Adaptivity in mimetic difference schemes: one-dimensional transient problems

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Adaptivity in mimetic difference schemes: one-dimensional transient problems

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Abstract. In this paper, we present an h-adaptive process that defines an optimal mesh to compute the solution transient of convection-diffusion-reaction boundary value problems by using mimetic numerical methods. The estimation of the error, in the spatial variable, is made from the discrete version of the gradient operator. The numerical experiment shows the good behavior of the procedure.

1. Introduction
In the last two decades, a new type of finite difference conservative schemes, known as support operators, and later as mimetic methods (MM) [1–3], has shown important advantages over the classic schemes of finite differences [4–6] in solving several problems that arise in engineering and science. However, little has been said about how to define an adaptive process that defines a mesh that is optimal to find a solution that meets a certain precision or error that is required by the problem to be solved.

A first step in this direction was given by [7] when constructing the gradient and divergent operators on non-uniform structured meshes, suggesting an adaptive process using equidistribution from a mesh-size function. On the other hand, in [8] and [9] is defined an adaptive process (of type h) for the stationary convection-diffusion equation and parabolic equations, respectively. In both works the approximation of the gradient is used to estimate the error in the spatial variable. No other satisfactory adaptivity results for the mimetic schemes proposed by [10] are known by the authors.

In this paper, an adaptive procedure is implemented that defines an optimal mesh to calculate the solution of problems modeled by the unidimensional equation of convection-diffusion-reaction in non-stationary regime. For this purpose, the non-uniform discrete operators proposed by [7] are used. In addition, to define an estimate of the error committed in the mimetic (spatial) approach, the mimetic discretization of the gradient operator is used without reference to the analytical solution of the boundary problem, which is generally unknown. In other words, an error estimate is made in the derivative of the solution, and not in the solution. This calculation does not merit any additional work, since the gradient has been previously defined to calculate the solution to the problem. Additionally, it can be said that the proposed process for estimating

the error follows the ideas of the residual SPR estimator (superconvergent patch recovery) introduced by [11] for smoothing tensions (derivatives), and [12] in the case of displacements (unknown variable of the problem); both versions were implemented in the past for the finite element method.

The error estimate and the adaptive algorithm are presented for one-dimensional problems. In the present, the authors develop the extension to multidimensional problems in structured meshes. On the other hand, the procedure for the case of unstructured meshes of quadrilateral elements represents, nowadays, an open problem.

The rest of the article is structured as follows. In the following section, the mimetic method used is briefly described and the boundary value problem considered is introduced along with its Robin-type boundary conditions. In the third section, the error estimator is introduced; later, in the fourth section, the adaptive process is defined. Finally, the numerical experimentation and the discussion of the results obtained together with the references of the work are presented.

2. Mimetic difference method

The mimetic difference methods are based on the discretization of the classical operators of the partial derivative equations (divergence, gradient and rotational) in such a way that they satisfy a discrete version of the Stokes Theorem or Green's identity [10]:

$$\langle \mathbf{D}v, f \rangle_Q + \langle v, \mathbf{G}f \rangle_P = \langle \mathbf{B}v, f \rangle_I. \tag{1}$$

In the Equation (1), $\mathbf{D}$, $\mathbf{G}$ and $\mathbf{B}$ are respectively the discrete versions of their corresponding continuous operators: gradient (∇), divergence ($\nabla\cdot$) and boundary operator $\partial/\partial n$. Functionals $\langle \cdot, \cdot \rangle$ represent a generalized internal product with Q, P and I weights. Using the identity (1), it is obtain the relation for the boundary operator $\mathbf{B} = Q\mathbf{D} + \mathbf{G}^{\mathrm{t}}P$.

For spatial discretization, a non necessarily uniform mesh is defined and whose geometry is given by the nodes x_i, with $i = 0, 1, \ldots, N$, and whose cells are the intervals $[x_{i-1}, x_i]$, with size $H_i := x_i - x_{i-1}$ for $i = 1, \ldots, N$. The intermediate nodes of the cells are given by $x_{i+1/2} = (x_i + x_{i+1})/2$, and the length between two consecutive intermediate nodes is given by $J_{x_i} := x_{i+1/2} - x_{i-1/2}$ for $i = 1, \ldots, N-1$. The cell $[x_{i-1}, x_i]$ will be referred to as the cell or element Ω_i. The solution and the divergence operator are defined in the center of the cells, while the operator gradient in the nodes x_i that define the cells (see Figure 1).
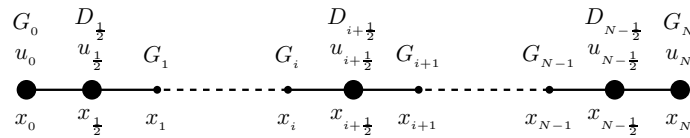

Figure 1. Non uniform one-dimensional mimetic mesh.

The discrete second-order gradient operator, introduced by [7] for non-uniform 1D meshes, is given by $\mathbf{G}u = \mathbf{J_G}\hat{\mathbf{G}}u$, where $\mathbf{J_G}$ is a diagonal matrix with the inverses of the lengths J_{x_i},

$$J_{x_0} = -\frac{8}{3}x_0 + 3x_{1/2} - \frac{1}{3}x_{3/2}, \qquad J_{x_N} = \frac{1}{3}x_{N-3/2} - 3x_{N-1/2} + \frac{8}{3}x_N,$$

and $\hat{\mathbf{G}}$ is the fixed part of the gradient operator for uniform meshes [10]. On the other hand, the second-order divergence operator, for non-uniform meshes 1D, is given by $\mathbf{D}v = \mathbf{J_D}\hat{\mathbf{D}}v$, where $\mathbf{J_D}$ is a diagonal matrix with the inverse of the lengths of the cells and $\hat{\mathbf{D}}$ the fixed part of the operator divergence for uniform meshes. The boundary operator $\mathbf{B}$ of dimension $[N+1 \times N+1]$ is given in [10].

2.1. Transient model problem

A boundary problem of the convection-diffusion-reaction type and time-dependent in its conservative form is given by the Equation (2),

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\nu(x)\frac{\partial}{\partial x}u\right) + f(x,t) \quad \text{en } \Omega \times [0,T), \tag{2}$$

where $\Omega = (a,b)$, $u(x,t)$ represents the variable of the problem (for example, temperature) at a point x of the domain Ω at a time t, $\nu > 0$ is the thermal transmission coefficient, and f is a scalar function that describes the existence of a source or sink in the problem. The Equation (2) is completed by defining the initial condition $u(x,0) = g(x)$ and the boundary conditions (Equation 3),

$$\alpha_a u(a,t) + \beta_a \frac{\partial}{\partial x}u(a,t) = \gamma_a, \qquad \alpha_b u(b,t) + \beta_b \frac{\partial}{\partial x}u(b,t) = \gamma_b, \tag{3}$$

with $\{\alpha_i, \beta_i, \gamma_i\}$, $i = a, b$, known real parameters, that depending on their value, determine boundary conditions of Dirichlet, Neumann or Robin type.

2.2. Mimetic discretization for the model problem

Using an implicit scheme for the time discretization with a time step k, and the discretization of the gradient and divergence operators, it is found the mimetic approximation for the convection-diffusion-reaction Equation (2) is given by Equation (4),

$$U^{n+1} - U^n = k\mathbf{D}(\nu\mathbf{G})U^{n+1} + kF^{n+1}, \tag{4}$$

where $U^n = \left(U(x_0, t_n), U(x_{1/2}, t_n), \ldots, U(x_{N-1/2}, t_n), U(x_N, t_n)\right)^{\mathrm{t}}$ represents the approximate mimetic solution in time $t_n = nk$ of the exact solution u of the problem, and $F^n = \left(f(x_0, t_n), f(x_{1/2}, t_n), \ldots, f(x_{N-1/2}, t_n), f(x_N, t_n)\right)^{\mathrm{t}}$ represents the restriction of f to the mimetic mesh.

Since the discretized divergence operator does not act on the boundary, then the Robin boundary conditions (Equation (3)) are obtained from Equation (5),

$$\left[[\alpha] + [\beta](\mathbf{B}\mathbf{G})\right]U^{n+1} = f_b, \tag{5}$$

where the vector f_b results from restricting the non homogeneous term of the boundary conditions to the mimetic mesh, that is, $f_b = (\gamma_a, 0, \ldots, 0, \gamma_b)^{\mathrm{t}}$. The arrays $[\alpha]$ and $[\beta]$ are such that $\alpha_{1,1} = \alpha_a$, $\alpha_{N+2,N+2} = \alpha_b$, $\beta_{1,1} = \beta_a$, $\beta_{N+2,N+2} = \beta_b$, and all other entries are zero.

From Equations (4) and (5), the mimetic scheme for the Equation (2) subject to the Robin boundary conditions (Equation (3)) is given by Equation (6),

$$\left[I + [\alpha] + [\beta]\mathbf{B}\mathbf{G} - k\mathbf{D}(\nu\mathbf{G})\right]U^{n+1} = U^n + kF^{n+1} + f_b. \tag{6}$$

3. Error estimation

When solving a problem numerically, it is convenient to control the quality of the approximated solution or the gradient of such a solution. This type of control can be achieved through a process of adaptivity of the mesh to efficiently approximate the solution of the problem. Likewise, in an adaptive process it is indispensable to have, throughout the domain, the local distribution of the error that is committed when using the approximate solution as a solution of the model. In other words, it is necessary to estimate the error committed in the approximation for each cell of the domain. In our case, the estimation of the error in the spatial variable is done on the gradient of the mimetic solution, that is, we must estimate the error that arises when using $\mathbf{G}U$ to approximate the exact gradient ∇u. The numerical error in the approximation $\mathbf{G}U$ of ∇u will be denoted by $e_G := \nabla u - \mathbf{G}U$.

3.1. Estimation of the error in space when using the gradient smoothing

The a posteriori error estimation process that is presented provides an approximation z^*, obtained by doing a postprocess on the solution $\mathbf{G}U$. The goal is to obtain the estimated error $e_{\mathrm{G}}^* = z^* - \mathbf{G}U$ in each cell of the Ω domain, such that $e_{\mathrm{G}}^* \approx e_G$.

Every cell Ω_i in the mesh has a patch of cells associated with it, ω_i, constituted by all the cells that surround it (see Figure 2). For the case of boundary elements, the patch of these cells is given by the border element and the two consecutive elements (previous) to it.

The calculation of z^* is done locally for each cell patch that is formed in the mesh. The values of $\mathbf{G}U$ in the nodes of the mesh are used as input to define a polynomial of higher order (interpolation). For one-dimensional problems, the patch of elements involves four nodes of the mesh (see Figure 2). In this case, a cubic polynomial is defined using interpolation on the four values of $\mathbf{G}U$. In particular, for any internal node x_j in the cell Ω_i (see Figure 2) it can be defined $z^*(x_j)$ in that cell. That is, the estimation of the error restricted to the cell Ω_i and evaluated in the node x_j is given by Equation (7),

$$e_{\mathrm{G}}^*\big|_i = z_j^* - I_h \mathbf{G}U, \tag{7}$$

where $I_h \mathbf{G}U$ represents the linear interpolation of $\mathbf{G}U$ evaluated in the node x_j, and z_j^* the value of z^* in the node x_j.
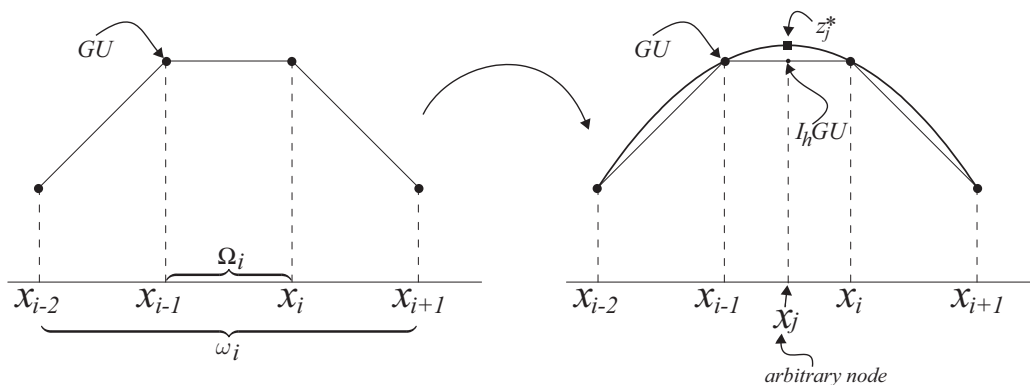

Figure 2. Illustration of the one-dimensional procedure. Each cell $]x_{i-1}, x_i[$ is associated with a patch $]x_{i-2}, x_{i+1}[$ and the corresponding values of $\mathbf{G}U$ in the mesh (nodes labeled with $\bullet$). It is passed a polynomial by these values (nodes $\bullet$). This polynomial is evaluated for the improved value z^* (node labeled with $\blacksquare$).

In L_2 norm, the error in each cell Ω_i is given by $\|e_{\mathrm{G}}^*\|_i^2 = \int_{\Omega_i} \psi_i(x)^2 dx$, with $\psi_i(x) = (z^* - I_h\mathbf{G}U)(x)$ for the element Ω_i. By Gaussian quadrature, it is established the Equation (8),

$$\|e_{\mathrm{G}}^*\|_i^2 = \frac{x_i - x_{i-1}}{2} \sum_{j=1}^{npG} \eta_j \Big(\psi_i \big(\frac{x_i - x_{i-1}}{2}\hat{x}_j + \frac{x_i + x_{i-1}}{2} \big) \Big)^2, \qquad (8)$$

where η_j and $\hat{x}_j$ represent the weights and points of the Gaussian quadrature (in our case, it is enough to take $npG = 2$). Continuing the process for all the cells Ω_i, it is possible to define the global estimated error $\|e_{\mathrm{G}}^*\|_2 = \sum_i \|e_{\mathrm{G}}^*\|_i$.

The smoothing proposed on the $\mathbf{G}U$ is able to improve the *curvature* of the approximate solution, that is, the smoothed solution z^* improves on its derivatives. However, this conclusion does not necessarily occur for the values without derivation (solution U of the problem). This fact justifies our selection, for the estimation of the error, in the gradient and not in the solution U of the problem.

4. Adaptive error control

The simplest strategy to control the error committed by using the approximate solution, $e := u - U$, consists of an iterative process that implements the estimation technique given in the previous section to define the distribution of the nodes (mesh) in the current time step, and keep such mesh in the following time steps until the tolerance of the error is not satisfied and it is necessary to redefine the mesh. This strategy is very general and does not require information on the type of problem to be addressed.

For the stopping criterion of the adaptive process, it is requested that $\|e\| \leq \texttt{TOL}$. However, although the error estimate is made in the solution gradient, there is no estimated value e^* for the error e. To solve this difficulty, it is used for each cell in the domain: $e_i = \int_{\Omega_i} e_{\mathrm{G}} dx \approx \int_{\Omega_i} e_{\mathrm{G}}^* dx$.

Thus,

$$\|e\| \leq \sum_i \|e\|_i = \sum_i \Big(\int_{\Omega_i} |e_{\mathrm{G}}|_i^2 dx \Big)^{1/2} \approx \sum_i \Big(\int_{\Omega_i} |e_{\mathrm{G}}^*|_i^2 dx \Big)^{1/2} = \sum_i \|e_{\mathrm{G}}^*\|_i. \qquad (9)$$

In practice, it can be used the estimated error of the gradient, $\|e_{\mathrm{G}}^*\|$, instead of the estimate $\|e^*\|$ of the error in the solution. However, this change can decrease the efficiency of the adaptive process, reaching to define meshes with many more nodes than necessary, but with a behavior similar to that achieved when using $\|e^*\|$.

5. Numerical results

Now, the numerical results obtained by applying the proposed adaptive algorithm are presented. The synthetic character of the analyzed example looks to justify the effectiveness of the estimator in cases where the problem has strong variations in its derivatives.

The estimation quality of e_{G}^* is measured using the quotient $\mathscr{I}^{\texttt{eff}} := \frac{\|e_{\mathrm{G}}^*\|}{\|e_{\mathrm{G}}\|} \times 100\%$, which is called *index of global effectiveness* or *index of local effectiveness*, in the case that it is measured on a specific cell. These indexes can be used to measure the quality of the estimate when the exact error is known (which is the case of the example analyzed); otherwise, a good approximation of it is required. For the analysis of the error, the maximum norm, $\|\cdot\|_\infty$, and the L_2 discrete norm $\|\cdot\|_2$, are considered.

5.1. Example

The model problem (Equations (2) and (3)) is solved with the mimetic scheme (Equation (6)) for a thermal transmission coefficient $\nu(x) = 1/\alpha + \alpha(x-x_0)^2$, with $\alpha = 250$ and $x_0 = 0.75$, and a source term $f(x,t)$ defined in such a way that the analytical solution of the problem is given as $u(x,t) = (1-x)\big[\arctan(\alpha(x-t)) + \arctan(\alpha t)\big]$. For this example, $u(0,t) = u(1,t) = 0$, which simplifies boundary conditions: $u'(0,t) = \alpha/(1+\alpha^2 t^2)$ y $u'(1,t) = -\arctan(\alpha(1-t)) - \arctan(\alpha t)$. The time interval is $t \in [0,0.9]$ and a time step given by $dt = 0.002$. In addition, no progress in time is made until an error tolerance of 0.001 for the gradient $\|e_G^*\|$ is met.

Figure 3(a) shows the approximate solution (line with ●) together with the analytical solution (solid line) for time $t = 0.5$. In the lower part, Figure 3(c), the meshes obtained (spatial distribution of the nodes) are shown during the adaptive process, for different time steps. The highest concentration of nodes occurs between the values where the gradient of the solution is more pronounced (as it could be expected). Figure 3(b) illustrates the number of nodes required in each time step.
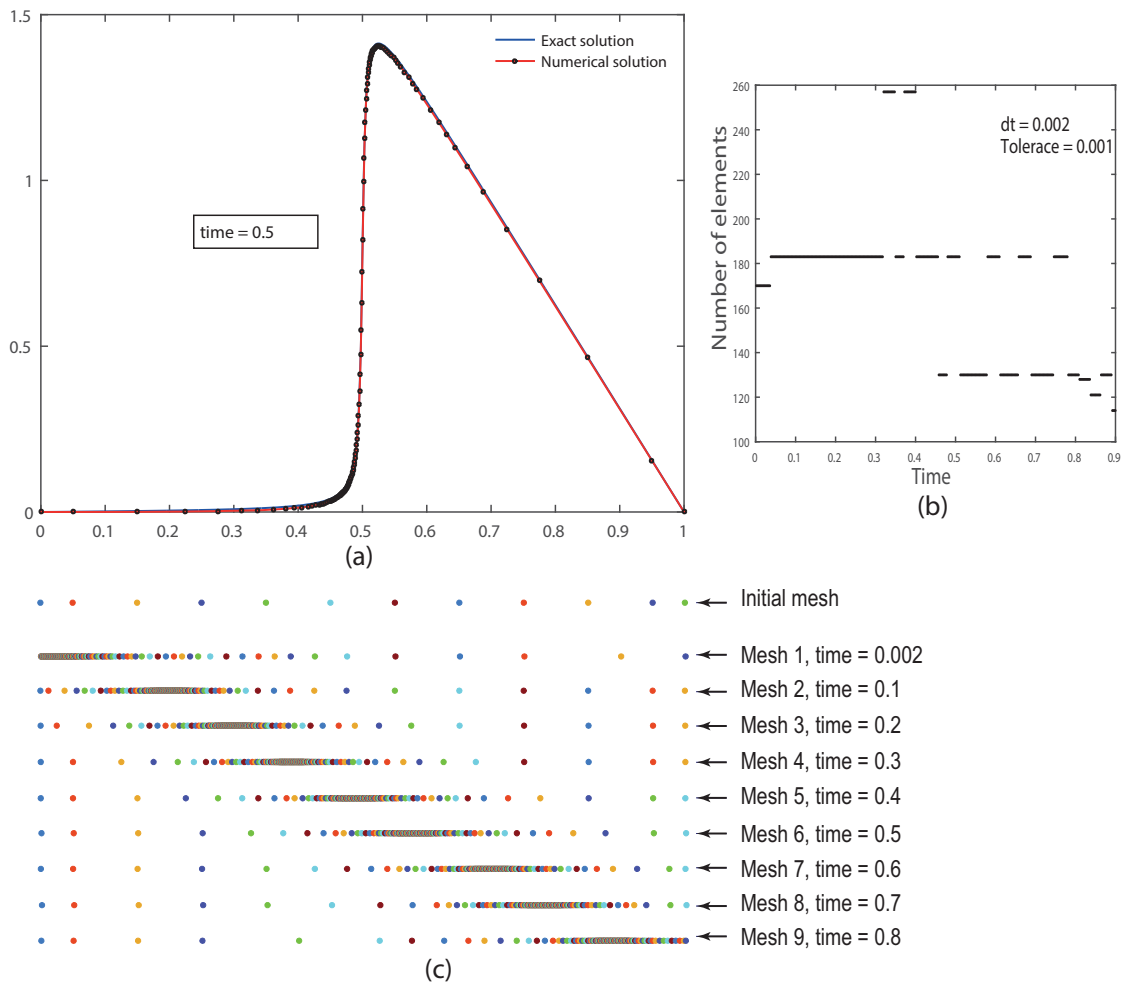

Figure 3. (a) Approximate (line with ●) and exact (continuous line) solutions for time $t = 0.5$. (b) Nodes required in each time step. (c) Spatial distribution of the nodes (meshes) for different time steps.

The adaptive process starts in a uniform mesh of 10 cells (11 nodes) and a relative error in the solution close to 30%. The relative error in the gradient is around 900%, and it is wanted to reach a solution in each step of time with an error lower than 0.1%. The numerical results for the succession of meshes obtained in some time steps, for an error tolerance of 10^{-3}, are presented in the Table 1.

In Table 1, the exact relative error in the gradient, $\|e_{\mathrm{G}}\|/\|Gu\|$, and its estimate, $\|e_{\mathrm{G}}^*\|/\|z^*\|$, are shown in the third and fourth columns, respectively. The relative error in the approach when using the mimetic solution, $\|e\|/\|u\|$, is given in the fifth column. In the last column, the global effectiveness index is presented. The results are shown only in the maximum norm, $\|\cdot\|_\infty$, because the results obtained in standard L_2 norm, $\|\cdot\|_2$, result, in general, analogues. In each time step shown in this table, the values obtained for the last mesh that defines the adaptive process are given. The fact that the prescribed tolerance is not reached, at each step of time, in the first iteration of the iterative process, does not imply that the adaptive process is functioning erratically or its effectiveness is low, this is mainly due to the additional conditions that are imposed on the process, for example, percentage of cells to be divided or number of divisions per cell.

Table 1. Tolerance 10^{-3}. Maximum norm. Values of the exact relative error in the gradient (third column), estimated relative error in the gradient (fourth column), exact relative error in the solution (fifth column) and global effectiveness index.

| Time | Exact relative error, estimated and effectiveness indexes | | | |
	Nodes	$\|e_{\mathrm{G}}\|/\|Gu\|$	$\|e_{\mathrm{G}}^*\|/\|z^*\|$	$\|e\|/\|u\|$	$\mathscr{I}^{\texttt{eff}}$
0	11	$0.920 \times 10^{+1}$	0.367	0.294	26.4%
0.002	171	0.762×10^{-2}	0.234×10^{-2}	0.281×10^{-1}	30.2%
0.1	184	0.353×10^{-2}	0.233×10^{-2}	0.249×10^{-1}	65.9%
0.3	184	0.272×10^{-2}	0.233×10^{-2}	0.887×10^{-2}	85.7%
0.5	184	0.861×10^{-2}	0.877×10^{-2}	0.988×10^{-2}	102.0%
0.7	131	0.723×10^{-2}	0.867×10^{-2}	0.645×10^{-2}	120.0%
0.9	115	0.748×10^{-2}	0.910×10^{-2}	0.610×10^{-2}	121.8%

Graphically, these results are shown in the Figure 4 for time $t = 0.3$. The estimated and exact relative errors (gradient) in the maximum and L_2 norms are shown in Figures 4. The asymptotic tendency of the estimated error, as the mesh is adjusted, reflects the good behavior of the proposed error estimator.

To define the performance of the adaptive process, the results are compared with a uniform mesh of 500 elements for all time steps. The error behavior for the uniform mesh and those obtained from the adaptive process turn out to be equivalent (see Figure 5). However, calculations made with uniform meshes with less than 500 elements show an oscillatory behavior in the error (Figure 5 shows the case of 300 elements), tending to lose stability as time advances.
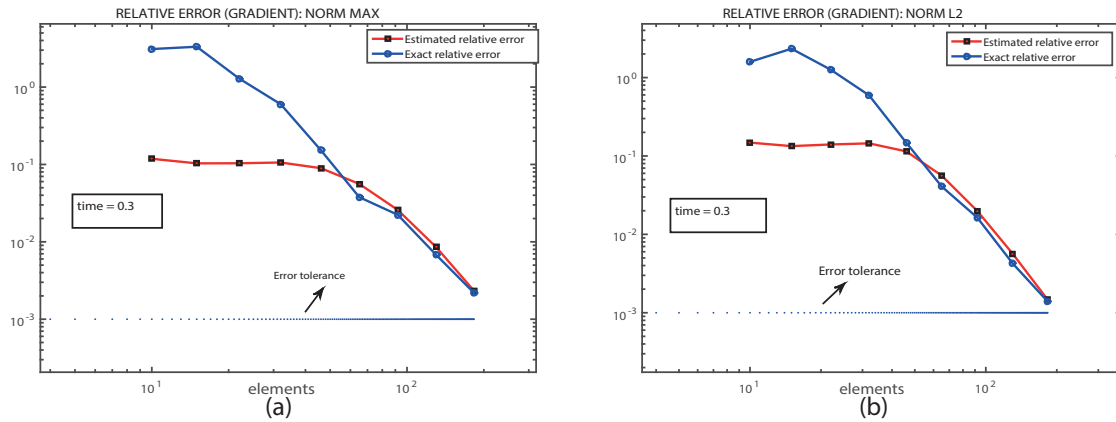
Figure 4. Convergence of the relative error of the gradient: ■ estimated error $\|e_{\mathrm{G}}^*\|/\|z^*\|$, ● real error $\|e_{\mathrm{G}}\|/\|Gu\|$. (a) Maximum norm, (b) L_2 norm.
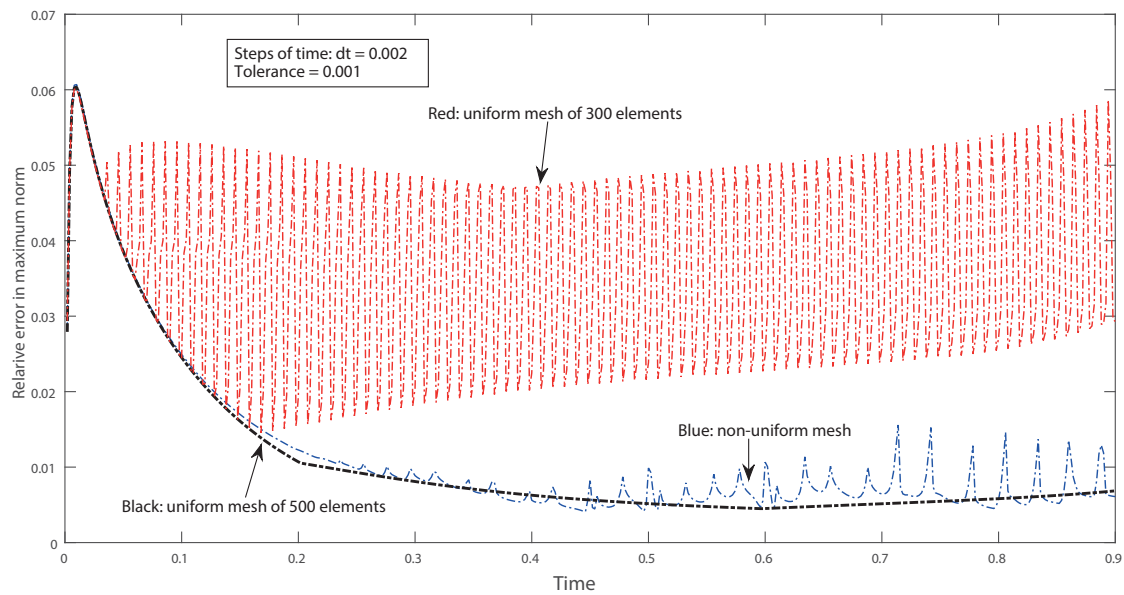

Figure 5. Maximum norm. Comparison of the error for uniform meshes and those given by the adaptive process.

6. Conclusions and final comments

An h-adaptive process has been established from an error estimate by softening the gradient for the spatial variable. The mesh is held fixed by successive time steps so long as it meets the prescribed error tolerance. Numerical experimentation verifies the good performance of error estimator by postprocess proposed, providing adaptive meshes which accelerate the accuracy (convergence) of the approximate solution compared to uniformly fine meshes.

References

[1] Shashkov M and Steinberg S 1995 Support-operator finite-difference algorithms for general elliptic problems *Journal of Computational Physics* **118(1)** 131–151

[2] Hyman J M, Shashkov M and Steinberg S 2002 Mimetic finite difference methods for diffusion equations *Computers Math. Applic.* **6(3-4)** 333–352

[3] Castillo J and Grone R D 2003 A matrix analysis approach to higher-order approximations for divergence and gradients satisfying a global conservation law *SIAM J. Matrix Anal. Appl.* **25(1)** 128–142

[4] Guevara J, Freites M and Castillo J 2005 A new second order finite difference conservative scheme, *Divulgaciones Matemáticas* **13(1)** 107–122

[5] Solano-Feo F, Guevara-Jordan J, Rojas O, Otero B and Rodriguez R 2016 A new mimetic scheme for the acoustic wave equation *Journal of Computational and Applied Mathematics* **295(1)** 2–12

[6] Sosa Jones G, Arteaga J and Jimnez O 2018 A study of mimetic and finite difference methods for the static diffusion equation *Computers and Mathematics with Applications* **76(1)** 633–648

[7] Batista E and Castillo J 2009 Mimetic schemes on non-uniform structured meshes *Electronic Transactions on Numerical Analysis* **34(1)** 152–162

[8] Calderón G and Lugo A 2015 Error estimation and adaptivity in mimetic schemes for boundary value problems *Boletín Venezolano de Matemáticas* **2** 109–124

[9] Calderón G, Carrillo E J, Villamizar J, Torres C and Castillo J 2019 Estimación de errores y adaptatividad en esquemas miméticos para un problema de tipo parabólico *Rev. UIS Ing.* submitted

[10] Castillo J and Yasuda M 2005 Linear systems arising for second-order mimetic divergence and gradient discretizations *Journal of Mathematical Modelling and Algorithms* **4(1)** 67–82

[11] Zienkiewicz O and Zhu J 1992 The superconvergent patch recovery (SPR) and a posteriori error estimates. Part 1: The recovery technique *Int. J. Num. Meth. Engrg.* **33** 1331–1364.

[12] Díez P and Calderón G 2007 Goal-oriented error estimation for transient parabolic problems *Computational Mechanics* **35(5)** 631–646.