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A Comparison of Third Order L_o - Stable Numerical Schemes for the Two –Dimensional Homogeneous Diffusion Problem Subject to Specification of Mass

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Abstract

This paper presents a numerical comparison of third order $L_o - stable$ numerical schemes for the two-dimensional parabolic partial differential equations subject to nonlocal boundary conditions. These numerical schemes are based on Pade` approximations to the matrix exponentials arising from the use of the method of lines and are tested on a model problem. The numerical comparison shows that the (0, 3) – Padé scheme is efficient and provide very accurate results as compared to (1, 2) – Padé scheme.

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Keywords: $L_o -$ stable, Parabolic Problems, nonlocal boundary conditions

1. Introduction

The two-dimensional parabolic partial differential equations with nonlocal boundary conditions arise in many important applications in sciences such as in heat transfer [3, 4, 16], medical science [4] and thermoelasticity [5]. In recent years, a number of numerical methods have been suggested in the literature for solving these equations (see, for instance, [7, 13, 14]), some of which (explicit methods) suffer stability restrictions. The one-dimensional diffusion problem was studied by Cannon et al. [4], Liu [19] and Ang [17]. A number of numerical methods for solving two dimensional diffusion equations with nonlocal boundary conditions are given in [11,13, 14, 15].

This work deals with a numerical comparison of third order numerical schemes based on (0,3) – Padé and (1, 2) – Padé approximants. Both numerical schemes will be applied on a model two-dimensional homogeneous diffusion problem with nonlocal boundary condition. The numerical solution of (0, 3) – Padé and (1, 2) – Padé schemes, exact solution and the absolute relative errors for the two experiments will be shown in the tabular form.

The outline of this paper is as follows: In section 2 we will give a brief review of Pade` approximants. In section 3 we will discuss the Pade` approximation of the matrix exponential. In section 4 we will consider two- dimensional diffusion equation with nonlocal boundary conditions and develop (0, 3) – Padé scheme. In section 5 we present numerical experiments. Concluding remarks are given in section 6.

2. Padé Approximants

In [12], the Padé approximant $R_{n,m}(z)$ to the exponential function $f(z) = e^{-z}$ is defined as follows: Let

$$R_{n,m}(z) = \frac{P_n(z)}{Q_m(z)} \tag{2.1}$$

where

$$P_n(z) = \sum_{j=0}^{n} \frac{(n+m-j)!n!}{(m+n)!\,j!(n-j)!}(-z)^n \tag{2.2}$$

and

$$Q_m(z) = \sum_{j=0}^{m} \frac{(n+m-j)!m!}{(m+n)!\,j!(n-j)!}(z)^n \tag{2.3}$$

satisfying

$$R_{n,m}(z) = e^{-z} + O(|\,z\,|^{n+m+1}) \qquad \text{as } |\,z\,| \to 0\,, \tag{2.4}$$

We will call $R_{n,m}(z)$ as $(n,m)-$Pade` scheme of order $(n+m)$.

3. $L_o -$ Stable Padé Schemes

In this section, we will discuss $L_o - stable$ Pade` schemes. The following definitions are given by G. D. Smith [9]:

Definition 3.1: A method is called $A_o - stable$ if $|R_{n,m}(-z)| < 1$ for all $z > 0$.

Definition 3.2: A method is called $L_o - stable$ if $|R_{n,m}(-z)| < 1$ for all $z > 0$ and $\lim_{z \to \infty} R_{n,m}(-z) = 0.$

The $(n, m) -$ Padé approximation schemes for parabolic problems are $L_o - stable$ when $n > m$ (see for details G. D Smith [9] page 122). It is well known fact that $L_o - stable$ methods are best suited for solving parabolic problems under nonsmooth data situation [2, 12]. $(0,1) -$ Padé, $(0,3) -$ Padé and $(1,2) -$ Padé are $L_o - stable$ methods.

The amplification symbol for (0, 1) – Pade` is given by

$$R(z) = \frac{1}{1+z} \tag{3.1}$$

The amplification symbol for (1,2) – Pade` is given by

$$R(z) = \frac{1 - \frac{1}{2}z}{1 + \frac{2}{3}z + \frac{1}{6}z^2} \tag{3.2}$$

The amplification symbol for (0,3) – Pade` is given by

$$R(z) = \frac{1}{1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3} \tag{3.3}$$

4. Padé Approximation of the Matrix Exponential

The $(n, m) -$ Padé approximation of e^{-kA} is approximated by

$$e^{-kA} \approx \{Q_m(kA)\}^{-1} P_n(-kA) \equiv R_{n,m}(kA), \tag{4.1}$$

where k is the time step.

The $(1, 2) -$ Padé approximation to the matrix exponential e^{-kA} is given by

$$v_{n+1} = \left(I - \frac{1}{3}kA\right)\left(I + \frac{2}{3}kA + \frac{1}{6}k^2A^2\right)^{-1} v_n \tag{4.2}$$

The $(0, 3) -$ Padé approximation to the matrix exponential e^{-kA} is given by

$$v_{n+1} = \left(I + kA + \frac{1}{2}k^2A^2 + \frac{1}{6}k^3A^3\right)^{-1} v_n \tag{4.3}$$

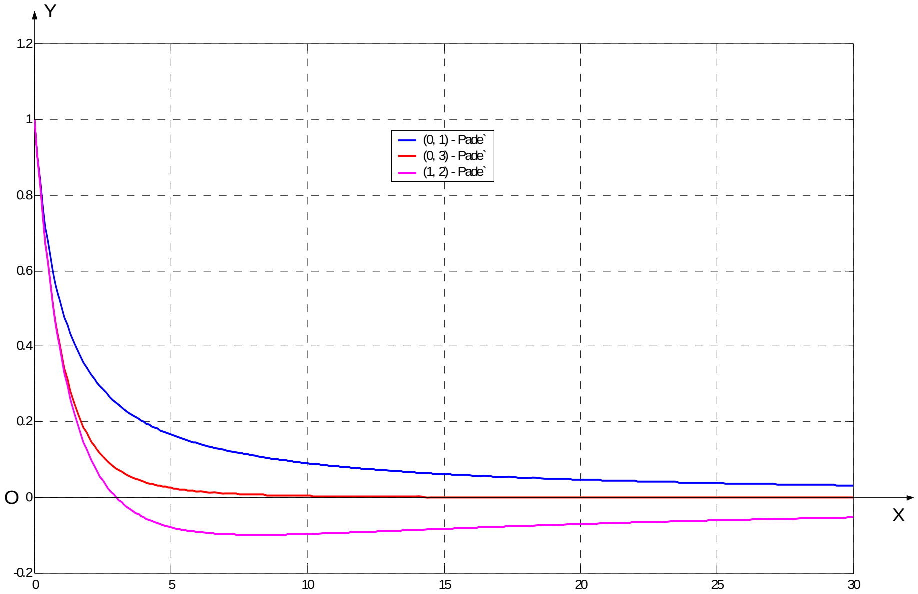

Figure 1. ***Graph of Amplification Symbol of (0,1) – Pade`, (0,3) – Pade and (1, 2) – Pade`***

The matrix A is a tridiagonal matrix. The number of diagonals of A increases with the powers of A. For example A^2 is a five diagonal matrix, A^3 is seven and A^4 is a nine diagonal matrix and so ill-cnditioning of the matrix A comes into picture.

Definition 4.1: The condition number of a matrix A denoted by $cond(A)$ and is defined by

$$cond(A) = \|A\| \|A^{-1}\|. \tag{4.4}$$

The condition number of a matrix measures the sensitivity of the solution of a system of linear equations to errors in the data. It gives an indication of the accuracy of the results from matrix inversion and the linear equations solutions. This can also cause computational difficulties and make the schemes computationally less efficient.

Partial fraction decomposition is a very useful technique of rewriting a rational function in simple terms. Gallopoulos and Saad [8] have used (m, m) – Padé (diagonal Padé) and constructed parallel algorithms using the factorizations. Khaliq et al. [1] discussed diagonal and subdiagonal Padé approximations in factored and partial fraction forms. They have used partial fraction forms of diagonal and subdiagonal Padé approximations to construct the following efficient parallel algorithm.

Algorithm 4.1

Step 1. For $i = 1, 2, \ldots, q_1 + q_2$, solve $(kA - c_i I) y_i = v_s$.

Step 2. If $n < m$, Compute

$$v_{n+1} = \sum_{i=1}^{q_1} w_i y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \mathrm{Re}(w_i y_i)$$

Step 3. If $n = m$, Compute

$$v_{n+1} = (-1)^m v_s + \sum_{i=1}^{q_1} w_i y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \mathrm{Re}(w_i y_i)$$

We have used partial fraction forms of subdiagonal Padé approximations to construct the $L_o - stable$ Pade` schemes.

5. Padé Numerical Schemes

We consider the homogeneous diffusion equation in two space variables, that is given by

$$u_t = \alpha(u_{xx} + u_{yy}); \qquad 0 < x, y < 1, \qquad t > 0 \tag{5.1}$$

in which we define $u = u(x, y, t)$ with the Dirichlet time-dependent boundary conditions

$$\begin{aligned} u(0, y, t) &= \psi_0(y, t), & 0 \le t \le T, \quad 0 \le y \le 1, \\ u(1, y, t) &= \psi_1(y, t), & 0 \le t \le T, \quad 0 \le y \le 1, \\ u(x, 0, t) &= \varphi_0(x, t), & 0 \le t \le T, \quad 0 \le x \le 1, \\ u(x, 1, t) &= \varphi_1(x, t), & 0 \le t \le T, \quad 0 \le x \le 1, \end{aligned} \tag{5.2}$$

The nonlocal boundary condition is

$$\int_0^1 \int_0^1 u(x, y, t) dxdy = \alpha(t), \qquad (x, y) \in \Omega \cup \partial\Omega, \tag{5.3}$$

and the initial condition is

$$u(x,y,0)=f(x,y), \qquad (x,y)\in\Omega\cup\partial\Omega, \tag{5.4}$$

where $f,\psi_o,\psi_1,\varphi_o,\varphi_1$ and α are known functions. The function $f(x,y)$ is continuous and will be discontinuous whenever initial and boundary conditions mismatch.

Following Gumel et. al. [11], we divide both intervals $0\le x\le X$ and $0\le y\le X$ into $N+1$ subintervals each of width h so that $h=\dfrac{X}{N+1}$ and the time t is discretized in steps of length k. At each time step $t=t_n=nk, n=0,1,2,\dots$ and we will have a square mesh with N^2 points within the square Ω and $N+2$ equally spaced points on each side of the boundary $\partial\Omega$. To approximate the solution $u(x,y,t)$ of (5.1) at each point (x_i,y_j,t_l) in $\Omega\times[t>0]$ where $i,j=1,2,\dots,N$ and $l=0,1,2,\dots$. Replacing the spatial derivatives in (5.1) by their second order central difference approximation leads to a system of N^2 first order, linear, ordinary differential equations of the form

$$\frac{dU}{dt}=AU+\beta(t), \qquad t>0, \quad U(x,y,0)=f(x,y) \tag{5.5}$$

where A is a matrix f order N^2 and can be split into block diagonal matrices A_1

and A_2 given by $A_1=\begin{bmatrix} A_1^* & & & & 0 \\ & A_1^* & & & \\ & & A_1^* & & \\ & & & \ddots & \\ 0 & & & & A_1^* \end{bmatrix}$

where A_1^* is the tridiagonal matrix of order N given by

$$A_1^*=\begin{bmatrix} -2 & 1 & & & 0 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 0 & & & 1 & -2 \end{bmatrix}$$

and

$$A_2=\frac{1}{h^2}\begin{bmatrix} -2I & I & & & 0 \\ I & -2I & I & & \\ & \ddots & \ddots & \ddots & \\ & & I & -2I & I \\ 0 & & & I & -2I \end{bmatrix}$$

where I is the identity matrix of order N.
Solving the system (5.5) subject to the initial condition $U(x,y,0)=f(x,y)$ yields [18], $U(t)=e^{tA}.f+\int_0^1 \mathrm{e}^{(t-s)A}.\beta(s)\,ds$, $t\geq 0$ and agrees with

$$U(t+k)=e^{kA}.U(t)+\int_t^{t+k}\mathrm{e}^{(t+k-s)A}.\beta(s)\,ds, \quad t=0,k,2k,\ldots \tag{5.6}$$

Approximating the quadrature in (5.6) by the trapezoidal rule yields

$$U(t+k)=e^{kA}.U(t)+\frac{k}{2}[\beta(t+k)+e^{kA}\beta(t)], \quad t=0,k,2k,\ldots \tag{5.7}$$

and may takes the form as

$$U(t+k)=e^{kA_1}.e^{kA_2}.U(t)+\frac{k}{2}[\beta(t+k)+e^{kA_1}.e^{kA_2}\beta(t)] \tag{5.8}$$

where the matrix A is replaced by A_1+A_2.

The approximation of the matrix exponential e^{-kA} by $(0,3)-$Padé and using partial fraction forms of subdiagonal Padé approximations yields the third order numerical scheme:

$$v_{n+1}=(\alpha_1+\alpha_2)[v_n+\frac{k}{2}\beta(t_n)]+\frac{k}{2}\beta(t_{n+1}) \tag{5.9}$$

where

$\alpha_1=\mathrm{w}_1(\mathrm{kA}-\mathrm{c}_1\mathrm{I})^{-1}$ and $\alpha_2=2\,\mathrm{Re}[\mathrm{w}_2(\mathrm{kA}-\mathrm{c}_2\mathrm{I})^{-1}]$
$\mathrm{c}_1=-1.596071637983321523112854143997$ (Real Pole)
$\mathrm{c}_2=-0.7019641810083392384435972928001 4-1.8073394944520218535764598429640\,\mathrm{i}$
$\mathrm{w}_1=1.4756865177957207165190465751319$
$\mathrm{w}_2=-0.7378432588978603582595232875659 2+0.3650178408010284724444376297914 5\,\mathrm{i}$

Gumel et. al. [2] developed an algorithm by using $(1,2)-$Padé to approximate the matrix exponential e^{-kA} and partial fraction forms of $(1,2)-$Padé (see for details Gumel et. al. [2] page 158). The parallel version of this algorithm was tested on model problems taken from the literature.

6. Numerical Experiments

In this section, we present a comparison between the numerical results of (1, 2) – Padé and (0, 3) – Padé schemes. The numerical results for (1, 2) – Padé are taken from [16] and the numerical results for (0, 3) – Padé are computed by using the numerical schemes (5.8). As in [2, 3, 13], the discretization parameters h and k are given values $h = \frac{1}{20}, k = \frac{1}{2400}$ in the first experiment and $h = \frac{1}{50}, k = \frac{1}{15000}$ in the second experiment so that $p = \frac{k}{h^2} = \frac{1}{6}$ in both experiments. The exact solution is known and used to test the accuracy of these numerical schemes. The absolute relative errors between the exact and numerical solutions are shown in the tables.

Problem. (Gumel et al. [2] and Ishak [10])
We consider the diffusion equation in two space variables given by

$$\frac{\partial u}{\partial t} = \alpha\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right); \qquad 0 < x, y < 1, \qquad t > 0 \tag{6.1}$$

The Dirichlet time-dependent boundary conditions are

$$\begin{aligned} u(0, y, t) &= e^{(y+2t)}, & 0 \le t \le T, \quad 0 \le y \le 1, \\ u(1, y, t) &= e^{(1+y+2t)}, & 0 \le t \le T, \quad 0 \le y \le 1, \\ u(x, 0, t) &= e^{(x+2t)}, & 0 \le t \le T, \quad 0 \le x \le 1, \\ u(x, 1, t) &= e^{(1+x+2t)}, & 0 \le t \le T, \quad 0 \le x \le 1, \end{aligned} \tag{6.2}$$

and nonlocal boundary condition

$$\int_0^1 \int_0^1 u(x, y, t)\,dx\,dy = (e-1)^2 e^{2t} \tag{6.3}$$

with initial conditions:

$$u(x, y, 0) = e^{(x+y)} \tag{6.4}$$

Theoretical solution is given by

$$u(x, y, t) = e^{(x+y+2t)}. \tag{6.5}$$

Here the PDE (5.1) subject to (5.2), (5.3) and (5.4) is solved numerically using (0, 3) – Padé and (1, 2)–Padé schemes which are L_o – stable schemes. As in [2, 3,13], the discretization parameters h and k are given the values $h = \frac{1}{20}$, $k = \frac{1}{2400}$. The absolute relative errors for the test problem are tabulated in Table 1, which shows that (0, 3) – Padé scheme gave superior results.

Table 1. Comparing Absolute Relative Error $h = \dfrac{1}{20}, k = \dfrac{1}{2400}$

X	Y	EXACT SOLUTION	(1, 2) – PADE`	(0, 3) – PADE`
0.1	0.1	9.02501350	3.3993 e-004	7.2921e-006
0.2	0.2	11.02317638	3.2676 e-004	1.7967e-005
0.3	0.3	13.46373804	2.6002 e-004	2.5890e-005
0.4	0.4	16.44464677	1.8408 e-004	2.9399e-005
0.5	0.5	20.08553692	1.1595 e-004	2.8601e-005
0.6	0.6	24.53253020	6.3782 e-005	2.4402e-005
0.7	0.7	29.96410005	2.9338 e-005	1.8015e-005
0.8	0.8	36.59823444	5.1982 e-006	1.0727e-005
0.9	0.9	44.70118449	3.3960 e-006	3.9328e-006

Following [2, 3, 13], the discretization parameters h and k are given the values $h = \frac{1}{50}$, $k = \frac{1}{15000}$. The absolute relative errors for the test problem are tabulated in Table 2. In this numerical experiment, the accuracy of (0, 3) – Padé compares well with (1, 2) – Padé scheme.

Table 2. Comparing Absolute Relative Errors $h = \dfrac{1}{50}, k = \dfrac{1}{15000}$

X	Y	EXACT SOLUTION	(1, 2) – PADE`	(0, 3) – PADE`
0.1	0.1	9.02501350	2.5562e-007	1.1707e-006
0.2	0.2	11.02317638	2.8302e-006	2.8809e-006
0.3	0.3	13.46373804	4.1114e-006	4.1507e-006
0.4	0.4	16.44464677	4.6798e-006	4.7135e-006
0.5	0.5	20.08553692	4.5541e-006	4.5858e-006
0.6	0.6	24.53253020	3.8804e-006	3.9129e-006
0.7	0.7	29.96410005	2.8540e-006	2.8895e-006
0.8	0.8	36.59823444	1.6804e-006	1.7220e-006
0.9	0.9	44.70118449	1.0154e-006	6.3346e-007

7. Conclusions

In this work, we employed $L_o - stable$ numerical scheme for the solution of two dimensional diffusion equations with nonlocal boundary conditions on four boundaries. To verify the accuracy of these schemes for parabolic problems with nonlocal boundary conditions, numerical solution, exact solution and the absolute relative errors are computed. In the first experiment we noticed that (0, 3) – Padé leads to higher accuracy but in the second experiment the accuracy level of both schemes is almost the same.

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