Least Squares Finite Element Method for 3D Unsteady Diffusion and Reaction-Diffusion problems

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Abstract - In this paper a study to application of Least Squares Finite Element Method (LSFEM) is made and with auxiliary equations (temperature derivatives) in the solution of Transient Three-dimensional Diffusion-Reaction. In order to do so, two applications are presented and discussed, one of them Pure Diffusion and another Diffusion-Reaction, both solved towards the constructive meshes with hexahedron of 8 and 27 nodes. This analysis uses the standard L_∞ (maximum error in all meshes) and L_2 (average error in all the meshes) to verify the numerical error committed in the solution.

Key-Words - LSFEM, Diffusion, Reaction-Diffusion, Hexaedrals, Error norms.

1 Introduction

Most of the activities and researches' related to engineering are not motivated exclusively by the human curiosity, but mainly by real needs which, in most of the cases, should be solved rapidly and precisely. The heat transfer has high importance in the engineering field and special interest in the knowledge of its mechanisms present in important equipments like; boilers, condensers, air pre-heaters, etc.. In refrigeration systems and air conditioning, for example, the heat transferring is crucial to a better understanding of mechanical engineering in terms of heat. Most of the real-physic problems are governed or either represented by Partial Differential Equations. Some mathematical methods are able to produce analytical solutions for physical problems, more precisely related to heat transfer problems (Arpaci [1], Bejan [2], Carslaw and Jaeger [3]). These methods are applied only for few problems and under a certain simplification. This fact brings the importance of the numerical methods in the heat transfer problems solution. For decades, the numerical methods is used in the solution of these problems, between the methods it is underlined the Method of Finite Differences (Smith [4]), of Finite Volumes (Chung [5]) and Finite Elements (Lewis [6], Donea and Huerta [7], Reddy [8]). In this paper is used the Finite Element Method in its variant of Quadratic Minimum. Since the beginning of 50´s, Turner [9], Clough [10], Argyris [11], Zienkiewicz and Cheung [12], Oden and Wellford [13] have used successfully the Finite Element Method in several branch of engineering.

In Donea and Quartapelle [14] the Finite Element Method is shown to solve transient problems governed by linear or either non-linear equations with advective dominant terms. Due to several numerical difficulties in the simulation of permanent and transient problems with dominants advective terms in the classical problems of Galerkin, the authors made use of alternative methods to solve such problems. The first method is the General Galerkin Method, which supplies expressive results due to the correct relation between the spatial and temporal variables expressed by the theory of the characteristics. The authors also refers to discretization with time, among them, as a solution. The Explicit Method of Euler does not provide good results when the problems are handled with non structured meshes in the finite element method. However, when methods based on the Series of Taylor with time are used, the Taylor-Galerkin has present significative advantages. Among them, a simple implementation and precision or third order in non-linear problems is present. To finalize, the Method of Least Squares presents the simplicity of the Taylor-Galerkin Method and the unconditional stability of the Method of Characteristics, however, its precision is jeopardized for the numbers of Courant higher than the unity.

Winterscheidt and Surana [15] showed a p-version of LSFEM to the two-dimensional convection-diffusion equation. The differential equation of second order which governs the convective-diffusive problem is reduced for a system of differential equations of first order. For this, the formulation of least squares is built and uses the same approximation order and for each dependable variable. At this article the authors made use of the Quadrature Rule of Gauss to calculate the numerical values of elements of matrixes and vectors. One of the advantages shown is the use of the rule of accurate integration, which generates functional much lower errors when compared to the rule of reduced integration.

It is important to highlight the work done by Burrel [16], where the authors presented the numerical solution via LSFEM in a case of advective transport of a pollutant in a one-dimensional domain. Making use of the Cranck-Nicolson Method formulation for temporal discretization, the authors compare the results obtained by LSFEM with the Galerkin Method, obtaining good results, mainly when using interpolation of forth order, fact described as fundamental by the authors. Howle [17] makes a study of computational efficiency of two numerical methods, based on the Galerkin/Finite Differences: Reduced Galerkin and Pseudo-Spectral in the solution of a problem of convection in permanent regime of Rayleigh-Bénard. The author, after showing the formulation in both methods, presented a numerical test where the Pseudo-Spectral uses a higher number of interactions than the Reduced Galerkin to converge the solution.

Bramble [18], introduce and analyze two Least Squares Methods for elliptic differential equations of second order in mixed boundary conditions. The main difference between the methods is the usage or not of an additional variable in the heat flux. The authors analyzed the convergence in two solutions, one soft and another singular, showing tables and comparing the mesh refinements, a discrete error L_2 and the Norm of maximum error. This example is solved without any additional variable.

Codina [19] compares several methods for the solution of diffusion-convection-reaction equation. Among them, the author showed that the Classical Method of *Streamline Upwind* Petrov-Galerkin (SUPG) is similar to the explicit version of Galerkin Characteristic (GC), and the Taylor-Galerkin (TG). This last has a similar effect of stabilization of the Sub-Mesh Scale (SGS); finally the author develops the Galerkin/Least Squares. After describing the basic concepts and the formulations of the cited methods and realize some numerical tests, the author makes a comparison among the methods and reaches interesting conclusions, like the Petrov-Galerkin who could generate a modification in the mass-matrix associated with the original Galerkin Method, making it non-symmetric, once the discretization with time is applied in the residual R. The same occurs with the Galerkin/Least Squares.

Vujicic e Brown [20] showed a numerical solution for a tridimensional transient heat conduction case, for which several discretization methods are tested, among them, the feature β-method where the β value is assumed as 0; 0.5; 0.75 and 1, beyond the Least Squares Method (LSM). In the spatial discretization by the finite element method, hexahedron linear elements are used (8 nodes) and quadratic (20 nodes), where comparison between the meshes with 1,000, 8,000, 27,000, 64,000 e 125,000 are made. Relevant results are reached and presented at this article, but the author did not compare the results with the analytical solution or either with the results obtained by other authors found in literature. Catabriga [21] present a numerical solution of problems of linear and non-linear convection-diffusion one –directional both in permanent regime. Despite the authors make use at this paper of finite element method as well as the finite differences for spatial discretization; the main focus is the method of solution for the linear system of spatial discretization. The main proposal is the use of LCD (left conjugate direction method), where, in order to validate the method, a comparison is made within the known GMRES (Generalized Minimal Residual). The authors conclude that the utilization of the GMRES the finite element method brings a “faster solution” while the LCD present itself faster when gathered with the finite differences method. Still in this year, Dag [22] showed a numerical solution of one-directional convection-diffusion transient by the LSFEM using interpolation functions and quadratics (*B-spline*). To validate the numerical results, the authors used the norm L_2 and norm L_∞ to compare with the analytical solution. How might be expected, the numerical results were better when using the quadratic interpolation functions, however the authors did not compare the precision/time in order to have an exact notion of which way is more advisable, linear or quadratic interpolation function.

Asensio [23] studied the transient one-directional advection- diffusion- reaction; the authors used the Crank-Nicolson Methods for the temporal discretization, while for the spatial discretization some schemes of finite element are used, among them Streamline-Upwind Petrov-Galerkin (SUPG), DWG Method (initially proposed by Douglas e Wang, 1989), the Galerkin-Least Squares (GLS) and underlined the strategy used by Link-Cutting Bubble (LCB). The authors also showed applications of advection- diffusion – reaction and pollutant dispersion 1D. The methods bring good results for refined meshes with special highlight for LCB, which in general presents better results. In Si [24] the authors made use of semi-discrete finite element method using the element P_1 to solve numerically problems of transient one-directional convection-diffusion; the obtained results are compared with the analytical solution and with the *finite difference streamline diffusion method.* Expressive results were obtained, even when more convective problems were treated. In this case, the authors tested some values to the term conductivity, keeping fixed and unitary the constant which follows the convective term. In Hannukainen [25] the authors presented an application of a scheme of finite elements with super convergence of 4th order to solve a problem of tridimensional diffusion in permanent regime. Two applications are shown where the maximum error is found in some mesh refinements. The analysis of maximum error committed is possible due to the fact the two cases have analytical solutions. Beyond of having the analysis in conforming to some types of refinements, the authors also analyzed the refinements realized, since certain types of elements, cube, tetrahedron and prism (this latter presents the better results) applied for all the refinements proposed in this paper. This paper aims to apply the Finite Element Method (LSFEM) with three auxiliary equations in the numerical solution of tridimensional diffusive-reactive phenomena in transient regime. In underline is LSFEM with three auxiliary equations which provide none only the numerical solution for temperature, *T*, how also the three partial derivatives. This proposal aims to enhance the literature mainly in terms of the LSFEM application, which, how was demonstrated in the introduction (bibliography) is still too much to come.

2 Model Equation

It is introduced here a numerical study of partial differential equation that models the phenomenon tridimensional diffusive-reactive transient and generic, defined in the domain $\Theta = \Xi \otimes \Omega \subset \Re^3$, $\Xi \subset \Re$, $\Omega \subset \Re^3$, for which Ξ e Ω are limited domains and closed, described as,

$$\psi \frac{\partial T}{\partial t} + k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} + k_z \frac{\partial^2 T}{\partial z^2} + BT = 0 \tag{1}$$

for which is assumed $k_x, k_y, k_z = \text{constants} \neq 0$, $T = T(x,y,z,t)$, $B = B(x,y,z)$ and $\psi = \psi(x,y,z)$ with $x, y, z, t \in \Re$ and boundary conditions of first and second type as well as the initial condition.

3 Formulation of LSFEM

The application of the LSFEM for tridimensional phenomena uses the sum of three auxiliary equations, generating a system of four partial differentials with four unknowns, defined as follow,

$$\psi \frac{\partial T}{\partial t} + k_x \frac{\partial q_x}{\partial x} + k_y \frac{\partial q_y}{\partial y} + k_z \frac{\partial q_z}{\partial y} + BT = 0 \tag{2}$$

$$q_x - \frac{\partial T}{\partial x} = 0 \tag{3}$$

$$q_y - \frac{\partial T}{\partial y} = 0 \tag{4}$$

$$q_z - \frac{\partial T}{\partial z} = 0 \tag{5}$$

First, doing the discretization in time the equations (2-5), and making use of approximate equations of *T*, q_x, q_y e q_z, respectively, by the equations $\tilde{T}$, $\tilde{q}_x$, $\tilde{q}_y$ e $\tilde{q}_z$ at the following way,

$$\psi \frac{\tilde{T}^{s+1} - \tilde{T}^{s}}{\Delta t} = \alpha \left[-k_x \frac{\partial \tilde{q}_x}{\partial x} - k_y \frac{\partial \tilde{q}_y}{\partial y} - k_z \frac{\partial \tilde{q}_z}{\partial z} - B\tilde{u} \right]^{s+1} + (1-\alpha)\left[-k_x \frac{\partial \tilde{q}_x}{\partial x} - k_y \frac{\partial \tilde{q}_y}{\partial y} - k_z \frac{\partial \tilde{q}_z}{\partial z} - B\tilde{T} \right]^{s} \quad (6)$$

$$\tilde{q}_x - \frac{\partial \tilde{T}}{\partial x} = 0 \quad (7)$$

$$\tilde{q}_y - \frac{\partial \tilde{T}}{\partial y} = 0 \quad (8)$$

$$\tilde{q}_z - \frac{\partial \tilde{T}}{\partial z} = 0 \quad (9)$$

In Eq. 6 was utilized the Cranck-Nicolson [8] for the temporal discretization. Now, some spatial approximations are done for each element of the functions $\tilde{T}$, $\tilde{q}_x$, $\tilde{q}_y$ e $\tilde{q}_z$ by the functions $\hat{T}^e$, $\hat{q}_x^e$, $\hat{q}_y^e$ e $\hat{q}_z^e$, at the following way,

$$\tilde{T} \cong \hat{T}^e = \sum_{i=1}^{Nnodes} N_i \hat{T}_i^e \quad (10)$$

$$\tilde{q}_x \cong \hat{q}_x^e = \sum_{i=1}^{Nnodes} N_i \hat{q}_{xi}^e \quad (11)$$

$$\tilde{q}_y \cong \hat{q}_y^e = \sum_{i=1}^{Nnodes} N_i \hat{q}_{y_i}^e \quad (12)$$

$$\tilde{q}_z \cong \hat{q}_z^e = \sum_{i=1}^{Nnodes} N_i \hat{q}_{zi}^e \quad (13)$$

for any step on time and with *Nnodes* being the number of nodes for each element. After defined the spatial approximations it is possible to write the residual equations for (6-9) as ahead (below, will be adopted $R_1 = R_1(x,y,z)$, $R_2 = R_2(x,y,z)$, $R_3 = R_3(x,y,z)$, $R_4 = R_4(x,y,z)$),

$$R_1 = \left\{ \frac{\psi}{\Delta t}\hat{T} + \alpha \left[k_x \frac{\partial \hat{q}_x}{\partial x} + k_y \frac{\partial \hat{q}_y}{\partial y} + k_z \frac{\partial \hat{q}_y}{\partial z} + B\hat{T} \right] \right\}^{s+1} + \left\{ -\frac{\psi}{\Delta t}\hat{T} + (1-\alpha) \left[k_x \frac{\partial \hat{q}_x}{\partial x} + k_y \frac{\partial \hat{q}_y}{\partial y} + k_z \frac{\partial \hat{q}_y}{\partial z} + B\hat{T} \right] \right\}^{s} \quad (14)$$

$$R_2 = \hat{q}_x - \frac{\partial \hat{T}}{\partial x} \quad (15)$$

$$R_3 = \hat{q}_y - \frac{\partial \hat{T}}{\partial y} \quad (16)$$

$$R_4 = \hat{q}_z - \frac{\partial \hat{T}}{\partial z} \quad (17)$$

Substituting the approximations (10-13) in equations (14-17), it is obtained,

$$R_1 = \alpha k_x \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \hat{q}_{xi}^{e,s+1} + \alpha k_y \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{q}_{yi}^{e,s+1} + \alpha k_z \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \hat{q}_{zi}^{e,s+1} + \left[\frac{\Psi}{\Delta t} + \alpha B \right] \sum_{i=1}^{Nnodes} N_i \hat{T}_i^{e,s} + (1-\alpha) k_x \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \hat{q}_{xi}^{e,s} + (1-\alpha) k_y \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{q}_{yi}^{e,s} + (1-\alpha) k_z \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \hat{q}_{zi}^{e,s} + \left[\frac{-\psi}{\Delta t} + (1-\alpha) B \right] \sum_{i=1}^{Nnodes} N_i \hat{T}_i^{e,s}$$

(18)

$$R_2(x,y,z) = \sum_{i=1}^{Nnodes} N_i \hat{q}_{xi}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \hat{T}_i^{e,s+1} \quad (19)$$

$$R_3(x,y,z) = \sum_{i=1}^{Nnodes} N_i \hat{q}_{yi}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{T}_i^{e,s+1} \quad (20)$$

$$R_4(x,y,z) = \sum_{i=1}^{Nnodes} N_i \hat{q}_{zi}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \hat{T}_i^{e,s+1} \quad (21)$$

Once this problem is composed for four equations, the functions are defined at the following manner [26],

$$I(R_1, R_2, R_3, R_4) = \int_{\Omega^e} R_1^2 d\Omega + \int_{\Omega^e} R_2^2 d\Omega + \int_{\Omega^e} R_3^2 d\Omega + \int_{\Omega^e} R_4^2 d\Omega$$

and its first variation is written at the way,

$$\delta I(R_1, R_2, R_3, R_4) = 2\int_{\Omega^e} (\delta R_1) R_1 \, d\Omega + 2\int_{\Omega^e} (\delta R_2) R_2 \, d\Omega + 2\int_{\Omega^e} (\delta R_3) R_3 \, d\Omega + 2\int_{\Omega^e} (\delta R_4) R_4 \, d\Omega = 0$$

or

$$\int_{\Omega^e} (\delta R_1) R_1 \, d\Omega + \int_{\Omega^e} (\delta R_2) R_2 \, d\Omega + \int_{\Omega^e} (\delta R_3) R_3 \, d\Omega + \int_{\Omega^e} (\delta R_4) R_4 \, d\Omega = 0 \quad (22)$$

with the following properties undependable of time,

$$\delta R_1 = \frac{\partial R_1}{\partial T_i^e}\delta T_i^e + \frac{\partial R_1}{\partial q_{xi}^e}\delta q_{xi}^e + \frac{\partial R_1}{\partial q_{y_i}^e}\delta q_{y_i}^e + \frac{\partial R_1}{\partial q_{zi}^e}\delta q_{zi}^e \tag{23}$$

$$\delta R_2 = \frac{\partial R_2}{\partial T_i^e}\delta T_i^e + \frac{\partial R_2}{\partial q_{xi}^e}\delta q_{xi}^e + \frac{\partial R_2}{\partial q_{y_i}^e}\delta q_{y_i}^e + \frac{\partial R_2}{\partial q_{zi}^e}\delta q_{zi}^e \tag{24}$$

$$\delta R_3 = \frac{\partial R_3}{\partial T_i^e}\delta T_i^e + \frac{\partial R_3}{\partial q_{xi}^e}\delta q_{xi}^e + \frac{\partial R_3}{\partial q_{y_i}^e}\delta q_{y_i}^e + \frac{\partial R_3}{\partial q_{zi}^e}\delta q_{zi}^e \tag{25}$$

$$\delta R_4 = \frac{\partial R_4}{\partial T_i^e}\delta T_i^e + \frac{\partial R_4}{\partial q_{xi}^e}\delta q_{xi}^e + \frac{\partial R_4}{\partial q_{y_i}^e}\delta q_{y_i}^e + \frac{\partial R_4}{\partial q_{zi}^e}\delta q_{zi}^e \tag{26}$$

with

$$\frac{\partial R_1}{\partial \hat{T}_i^e} = \left(\frac{\psi}{\Delta t} + \alpha\, B\right)\sum_{i=1}^{Nnodes} N_i \tag{27}$$

$$\frac{\partial R_1}{\partial \hat{q}_{xi}^e} = \alpha k_x \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \tag{28}$$

$$\frac{\partial R_1}{\partial \hat{q}_{y_i}^e} = \alpha k_y \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \tag{29}$$

$$\frac{\partial R_1}{\partial \hat{q}_{zi}^e} = \alpha k_z \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \tag{30}$$

$$\frac{\partial R_2}{\partial \hat{T}_i^e} = -\sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \tag{31}$$

$$\frac{\partial R_2}{\partial \hat{q}_{xi}^e} = \sum_{i=1}^{Nnodes} N_i \tag{32}$$

$$\frac{\partial R_2}{\partial \hat{q}_{y_i}^e} = 0 \tag{33}$$

$$\frac{\partial R_2}{\partial \hat{q}_{zi}^e} = 0 \tag{34}$$

$$\frac{\partial R_3}{\partial \hat{T}_i^e} = -\sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \tag{35}$$

$$\frac{\partial R_3}{\partial \hat{q}_{xi}^e} = 0 \tag{36}$$

$$\frac{\partial R_3}{\partial \hat{q}_{y_i}^e} = \sum_{i=1}^{Nnodes} N_i \tag{37}$$

$$\frac{\partial R_3}{\partial \hat{q}_{zi}^e} = 0 \tag{38}$$

$$\frac{\partial R_4}{\partial \hat{T}_i^e} = -\sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \tag{39}$$

$$\frac{\partial R_4}{\partial \hat{q}_{xi}^e} = 0 \tag{40}$$

$$\frac{\partial R_4}{\partial \hat{q}_{y_i}^e} = 0 \tag{41}$$

$$\frac{\partial R_3}{\partial \hat{q}_{zi}^e} = \sum_{i=1}^{Nnodes} N_i \tag{42}$$

Substituting the Eqs. (23-26) and (27-42) into Eq. (22) have,

$$\begin{aligned}
&\int_\Omega \left\{ \left[\left(\frac{\psi}{\Delta t} + \alpha\, B\right) \sum_{i=1}^{Nnodes} N_i \right] \delta\, \hat{T}_i^{e,s+1} + \alpha k_x \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \delta\, \hat{q}_{x\,i}^{e,s+1} + \right. \\
&\left. \alpha k_y \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \delta\, \hat{q}_{y\,i}^{e,s+1} + \alpha k_z \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \delta\, \hat{q}_{z\,i}^{e,s+1} \right\} \times \\
&\left\{ \alpha k_x \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \hat{q}_{xi}^{e,s+1} + \alpha k_y \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{q}_{yi}^{e,s+1} + \right. \\
&\alpha k_z \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \hat{q}_{zi}^{e,s+1} + \left[\frac{\psi}{\Delta t} + \alpha\, B\right] \sum_{i=1}^{Nnodes} N_i \hat{T}_i^{e,s+1} + \\
&(1-\alpha) k_x \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \hat{q}_{xi}^{e,s} + (1-\alpha) k_y \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{q}_{yi}^{e,s} + \\
&(1-\alpha) k_z \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{q}_{zi}^{e,s} + \left[\frac{-\psi}{\Delta t} + (1-\alpha)\, B\right] \times \\
&\left. \sum_{i=1}^{Nnodes} N_i \hat{T}_i^{e,s} \right\} d\Omega + \int_{\Omega^e} \left[-\sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \delta\, \hat{T}_i^{e,s+1} + \right. \\
&\left. \sum_{i=1}^{Nnodes} N_i \delta\, \hat{q}_{x\,i}^{e,s+1} \right] \times \left[\sum_{i=1}^{Nnodes} N_i \hat{q}_{xi}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \hat{T}_i^{e,s+1} \right] d\Omega + \\
&+ \int_{\Omega^e} \left[-\sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \delta\, \hat{T}_i^{e,s+1} + \sum_{i=1}^{Nnodes} N_i \delta\, \hat{q}_{y\,i}^{e,s+1} \right] \times \\
&\left[\sum_{i=1}^{Nnodes} N_i \hat{q}_{yi}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{T}_i^{e,s+1} \right] d\Omega + \\
&+ \int_{\Omega^e} \left[-\sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \delta\, \hat{T}_i^{e,s+1} + \sum_{i=1}^{Nnodes} N_i \delta\, \hat{q}_{z\,i}^{e,s+1} \right] \times \\
&\left[\sum_{i=1}^{Nnodes} N_i \hat{q}_{zi}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \hat{T}_i^{e,s+1} \right] d\Omega = 0
\end{aligned}$$

Reorganizing the previous equation, it is seen,

$$\delta \hat{T}_i^{e,s+1} \times \int_{\Omega^e} \left(U_1 \times U_2 + U_3 + U_4 + U_5\right) d\Omega + \delta \hat{q}_{x\,i}^{e,s+1} \times \int_{\Omega^e} \left(U_6 \times U_2 + U_7\right) d\Omega + \delta \hat{q}_{y\,i}^{e,s+1} \times \int_{\Omega^e} \left(U_8 \times U_2 + U_9\right) d\Omega + \delta \hat{q}_{z\,i}^{e,s+1} \times \int_{\Omega^e} \left(U_{10} \times U_2 + U_{11}\right) d\Omega = 0 \quad (43)$$

for which

$$U_1 = \left[\frac{\psi}{\Delta t} + \alpha B\right] \sum_{i=1}^{Nnodes} N_i \quad (44)$$

$$U_2 = \alpha k_x \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \hat{q}_{x\,i}^{e,s+1} + \alpha k_y \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{q}_{y\,i}^{e,s+1} + \alpha k_z \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \hat{q}_{z\,i}^{e,s+1} + \left[\frac{\psi}{\Delta t} + \alpha B\right] \sum_{i=1}^{Nnodes} N_i \hat{T}_i^{e,s+1} + (1-\alpha) \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \hat{q}_{x\,i}^{e,s} + (1-\alpha) \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{q}_{y\,i}^{e,s} + (1-\alpha) \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \hat{q}_{z\,i}^{e,s} + \left[\frac{-\psi}{\Delta t} + (1-\alpha) B\right] \sum_{i=1}^{Nnodes} N_i \hat{T}_i^{e,s} \quad (45)$$

$$U_3 = -\sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \times \left[\sum_{i=1}^{Nnodes} N_i \hat{q}_{x\,i}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \hat{T}_i^{e,s+1}\right] \quad (46)$$

$$U_4 = -\sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \times \left[\sum_{i=1}^{Nnodes} N_i \hat{q}_{y\,i}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{T}_i^{e,s+1}\right] \quad (47)$$

$$U_5 = -\sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \times \left[\sum_{i=1}^{Nnodes} N_i \hat{q}_{z\,i}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \hat{T}_i^{e,s+1}\right] \quad (48)$$

$$U_6 = \alpha k_x \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \quad (49)$$

$$U_7 = \sum_{i=1}^{Nnodes} N_i \times \left[\sum_{i=1}^{Nnodes} N_i \hat{q}_{x\,i}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial x} \hat{T}_i^{e,s+1}\right] \quad (50)$$

$$U_8 = \alpha k_y \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \quad (51)$$

$$U_9 = \sum_{i=1}^{Nnodes} N_i \times \left[\sum_{i=1}^{Nnodes} N_i \hat{q}_{y\,i}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial y} \hat{T}_i^{e,s+1}\right] \quad (52)$$

$$U_{10} = \alpha k_z \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \quad (53)$$

$$U_{11} = \sum_{i=1}^{Nnodes} N_i \times \left[\sum_{i=1}^{Nnodes} N_i \hat{q}_{z\,i}^{e,s+1} - \sum_{i=1}^{Nnodes} \frac{\partial N_i}{\partial z} \hat{T}_i^{e,s+1}\right] \quad (54)$$

In order to satisfy the Equation (43) it is required simultaneously,

$$\int_{\Omega^e} \left(U_1 \times U_2 + U_3 + U_4 + U_5\right) d\Omega = 0 \quad (55)$$

$$\int_{\Omega^e} \left(U_6 \times U_2 + U_7\right) d\Omega = 0 \quad (56)$$

$$\int_{\Omega^e} \left(U_8 \times U_2 + U_9\right) d\Omega = 0 \quad (57)$$

$$\int_{\Omega^e} \left(U_{10} \times U_2 + U_{11}\right) d\Omega = 0 \quad (58)$$

in order words;, $\delta T_i^{s+1,e}$, $\delta q_{x\,i}^{s+1,e}$, $\delta q_{y\,i}^{s+1,e}$ e $\delta q_{z\,i}^{s+1,e}$ are not identically nulls in all the domain.

The Eqs. (55-58) generate the follow linear system,

$$\begin{bmatrix} A & B & C & D \\ B^T & E & G & H \\ C^T & G^T & I & J \\ D^T & H^T & J^T & K \end{bmatrix} \begin{Bmatrix} \hat{T}^{e,s+1} \\ \hat{q}_x^{e,s+1} \\ \hat{q}_y^{e,s+1} \\ \hat{q}_z^{e,s+1} \end{Bmatrix} + \begin{bmatrix} L & M & N & O \\ P & Q & R & S \\ T & U & V & X \\ Z & W & Y & \beta \end{bmatrix} \begin{Bmatrix} \hat{T}^{e,s} \\ \hat{q}_x^{e,s} \\ \hat{q}_y^{e,s} \\ \hat{q}_z^{e,s} \end{Bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (59)$$

Once the variables $\hat{T}^{e,s}$, $\hat{q}_x^{e,s}$, $\hat{q}_y^{e,s}$ and $\hat{q}_z^{e,s}$ are already known from the previous step on time "s", the system (13) stays at the following way,

$$\begin{bmatrix} A & B & C & D \\ B^T & E & G & H \\ C^T & G^T & I & J \\ D^T & H^T & J^T & K \end{bmatrix} \begin{Bmatrix} \hat{T}^{e,s+1} \\ \hat{q}_x^{e,s+1} \\ \hat{q}_y^{e,s+1} \\ \hat{q}_z^{e,s+1} \end{Bmatrix} = - \begin{bmatrix} L & M & N & O \\ P & Q & R & S \\ T & U & V & X \\ Z & W & Y & \beta \end{bmatrix} \begin{Bmatrix} \hat{T}^{e,s} \\ \hat{q}_x^{e,s} \\ \hat{q}_y^{e,s} \\ \hat{q}_z^{e,s} \end{Bmatrix} \quad (60)$$

for which,

$$A_{ij} = \int_{\Omega^e} \left\{ \left(\frac{\psi}{\Delta t} + \alpha\, B \right)^2 N_i N_j + \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z} \right\} d\Omega \qquad (61)$$

$$B_{ij} = \int_{\Omega^e} \left\{ \left[\left(\frac{\psi}{\Delta t} + \alpha\, B \right) N_i \right] \times \left[\alpha k_x \frac{\partial N_j}{\partial x} \right] - \frac{\partial N_i}{\partial x} N_j \right\} d\Omega \qquad (62)$$

$$C_{ij} = \int_{\Omega^e} \left\{ \left[\left(\frac{\psi}{\Delta t} + \alpha\, B \right) N_i \right] \times \left[\alpha k_y \frac{\partial N_j}{\partial y} \right] - \frac{\partial N_i}{\partial y} N_j \right\} d\Omega \qquad (63)$$

$$D_{ij} = \int_{\Omega^e} \left\{ \left[\left(\frac{\psi}{\Delta t} + \alpha\, B \right) N_i \right] \times \left[\alpha k_z \frac{\partial N_j}{\partial z} \right] - \frac{\partial N_i}{\partial z} N_j \right\} d\Omega \qquad (64)$$

$$E_{ij} = \int_{\Omega^e} \left[\alpha^2 k_x^2 \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + N_i N_j \right] d\Omega \qquad (65)$$

$$G_{ij} = \int_{\Omega^e} \alpha^2 k_x k_y \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial y}\, d\Omega \qquad (66)$$

$$H_{ij} = \int_{\Omega^e} \alpha^2 k_x k_z \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial z}\, d\Omega \qquad (67)$$

$$I_{ij} = \int_{\Omega^e} \left[\alpha^2 k_y^2 \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} + N_i N_j \right] d\Omega \qquad (68)$$

$$J_{ij} = \int_{\Omega^e} \alpha^2 k_y k_z \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial z}\, d\Omega \qquad (69)$$

$$K_{ij} = \int_{\Omega^e} \left[\alpha^2 k_z^2 \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z} + N_i N_j \right] d\Omega \qquad (70)$$

$$L_{ij} = \int_{\Omega^e} \left\{ \left[\left(\frac{\psi}{\Delta t} + \alpha\, B \right) N_i \right] \times \left[\left(\frac{-\psi}{\Delta t} + (1-\alpha)\, B \right) N_j \right] \right\} d\Omega \qquad (71)$$

$$M_{ij} = \int_{\Omega^e} \left[\left(\frac{\psi}{\Delta t} + \alpha\, B \right) N_i \right] \times (1-\alpha) k_x \frac{\partial N_j}{\partial x}\, d\Omega \qquad (72)$$

$$N_{ij} = \int_{\Omega^e} \left[\left(\frac{\psi}{\Delta t} + \alpha\, B \right) N_i \right] \times (1-\alpha)\, k_y \frac{\partial N_j}{\partial y}\, d\Omega \qquad (73)$$

$$O_{ij} = \int_{\Omega^e} \left[\left(\frac{\psi}{\Delta t} + \alpha\, B \right) N_i \right] \times (1-\alpha)\, k_z \frac{\partial N_j}{\partial z}\, d\Omega \qquad (74)$$

$$P_{ij} = \int_{\Omega^e} \alpha k_x \frac{\partial N_i}{\partial x} \times \left[\left(-\frac{\psi}{\Delta t} + (1-\alpha)\, B \right) N_j \right] d\Omega \qquad (75)$$

$$Q_{ij} = \int_{\Omega^e} (1-\alpha)\alpha\, k_x^2 \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}\, d\Omega \qquad (76)$$

$$R_{ij} = \int_{\Omega^e} (1-\alpha)\alpha\, k_x k_y \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial y}\, d\Omega \qquad (77)$$

$$S_{ij} = \int_{\Omega^e} (1-\alpha)\alpha\, k_x k_z \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial z}\, d\Omega \qquad (78)$$

$$T_{ij} = \int_{\Omega^e} \alpha\, k_y \frac{\partial N_i}{\partial y} \times \left[\left(-\frac{\psi}{\Delta t} + (1-\alpha)\, B \right) N_j \right] d\Omega \qquad (79)$$

$$U_{ij} = \int_{\Omega^e} \alpha(1-\alpha) k_x k_y \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial x}\, d\Omega \qquad (80)$$

$$V_{ij} = \int_{\Omega^e} (1-\alpha)\alpha\, k_y^2 \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}\, d\Omega \qquad (81)$$

$$X_{ij} = \int_{\Omega^e} \alpha(1-\alpha) k_y k_z \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial z}\, d\Omega \qquad (82)$$

$$Z_{ij} = \int_{\Omega^e} \alpha\, k_z \frac{\partial N_i}{\partial z} \times \left[\left(-\frac{\psi}{\Delta t} + (1-\alpha)\, B \right) N_j \right] d\Omega \qquad (83)$$

$$W_{ij} = \int_{\Omega^e} \alpha(1-\alpha) k_x k_z \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial x}\, d\Omega \qquad (84)$$

$$Y_{ij} = \int_{\Omega^e} \alpha(1-\alpha) k_y k_z \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial y}\, d\Omega \qquad (85)$$

$$\beta_{ij} = \int_{\Omega^e} \alpha(1-\alpha) k_z^2 \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z}\, d\Omega \qquad (86)$$

In order to use the Quadrature of Gauss-Legendre to calculate the integrals in the coefficients of the linear system described in (60), the transformations from global coordinates to local coordinates are required ($x \to \xi$, $y \to \eta$, $z \to \zeta$), and more details about the transformations can be found in [27].

4 Numerical Applications

All formulations shown in this paper were implemented in a computational code written in FORTRAN. To solve the linear system (60) is used a routine DL2LXG of IMSL FORTRAN. Thus, only the coefficients non null in the linear system (60) were stored. For the two proposed applications is adopted the following analytical solution,

$$T(x,y,z,t) = e^t (e^x + e^y + e^z)$$

$$\frac{\partial T}{\partial x} = e^t e^x, \quad \frac{\partial T}{\partial y} = e^t e^y, \quad \frac{\partial T}{\partial z} = e^t e^z.$$

To evaluate the error committed in the numerical solution, two Norms were adopted; norm L_∞ which represents the maximum error committed in all the mesh found by the higher value calculated by the expression $\| e_i \| = | T_i^{an} - T_i^{num} |$ where T_i^{an} is the analytical solution, and T_i^{num} being the numerical solution for both at the node "*i*" and norm L_2 which represents a view of average error committed in all the mesh and can be calculated by the expression; $\| e \|_2 = \sqrt{\left(\sum_{i=1}^{NNost} e_i^2 \right) / NNost}$ with *Nnost* being the total number of nodes of the mesh.

Application 1 – Diffusion Equation. For this case, the following equation is adopted as model,

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} = \frac{\partial T}{\partial t}$$

in a domain of unity cube.

To analyze the results of this application, it was taken as the main factor for comparison the usage of hexahedron elements with 8 or 27 nodes and the quantity of nodes in all the mesh. Thereby, the numerical value of h, which in this application and others is adopted as h = $\Delta x = \Delta y = \Delta z$, was analyzed in such way to generate situations with the same total number of nodes in all mesh for both 8 and 27 nodes. For instance, in a situation where h = 1/6 (8 nodes) and h = 1/3 (27 nodes) in both cases the mesh has 343 nodes.

From this proposal it is expected a comparison of results of the two hexahedron adopted at this paper, the most conclusive possible, once at this way, situations with global matrixes with same size and with the same freedom degrees in all domain will be present.

In Tables 1 and 2 are shown the results from the two proposed norms in the analysis of error to the solution of the variable *T*. In those is noted better numerical results for two temporal refinements adopted (Δt = 0.1 e Δt = 0.01) with hexahedron of 8 nodes. On the other hand, for the solution of the variables T_x, T_y e T_z (Tables 3 e 4), which at this paper presented very similar results in a point of being considered equals. The hexahedron with 27 nodes showed the best results, reaching situations where the precision order is higher than the hexahedron of 8 nodes (for example, case h = 1/7 e Δt = 0.01). It should be also underlined that for the temporal refinement Δt = 0.1 the proposed spatial refinement presented few enhanced in precision for two hexahedrons.

Table 1. Norm L_∞ of error committed in *T* by LSFEM in *t* = 1.

NNost	8 nodes			27 nodes		
	h	**Δt = 0.1**	**Δt = 0.01**	**h**	**Δt = 0.1**	**Δt = 0.01**
343	1/6	3.10E-03	5.64E-03	1/3	5.33E-03	1.60E-02
729	1/8	3.35E-03	2.74E-03	1/4	4.17E-03	6.29E-03
1331	1/10	3.53E-03	1.48E-03	1/5	4.13E-03	2.92E-03
2197	1/12	3.65E-03	9.47E-04	1/6	3.93E-03	1.53E-03
3375	1/14	3.73E-03	6.98E-04	1/7	4.00E-03	8.78E-04

Table 2. Norm L_2 of error committed in *T* by LSFEM in *t* = 1.

NNost	8 nodes			27 nodes		
	h	**Δt = 0.1**	**Δt = 0.01**	**h**	**Δt = 0.1**	**Δt = 0.01**
343	1/6	1.13E-03	1.14E-03	1/3	1.76E-03	4.64E-03
729	1/8	1.38E-03	6.51E-04	1/4	1.67E-03	1.94E-03
1331	1/10	1.52E-03	4.18E-04	1/5	1.70E-03	9.20E-04
2197	1/12	1.61E-03	2.91E-04	1/6	1.73E-03	4.83E-04
3375	1/14	1.67E-03	2.15E-04	1/7	1.75E-03	2.75E-04

Table 3. Norm L_∞ of error committed in $T_x \cong T_y \cong T_z$ by LSFEM in t = 1.

NNost	8 nodes			27 nodes		
	h	Δt = 0.1	Δt = 0.01	h	Δt = 0.1	Δt = 0.01
343	1/6	1.23E-03	1.59E-03	1/3	6.88E-04	6.06E-04
729	1/8	4.87E-04	7.58E-04	1/4	5.50E-04	2.78E-04
1331	1/10	2.06E-04	4.18E-04	1/5	5.23E-04	1.27E-04
2197	1/12	2.56E-04	2.63E-04	1/6	5.16E-04	7.17E-05
3375	1/14	3.17E-04	1.94E-04	1/7	5.06E-04	4.78E-05

Table 4. Norm L_2 of error committed in $_x \cong T_y \cong T_z$ by LSFEM in t = 1.

NNost	8 nodes			27 nodes		
	h	Δt = 0.1	Δt = 0.01	h	Δt = 0.1	Δt = 0.01
343	1/6	4.10E-04	5.55E-04	1/3	2.81E-04	1.76E-04
729	1/8	1.49E-04	3.20E-04	1/4	2.69E-04	7.19E-05
1331	1/10	8.58E-05	2.07E-04	1/5	2.70E-04	3.47E-05
2197	1/12	1.24E-04	1.45E-04	1/6	2.74E-04	1.95E-05
3375	1/14	1.63E-04	1.06E-04	1/7	2.77E-04	1.23E-05

From Tables 1 to 4, in general was fixed two refinements in time and changed some spatial refinements.

On the other hand, in the Figures 1 and 2 were fixed two spatial refinements and changed the steps from 10 to 100 in time; in order to analyze till when would be advantageous refine in time for a determined spatial refinement. It is noted in Figure 1 that the numerical results for the solution of T are better for h = 1/10 with a hexahedron with 8 nodes, and more, at this the refinement reached of 30 steps in time showed advantageous; from that point on the results worsen. Now the Figure 2, the best results in the derivatives solution occurs in h=1/5 in a hexahedron with 27 nodes, where is also advantageous to refine the mesh till 30 steps in time. It is important underline that by the Figure 2 it is noted for hexahedron with 8 nodes, being to h = 1/8 as also for h = 1/10, the temporal refinement, at this case is always damaging.

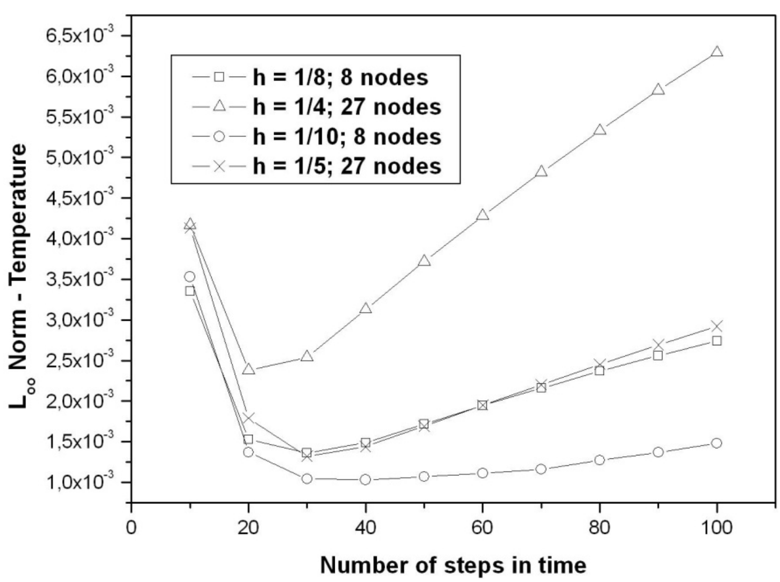

Fig. 1 Norm L_∞ of error committed changing the number of steps in time for temperature solution .

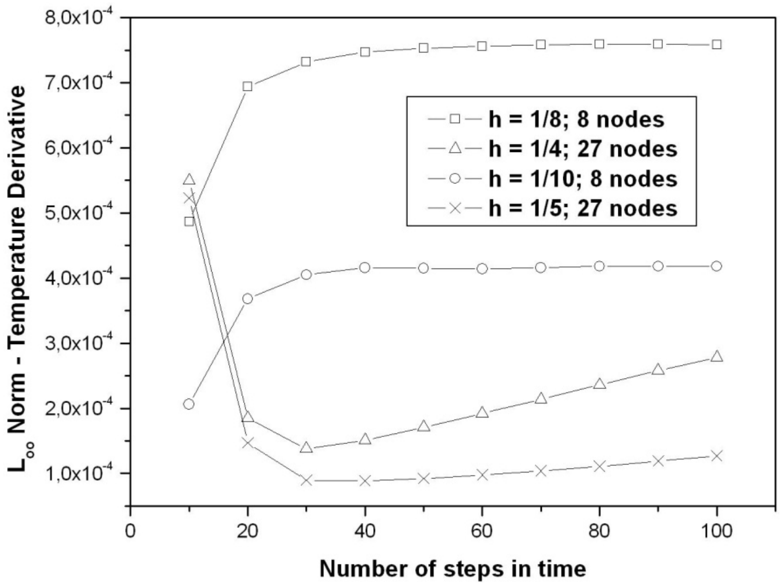

Fig. 2 Norm L_∞ of error committed changing the number of steps in time for the solution of first derivatives of temperature.

Application 2 – Reaction-Diffusion Equation. For this case the following equation is adopted as a model;

$$2\frac{\partial^2 T}{\partial x^2}+2\frac{\partial^2 T}{\partial y^2}+2\frac{\partial^2 T}{\partial z^2}-T=\frac{\partial T}{\partial t}$$

in an unity domain.

From Table 5 to 8 it is noted that for the case of diffusive-reactive the usage of hexahedron with 8 and 27 nodes presented superior results with meshes relatively coarse, and more, in a general view, on both proposed hexahedron. The precision order was the same, demonstrating that whether the focus is the numerical precision, being hexahedron with 8 or 27 nodes the results are equivalent and considered good. Thus, per the application 1, for Δt = 0.1, the numerical results of temperature few enhance with the spatial refinement, but for the derivatives the hexahedron with 8 nodes shows a slight improvement.

Table 5. Norm L_∞ of error committed in T by LSFEM in t = 1.

NNost	8 nodes			27 nodes		
	h	**Δt = 0.1**	**Δt = 0.01**	**h**	**Δt = 0.1**	**Δt = 0.01**
343	1/6	4.27E-03	1.52E-02	1/3	6.45E-03	3.57E-02
729	1/8	3.79E-03	7.20E-03	1/4	4.55E-03	1.32E-02
1331	1/10	3.72E-03	4.35E-03	1/5	4.28E-03	6.14E-03
2197	1/12	3.73E-03	2.98E-03	1/6	3.97E-03	3.17E-03
3375	1/14	3.76E-03	2.13E-03	1/7	4.04E-03	1.75E-03

Table 6. Norm L_2 of error committed in T by LSFEM in t = 1.

NNost	8 nodes			27 nodes		
	h	**Δt = 0.1**	**Δt = 0.01**	**h**	**Δt = 0.1**	**Δt = 0.01**
343	1/6	1.23E-03	3.45E-03	1/3	1.95E-03	9.47E-03
729	1/8	1.35E-03	2.05E-03	1/4	1.63E-03	4.02E-03
1331	1/10	1.47E-03	1.35E-03	1/5	1.63E-03	1.92E-03
2197	1/12	1.54E-03	9.56E-04	1/6	1.66E-03	1.01E-03
3375	1/14	1.60E-03	7.12E-04	1/7	1.69E-03	5.80E-04

Table 7. Norm L_∞ of error committed in $T_x \cong T_y \cong T_z$ by LSFEM in t = 1.

NNost	8 nodes			27 nodes		
	h	**Δt = 0.1**	**Δt = 0.01**	**h**	**Δt = 0.1**	**Δt = 0.01**
343	1/6	1.58E-03	2.30E-03	1/3	3.52E-04	6.26E-04
729	1/8	7.21E-04	1.27E-03	1/4	3.61E-04	3.77E-04
1331	1/10	3.55E-04	8.13E-04	1/5	3.45E-04	1.98E-04
2197	1/12	1.68E-04	5.53E-04	1/6	3.51E-04	1.06E-04
3375	1/14	7.53E-05	4.55E-04	1/7	3.53E-04	5.87E-05

Table 8. Norm L_2 of error committed in $T_x \cong T_y \cong T_z$ by LSFEM in t = 1.

NNost	8 nodes			27 nodes		
	h	**Δt = 0.1**	**Δt = 0.01**	**h**	**Δt = 0.1**	**Δt = 0.01**
343	1/6	6.65E-04	1.02E-03	1/3	1.15E-04	2.00E-04
729	1/8	3.33E-04	6.14E-04	1/4	1.37E-04	8.61E-05
1331	1/10	1.67E-04	4.07E-04	1/5	1.46E-04	4.05E-05
2197	1/12	7.50E-05	2.88E-04	1/6	1.50E-04	2.11E-05
3375	1/14	2.67E-05	2.14E-04	1/7	1.53E-04	1.19E-05

On the other hand, in Figures 3 and 4 with the temporal refinement for two spatial refinements, it is noted that as the solution of T as its derivatives, the case h = 1/6 with 27 nodes presents the best results and again around 30 steps in time, it means it is not necessary higher refinements in time for this h.

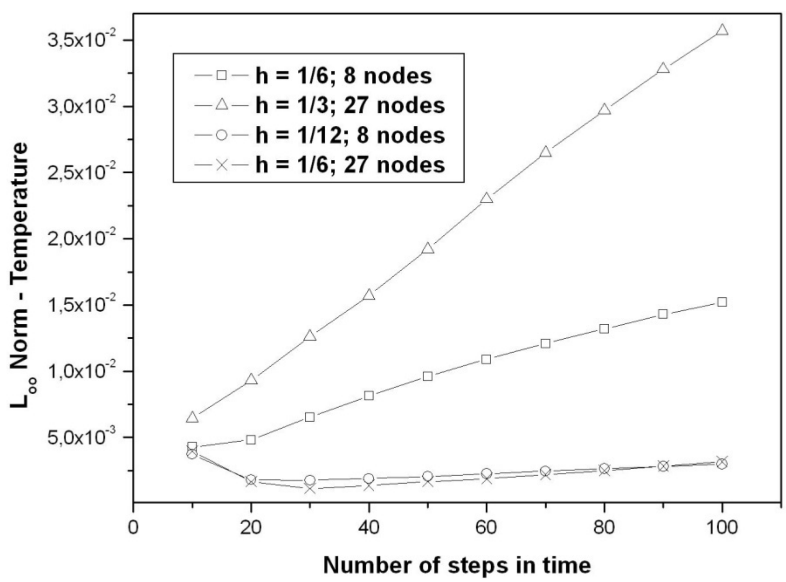

Fig. 3 Norm L_∞ of error committed changing the number of steps in time for the temperature solution.

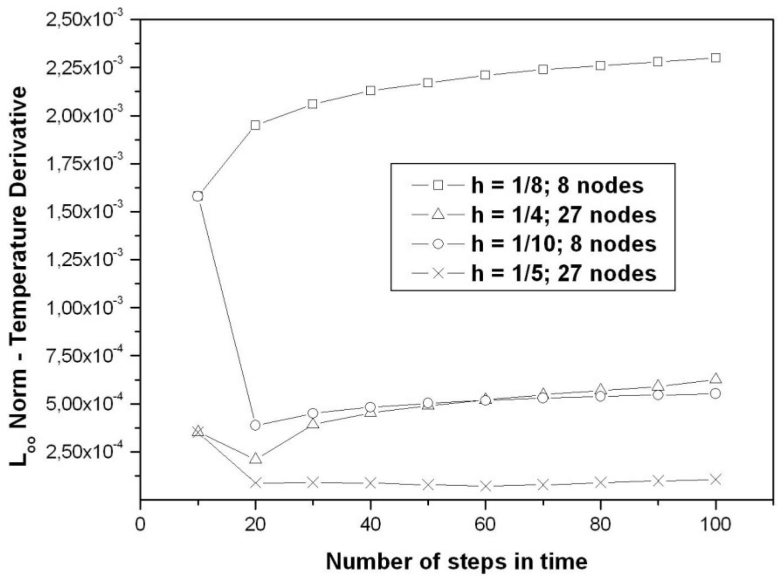

Fig. 4 Norm L_∞ of error committed changing the number of steps in time for the solution of first derivatives of temperature.

5 Conclusions

The LSFEM showed very efficient in the solution of unsteady tridimensional diffusive-reactive problems. The auxiliary equations create an advantage in obtain the derivative of temperature in three spatial directions at the same order of precision than the numerical solution of T. It would not happen whether it was necessary a routine which calculated the derivatives from only the results obtained of temperature. In heat transfer problem is true that the unique variable is the temperature, and other three are inserted (the derivatives). It is the same as insert three new freedom degrees in the problem, but the numerical efficiency compensate the cost (see [28-31] what happens with the Galerkin method in terms of calculus of derivatives). To the same number of nodes in the mesh it is important to mention that the use of 8 or 27 nodes result in equivalent results. For real problems of diffusion-reaction it is advisable the use of hexahedron with 8 nodes, once the matrix of the element for this case is of order 32, while to the hexahedron with 27 nodes is of order 108. It means that, despite of the comparison of two hexahedrons in global matrix presents equivalent results; the quantity of coefficients non nulls in a global matrix is lower in cases with hexahedron with 8 nodes. The cost of storage within a computational time, are both smaller than the hexahedron with 27 nodes.

Acknowledgments

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