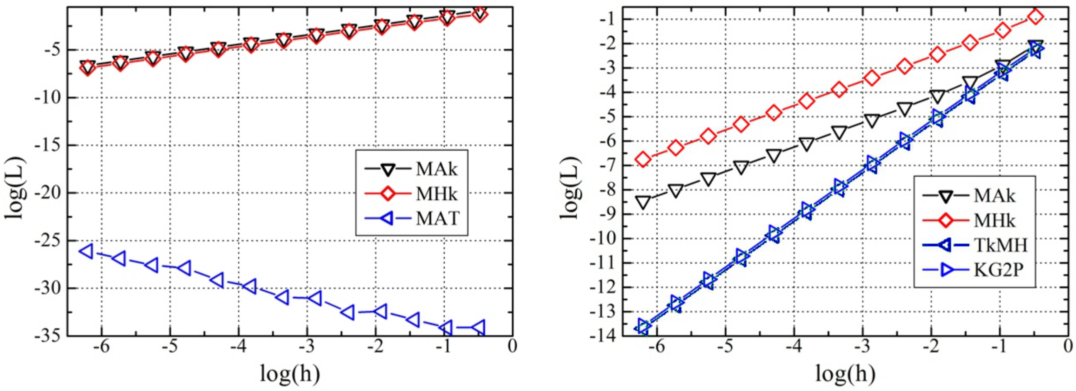
Table 3. Comparison of the CPU Times.

mesh		T_{cpu} (s)	R										
N	Problem	**MAk**	MHk	MAT	LTMH	TkMH	KG2P	KG3P	Lk2M	KG4P	KG6P	DK1D	AD1D
1,024	A	**0.017**	1.046	1.129	1.491	1.639	2.018	2.296	1.694	3.629	4.064	1.268	-
	B	**0.125**	1.031	1.054	1.336	1.440	1.760	1.954	1.488	2.943	3.275	1.092	-
	C	**0.002**	1.103	1.000	1.199	1.103	1.000	1.000	1.500	1.199	1.199	1.199	-
	D	**0.020**	1.039	1.126	1.481	1.606	1.890	2.150	1.654	3.276	3.701	1.229	-
	E	**0.107**	1.013	1.016	1.101	1.137	1.242	1.308	1.152	1.634	1.740	1.095	1.338
1,048,576	A	**17.854**	1.048	1.091	1.482	1.601	1.989	2.249	1.670	3.524	3.992	1.241	-
	B	**129.028**	1.040	1.038	1.309	1.410	1.714	1.892	1.466	2.852	3.277	1.092	-
	C	**1.716**	1.055	0.986	1.109	1.132	0.986	0.991	1.314	1.086	1.118	1.055	-
	D	**20.623**	1.043	1.152	1.494	1.609	1.917	2.173	1.660	3.239	3.705	1.248	-
	E	**110.098**	1.023	1.010	1.095	1.129	1.235	1.295	1.147	1.623	1.721	1.099	1.330

The CPU time spent in Problem C is very short, therefore all schemes presented very similar results. It can be observed of Tab. 3 that Problem C presents,the MAT scheme for mesh $N = 1,048,576$, CPU time shorter than the other schemes. For other problems, the MAk had the shortest computational time.

Table 3 allows a qualitative assessment of the computational time when calculating schemes k. Thus, it is demonstrated that for Problems A, B and D, whose thermal conductivity functions require more calculations in the numerical integration, the schemes KG2P, KG3P, KG4P and KG6P present, from shortest to longest, in that order, the longest computational times.

4.7 Problems C and D with material change in a node



(a) Results for Problem C. (b) Results for problem D.

Figure 7. Average of norm l_1 for the true errors (E), C and D Problems with material change in a node.

The results of the discretization error of Problem C is classified in two distinct groups. The first one consists of schemes which do not present discretization error and the second group for schemes with discretization errors. The schemes with discretization errors are the MAk and MHk. In this analysis the ratio of mesh refining is equal to three. Of the two schemes that have discretization error, MAk is the one with the highest values and MHk with the lowest. Figure 7(a) shows the behavior of these two schemes with discretization errors. The other schemes do not present any discretization errors, except for rounding errors. For schemes MAk and MHk, the effective order of discretization error is close to unity when h tends to zero. In the outstanding schemes do not present discretization errors, as a result the effective order was not calculated.

The analysis of Problem D demonstrated that all schemes have discretization errors. The scheme with the highest discretization error is MHk and TkMH presented the lowest. Figure 7(b) shows the curves of $log(L)$ versus $log(h)$ for the four schemes evaluated. The ratio of mesh refining used for all analyzes is equal to three. For schemes MAk and MHk the effective order of the discretization error is close to unity when h tends to zero. For the remaining schemes the order effective is close to two when h tends to zero.

5. CONCLUSION

To the FVM the schemes normally used to calculate the thermal conductivity in the face of CV are MAk and MHk. The MAk scheme provides good results for diffusive problems in which the thermal conductivity is constant or varies

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smoothly as a function of temperature. The MHk provides good results for diffusion problems in two dissimilar media, where the variation of the thermal conductivity should take place at the face of the CV.

As a contribution of this study was the analysis of five problems with different characteristics. The problems A, B and E with thermal conductivity dependent on the temperature and uniform all the way through the calculation domain. Problems C and D have two different media and with different thermal conductivities, in these problems have been possible to assess the effect of the change of thermal conductivity at the face or in a node of the mesh.

As a result of the analyzes, it is possible to conclude :

1. The evaluation the calculating schemes of k should not be performed for only one or two meshes. So that the results can be compared to the numerical solution in each of the meshes assessed should be in the convergent interval.

2. From the seven proposed schemes, excluding AD1D, all of them showed better results than those obtained with MHk. The schemes KG4P and KG6P showed a greater processing time in comparison to the other schemes.

3. AD1D, despite being based on the exact solution to the advection-diffusion problem, does not present good results in comparison to the other schemes.

4. Schemes KG2P and KG3P proposed by Voller (2001), do not provide good results when there is discontinuity in the thermal conductivity.

5. For problems which have discontinuity in thermal conductivity, schemes that maintain the consistency of results for whatever the position change of the thermal conductivity, face or node, are schemes LTMH, TkMH, Lk2M, KG4P, KG6P and DK1D. MAk does not present good results no matter what configuration used.

6. Problems when thermal conductivity is independent of temperature: the only problem assessed in this study was Problem C. In this case, it is suggested for the calculation of k schemes : LTMH, TkMH, KG4P and KG6P. It is recommended as the only suggestion scheme LTMH because of the simplicity in computational implementation.

7. Problems with thermal conductivity dependent of temperature : in this study were studied Problems A, B, D and E. The results presented in relation to the discretization error and computational cost, it is suggested the use of DK1D scheme for this type of problem.

The scheme for calculation of k at the face of CV, where necessary, should be transparent to the analyst of the problem. That is,it should not be a concern the fact that there is influence of meshing in the result or if the computational cost is high for a particular scheme. Therefore, it is indicated, in general, the scheme LTMH for problems where k is independent of temperature and DK1D where k is temperature dependent.

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7. RESPONSIBILITY NOTICE

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