FARAUTE Ciens. y Tec., 3(1): 64-70, 2008.

ISSN 1698-7418
Depósito Legal PP200402CA1617

A NUMERICAL STUDY OF A MIMETIC SCHEME FOR UNSTEADY HEAT EQUATION

Un Estudio Numérico de un Esquema Mimético para la Ecuación No Estática del Calor

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Fecha de recepción: 08/10/2007, **Fecha de Revisión:** 19/11/2007, **Fecha de Aceptación:** 09/05/2008

Abstract

A new mimetic scheme for the unsteady heat equation is presented. It combines recently developed mimetic discretizations for gradient and divergence operators in space with a Crank- Nicolson approximation in time. A comparative numerical study against standard finite difference shows that the proposed scheme achieves higher convergence rates, better approximations, and it does not require ghost points in its formulation.

Key words: mimetic scheme, finite differences, gradient operator, divergence operator, heat equation.

Resumen

Se presenta un nuevo esquema mimético para resolver la ecuación no estática del calor. El esquema combina discretizaciones miméticas de los operadores gradiente y divergencia, recientemente desarrolladas, en el espacio con una aproximación tipo Crank-Nicolson en el tiempo. Un estudio numérico comparativo contra el esquema de diferencias finitas tradicionales muestra la superioridad del esquema propuesto obteniéndose órdenes de convergencia superiores, mejores aproximaciones y la ausencia de puntos fantasmas en su formulación.

Palabras clave: esquema mimético, diferencias finitas, operador gradiente, operador divergencia, ecuación del calor.

1. Introduction

Mimetic schemes are a new type of numerical methods for solving partial differential equations. They are based on the discretizations of the main continum differential operators, which are combined to obtain the mimetic schemes for the most common equations in mathematical physics. A key feature of the mimetic discretizations is that they satisfy discrete versions of the Green-Gauss-Stokes theorem. This property guaranties the conservative character of the numerical schemes. Mimetic methods could be considered as a hybrid between finite element and finite difference methods with the advantage that their computer implementation are not harder than standard finite differences, while quality of their numerical approximations are comparable to those obtained by finite element in hard problems. These characteristics of mimetic schemes are principal incentives to continue their research and improvement.

In this article a new mimetic scheme for the unsteady heat equation is presented. Its content has been distributed in the following way. In the next section we give a short bibliographic review. After that the second order mimetic discretization for gradient and divergence operators are described. Next, we present the unsteady heat equation and the new mimetic scheme for its solution in the most general context. As a continuation the new scheme is adapted to the one dimensional case. Finally, a comparative numerical study and its conclusion are given.

2. Review of previous works

In (Castillo *et al.*, 2003) a systematic approach using uniform one dimensional grid to obtain new higher order mimetic schemes for gradient and divergence operators with the same order of convergence at the boundary and inner grid points is presented. Its second order version was used to solve the static heat equation (Freites *et al.*, 2004; Castillo *et al.*, 2005) and numerical results showed that they produced better approximated solutions than support operators conservative schemes presented in (Shashkov, 1996) and standard finite differences based on ghost points. An analytic proof of convergence for this scheme was reported in (Guevara *et al.*, 2007). Applications of mimetic discretizations developed in (Castillo et al., 2003) to transient problems have been only published for one dimensional Navier Stokes equation with encouraging results (Fagundez *et al.*, 2004). Combination of second order mimetic discretization with Crank Nicolson approach in time has not been reported in the context of transient heat equation to the best of our knowledge. Therefore, numerical study and mimetic scheme presented in this article are original contributions developed in (Mannarino, 2007).

3. Basic Mimetic Operators

A mimetic scheme should provide matrix discretizations $[G]$ and $[D]$ for gradient (∇) and divergence $(\nabla .)$ operators respectively. It is well known that the Green-Gauss-Stokes theorem is represented by the relation

$$\int_{\Omega} (\nabla \cdot u) v dx + \int_{\Omega} u \nabla v dx = \int_{\partial\Omega} \langle u, \vec{n} \rangle v ds \quad (1)$$

between the operators ∇ and $\nabla .$ at the continuous level. In the context of the heat equation only gradient and divergence discretizations, $[G]$ and $[D]$, are required. They satisfy a discrete version of Green-Gauss-Stokes theorem

$$\langle [D]u, v \rangle_Q + \langle u, [G]v \rangle_W = \langle [B]u, v \rangle_I \quad (2)$$

In this expression brackets represent generalized inner products with weights Q, W, I, and the matrix associated to the complete operator $[B]$ is defined by the explicit formula

$$[B] = Q[D] + [G]^t W \quad (3)$$

A comparison of equations (1) and (3) reveals that $[B]$ represents the boundary operator in the Green-Gauss-Stokes Theorem. It will play a fundamental role in boundary conditions mimetic discretizations. Mimetic methods have been specially designed for logically rectangular grids, so description of operators $[G]$ and $[D]$ are best defined in one dimensional context. In order to obtain these expressions a one dimensional mimetic or staggered grid has been sketched in Fig. 1.

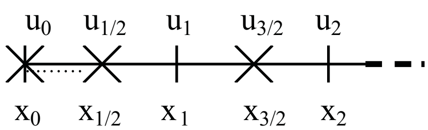

Fig. 1. 1-d mimetic or staggered grid

In this figure, a typical left boundary of the grid is displayed. Right boundary configuration is easily obtained by symmetry. Crosses represent nodes and vertical lines are grid blocks edges. Nodes positions are represented by $\{x_\alpha\}$ with α as a fraction if they are block centers. Edges positions are given by $\{x_\alpha\}$ with α as an integer if they are inner edges. Nodes and edges agree at the boundaries and they are represented by x_0 and x_n if the grid has n blocks. For simplicity, it will be assumed tha $x_0=0$, $x_n=1$, $x_{\alpha+1}-x_\alpha = 1/n \equiv h$ when α is integer or fraction, and $x_{1/2}-x_0 = x_n - x_{n-1/2} = h/2$. Sequence $\{x_\alpha\}$ represents generic functional values at edges or nodes $u_\alpha = f(x_\alpha)$ Description of operators $[G]$ and $[D]$ should be addressed in relation with a mimetic or staggered grid. On the above grid, the boundary entries for $[G]$ have the form

$$
\begin{aligned}
(Gu)_0 &= \frac{-(8/3)u_0 + 3u_{1/2} - (1/3)u_{3/2}}{h} \\
(Gu)_n &= \frac{(8/3)u_n - 3u_{n-1/2} + (1/3)u_{n-3/2}}{h}
\end{aligned}
\tag{4}
$$

while at inner edges its entries are just standard central difference

$$
(Gu)_i = \frac{u_{i+1/2} - u_{i-1/2}}{h} \tag{5}
$$

On the other hand, entries for mimetic divergence discretization $[D]$ are defined at the block centers and they reduce to standard central difference

$$
(Du)_{i+1/2} = \frac{u_{i+1} - u_i}{h} \tag{6}
$$

It is important to notice that equations (4), (5), and (6) are all second order and they define the only possible global second order mimetic discretizations for gradient and divergence operators. These observations are the main contribution of references (Castillo *et al.*, 2003; Castillo *et al.*, 2005).

4. Mimetic Scheme for Heat Equation

In its most general form the heat equations is represented by

$$
\frac{\partial u}{\partial t} - \nabla \cdot \left(K \nabla u\right) = F \tag{7}
$$

where *u* is temperature, *K* heat transfer diffusivity coefficient, *F* is known source term. In order to obtain a solution for heat equations initial and boundary conditions are required. The initial condition represents the values of temperature, $c(x)$, at a certain time which is usually assumed equal to zero. In symbols this takes the form.

$$
u(x,0) = c(x) \tag{8}
$$

There are several options to prescribe boundary conditions. However, a non trivial and general Robin's boundary condition

$$
\alpha(x)u + \frac{\partial u}{\partial \vec{n}} = f(x,t) \tag{9}
$$

Our scheme applies to any other boundary condition but Robin's conditions produce the best results and this justifies our choice. Moreover, no time dependent mimetic scheme based in (Castillo & Grone, 2003) have been applied to this type of boundary condition. Combination of equations (7), (8) and (9) is a well posed problem and an approximation of its solutions by numerical methods is well motivated.

The new mimetic scheme for the heat equation is based in Crank Nicolson approach. It is obtained by combinations of an implicit scheme, an explicit scheme, boundary conditions approximation and superposition of all them. The explicit scheme is developed from (7) by changing the continuous spatial operators by the mimetic approximations presented in section 3 and the forward difference for the time derivative. In matrix form it takes the form.

$$(1/2)[T]\left(U^{n+1/2}-U^{n}\right)-[D][K][G]U^{n}=F^{n} \quad (8)$$

In this expression $[T]$ is a diagonal matrix whose nonzero entries are $(1/dt)$ and dt is the time step. Similarly $[K]$ is a diagonal matrix whose nonzero entries are approximation of K on the mimetic grid edges. Vectors $U^{n+1\, or\, n}$ and F^{n} are the approximations to temperature and the source term on the mimetic grid nodes, their upper indexes denote the time level. The implicit scheme is obtained in a similar fashion, but the time derivative is backward difference. Its matrix formulation is

$$(1/2)[T]\left(U^{n+1}-U^{n+1/2}\right)-[D][K][G]U^{n+1}=F^{n+1} \quad (9)$$

and its description follows word by word the explicit approximations with straightforward changes in the time levels. Next, the boundary condition approximations are required at time step $n+1$ and n. This discretization is accomplished by combining operators $[G]$ and $[B]$ to approximate normal derivatives in (9). In symbols, a mimetic boundary conditions approximation takes the forms

$$\begin{aligned}
&[A]U^{n+1}+[B][G]U^{n+1}=f^{n+1}\\
&[A]U^{n}+[B][G]U^{n}=f^{n}
\end{aligned} \quad (10)$$

In these expression $[A]$ is a diagonal matrix and its nonzero entries are α values along the boundary. Vectors $f^{n \text{ or } n+1}$ are f approximations on the grid nodes at the boundary and zero elsewhere. By the superposition principle equations (8), (9) and (10) can be added to obtain the new mimetic scheme for the heat equation.

$$\begin{aligned}
&[CN]U^{n+1}=-[CN]U^{n}+\\
&+\frac{1}{2}\left(F^{n+1}+f^{n+1}+F^{n}+f^{n}\right)
\end{aligned} \quad (11)$$

In this expression

$$[CN]\equiv[T]-([D][K][G]-[A]-[B][G])/2 \quad (12)$$

which guaranties the mimetic character of the discretizations. The linear system in one dimension for [CN] associated with the staggered grid in Fig. 1 is $(n+2)\times(n+2)$. This means that the new scheme contains n linear equations, one for each internal node, and two equations for boundary conditions. Explicit expressions for these equations will be present to give consistence to this article. Due to symmetric considerations only five linear equations need to be listed. The first equation will be associated to node x_o and it takes the form.

$$\begin{aligned}
&\left(\frac{\alpha}{2}+\frac{4}{2h}\right)U_0^{n+1}-\frac{3}{2h}U_{1/2}^{n+1}+\frac{1}{6h}U_{3/2}^{n+1}=\\
&-\left(\frac{\alpha}{2}+\frac{4}{3h}\right)U_0^{n}+\frac{3}{2h}U_{1/2}^{n}-\frac{1}{6h}U_{3/2}^{n}+\frac{(f_o^{n+1}+f_0^{n})}{2}
\end{aligned} \quad (13)$$

notice that the three terms in this expression denotes the effect of the one hand side gradient definition in (4). Second equation is centered in $x_{1/2}$ and it is given by

$$\begin{aligned}
&-\left(\frac{1}{6}+\frac{4}{3h^2}\right)U_o^{n+1}+\left(\frac{1}{4h}+\frac{2}{h^2}+\frac{1}{dt}\right)U_{1/2}^{n+1}\\
&-\left(\frac{1}{12h}+\frac{2}{3h^2}\right)U_{3/2}^{n+1}=\left(\frac{1}{6}+\frac{1}{3h^2}\right)U_0^{n}\\
&-\left(\frac{1}{4h}+\frac{2}{h^2}-\frac{1}{dt}\right)U_{1/2}^{n}+\left(\frac{1}{12h}+\frac{2}{3h^2}\right)U_{3/2}^{n}\\
&+\frac{(F_{1/2}^{n+1}+F_{1/2}^{n})}{2}
\end{aligned} \quad (14)$$

There is an analog expression for symmetric node $x_{n-1/2}$. It is worth to mention that these equations are relations between values at three consecutive nodes with no uniform spaces among them. Third equation is not standard because it contains four terms in his expression. It is centered in $x_{3/2}$ and its symmetric contra part is associated to node $x_{n-5/2}$.

$$\frac{1}{6h}U_0^{n+1}-\left(\frac{1}{4h}+\frac{1}{2h^2}\right)U_{1/2}^{n+1}+\left(\frac{1}{12h}+\frac{1}{h^2}+\frac{1}{dt}\right)U_{3/2}^{n+1}$$
$$-\frac{1}{2h^2}U_{5/2}^{n+1}=-\frac{1}{6h}U_0^{n}+\left(\frac{1}{4h}+\frac{1}{2h^2}\right)U_{1/2}^{n} \qquad (15)$$
$$-\left(\frac{1}{12h}+\frac{1}{h^2}-\frac{1}{dt}\right)U_{3/2}^{n}+\frac{1}{2h^2}U_{5/2}^{n}+\frac{(F_{3/2}^{n+1}+F_{3/2}^{n})}{2}$$

Finally, we give the standard Crank Nicolson equation whose expression is valid for all inner nodes in the range $3/2<i+1/2<n-3/2$ for i=1,2,…,n-3

$$-\frac{1}{2h^2}U_{i-1/2}^{n+1}+\left(\frac{1}{h^2}+\frac{1}{dt}\right)U_{i+1/2}^{n+1}-\frac{1}{2h^2}U_{i+3/2}^{n+1}=$$
$$\frac{1}{2h^2}U_{i-1/2}-\left(\frac{1}{h^2}-\frac{1}{dt}\right)U_{i+1/2}^{n}+\frac{1}{2h^2}U_{i+3/2}^{n}+$$
$$\frac{(F_{i+1/2}^{n+1}+F_{i+1/2}^{n})}{2} \qquad (16)$$

In view of equations (13), (14), (15) and (16) then the matrix structure of [CN] is almost tridiagonal in one dimension and a banded matrix in higher dimensions. This gives evidence that the new scheme is not more computational intensive than standard finite difference.

An analytical study of the new scheme convergence has been performed in (Mannarino, 2007) by the Lax's equivalence theorem. However, (Mannarino, 2007) does not provide the convergence orders developed here.

5. Comparative Numerical Study

This study presents and analyzes two test problems which are solved with the new scheme, which will be called mimetic from now on, and standard finite difference scheme based on ghost points denoted by (FD). In order to be consistent with the theoretical development of this article, both test problems will be one dimensional. However, our results hold in a higher dimensional context (Mannarino, 2007).

The first test problem is a non homogeneous heat equation $\partial_t^u - \partial_{xx} = -e^{-t}x$ with initial condition $u(x,0)=x$ and boundary conditions

$$u(0)-\frac{\partial u}{\partial x}(0)=-e^{-t}, u(1)+\frac{\partial u}{\partial x}(1)=2e^{-t}$$

Errors in the modulus maximum norm are showed in Fig. 2. In this figure the better approximation is represented by the lower line. It is observed that line with crosses is above the line with circles associated with the mimetic scheme. This means that errors between analytical solution and numerical solutions computed by the mimetic scheme are always smaller than the errors obtained from the FD scheme.

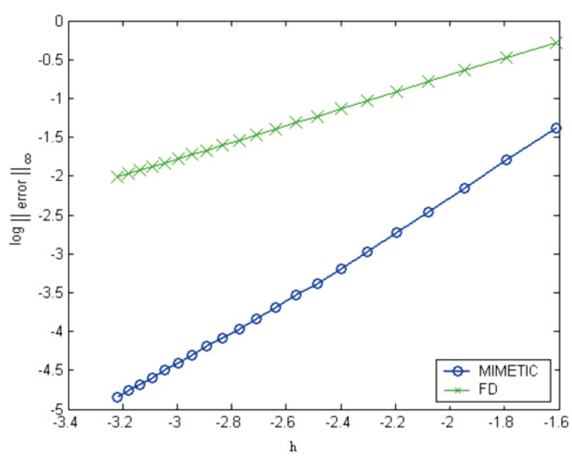

Fig. 2. Errors in first test problem.

Table 1 gives the values of these errors for a set of grid sizes. It can be seen that errors computed with the mimetic scheme are three orders of magnitude smaller than those registered by FD scheme

Methods	Grid size	Errors
MIMETIC	30	1.4022×10^{-5}
	60	3.5048×10^{-6}
	100	1.2618×10^{-6}
FD	30	1.6500×10^{-2}
	60	8.3000×10^{-3}
	100	5.0000×10^{-3}

Table 1. Errors in infinity norm

Fig. 2 shows that the slope for error curve associated to the mimetic scheme is higher than the one for FD scheme. A quantification of these slopes is presented in Table 2. It gives evidence that new mimetic scheme achieves a second order convergence rate while standard FD scheme in only first order.

Methods	Grid size	Orders
MIMETIC	30	2.0008
	60	2.0004
	100	2.0002
FD	30	1.1167
	60	1.0802
	100	1.0607

Table 2. Convergence Orders

The second test problem is defined by a non homogeneous heat equation $\partial_t^u - \partial_{xx} = (-1/10 + 4\pi^2)e^{-t/10} sen(2\pi x)$ initial condition $u(x,0) = e^{-t/10} sen(2\pi x)$ and boundary conditions given by

$$u(0) - \frac{\partial u}{\partial x}(0) = -2\pi e^{\frac{-t}{10}}, u(1) + \frac{\partial u}{\partial x}(1) = 2\pi e^{\frac{-t}{10}}.$$

Graphical representation of errors computed in the modulus maximum norm is displayed in Fig. 3.

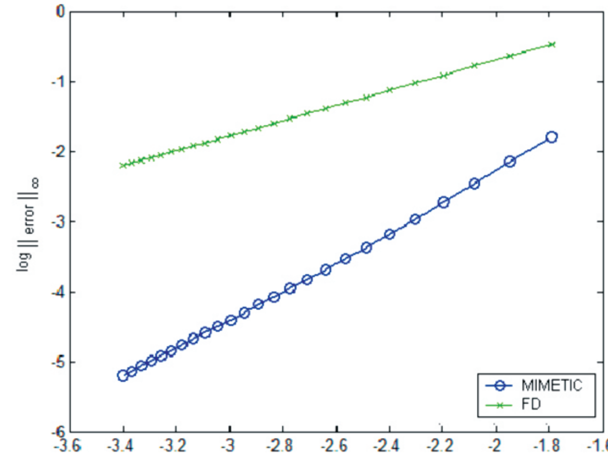

Fig. 3. Errors in second test problem

This figure shows the same behavior described in the first test problem. However, the gap between both curves is smaller in the second test problem, because the right hand side in the differential equation in an oscillatory function which produces a more difficult problem. The specific errors obtained for this problem are given in Table 3. It shoes that mimetic scheme errors are one order of magnitude smaller than those obtained by FD.

Methods	Grid size	Errors
MIMETIC	30	5.5000×10^{-3}
	60	1.4000×10^{-3}
	100	5.0298×10^{-4}
FD	30	1.0980×10^{-1}
	60	5.3500×10^{-2}
	100	3.1800×10^{-2}

Table 3. Errors in infinity norm

The convergence rates for both schemes are reported in Table 4. It gave a second order convergence rate for the mimetic scheme and first order for FD.

Methods	Grid size	Orders
MIMETIC	30	2.1108
	60	2.0445
	100	2.0202
FD	30	1.0758
	60	1.0620
	100	1.0503

Table 4. Convergence Orders

The explanation for the excellent results presented in these tests problems could be attributed to the use of ghost points in standard FD scheme. Ghost point in FD discretizations produces finite difference stencils centered in $x_{1/2}$ and $x_{n-1/2}$ whose first order approximations at the boundaries. Such phenomenon is not reproduced in the mimetic scheme because its staggered grid does not require any ghost point or extension in its formulation.

6. Discussion and Conclusions

A new mimetic scheme for approximation of the heat equation has been presented. Explicit expressions of its equations on a one dimensional staggered grid were developed. They show that linear systems associated to the new scheme are banded and very similar to those obtained from standard FD. Extensions of the mimetic scheme to multidimensional problems on logical rectangular grid can be easily achieved by Cartesian product of the equations developed in one dimensional problem. The comparative numerical study showed that the mimetic scheme produces smaller errors and faster convergence rates than standard FD based on ghost points. Since new mimetic scheme has solid theoretical foundations, its computer implementation is not harder than standard FD, and it produces high quality approximated solutions, then it seems fair to claim that it represents a new alternative for solving heat transfer problem in engineering.

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