Solving Two –Dimensional Diffusion Equations with Nonlocal Boundary Conditions by a Special Class of Padé Approximants

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ABSTRACT

Parabolic partial differential equations with nonlocal boundary conditions arise in modeling of a wide range of important application areas such as chemical diffusion, thermoelasticity, heat conduction process, control theory and medicine science. In this paper, we present the implementation of positivitypreserving Padé numerical schemes to the two-dimensional diffusion equation with nonlocal time dependent boundary condition. We successfully implemented these numerical schemes for both Homogeneous and Inhomogeneous cases. The numerical results show that these Padé approximation based numerical schemes are quite accurate and easily implemented.

1. INTRODUCTION

The two-dimensional parabolic partial differential equations with nonlocal boundary conditions arise in many important applications in sciences [4,5,7,8,12]. In recent years, a number of numerical techniques for solving two-dimensional parabolic partial differential equations with nonlocal boundary conditions have been studied [10, 11, 15].

In this paper, we consider the implementation of positivitypreserving Padé schemes for two dimensional diffusion equations with nonlocal boundary conditions. (0, 2m-1) – Padé schemes are known as positivity-preserving Padé schemes. The name "Positivity-Preserving Padé" was given by Wade et al. [13]. The positivity-preserving Padé schemes are relatively a new research area; they have captured the interest of mathematicians and scientists. In the past few years, much attention has been devoted to the development of positivity-preserving schemes. The concept of positivity has emerged prominently because it has been found to be an important factor in controlling spurious oscillations.

The outline of this paper is as follows: In section 2 we will give a brief review of Padé approximants. In section 3 we will discuss the positivity-preserving Padé schemes. In section 4 we present numerical experiments. Concluding remarks are given in section 5.

2. PADE` APPROXIMANTS

Padé approximants are generalizations to power series approximations. If $P_n(x)$ and $Q_m(x)$ are polynomials of

degree *n* and *m* respectively, then " $\frac{P_n(x)}{Q_m(x)}$ is a Padé

approximation of a function f(x) " means that

$$f(x) = \frac{P_n(x)}{Q_m(x)} + O(x^{n+m+1})$$
(2.1)

As in [34], Padé proposed that one can find the closest approximation to a given series $\sum_{k=0}^{\infty} c_k x^k$ by defining a rational function

$$R_{n,m}(x) = \frac{P_n(x)}{Q_m(x)}$$
(2.2)

where

$$P_n(x) = \sum_{k=0}^n a_k x^k$$
 (2.3)

and

$$Q_m(x) = 1 + \sum_{k=1}^m b_k x^k$$
(2.4)

Let f(z) be analytic in a region of the complex plane containing the origin z = 0. A Padé approximation $R_{n,m}(z)$ to the function f(z) is defined by

$$R_{n,m}(z) = \frac{P_n(z)}{Q_m(z)}$$
(2.5)

where $P_n(x)$ and $Q_m(x)$ are polynomials in z of degree n and m respectively with leading coefficients unity. For each pair of non-negative integers n and m, $P_n(x)$ and $Q_m(x)$ are those polynomials for which the Taylor series expansion of $R_{n,m}(z)$ about the origin agrees with the Taylor series

expansion of f(z) for as many terms as possible. Since the ratio contains essentially (n + m + 1) unknown coefficients, the requirement that

$$Q_m(z)f(z) - P_n(z) = O(|z|^{n+m+1}), |z| \to 0$$
 gives rise to $(n+m+1)$ linear equations for these coefficients.

In the present work, we utilized (n,m) – Padé approximations for e^{-z} following [36, 37]. In [38], the Padé approximant $R_{n,m}(z)$ to the exponential function $f(z) = e^{-z}$ is defined as follows: Let

$$R_{n,m}(z) = \frac{P_n(z)}{Q_m(z)}$$
(2.6)

where

$$P_n(z) = \sum_{j=0}^n \frac{(n+m-j)!n!}{(m+n)!j!(n-j)!} (-z)^n$$
(2.7)

and

$$Q_m(z) = \sum_{j=0}^m \frac{(n+m-j)!m!}{(m+n)!j!(n-j)!} (z)^n$$
(2.8)

satisfying

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

We will call $R_{n,m}(z)$ as (n,m) – Padé scheme of order (n+m).

3. POSITIVITY-PRESERVING PADE' SCHEMES

The positivity-preserving schemes are relatively a new research area; they have captured the interest of mathematicians and scientists. The notion of a positive scheme was introduced as a refinement of L_0 - stability. A positive scheme has a positive symbol on the positive real axis and is monotonically decreasing to 0. In the past few years, much more attention has been devoted to the development of positivity preserving schemes and the concept of positivity has come out prominently because it has been found to be an important factor in controlling spurious oscillations. Wade et al. [13] has discussed many application problems, taken from the literature, reflecting the importance of positivity-preserving schemes and concluded the increasing interest of researchers in the development and application of positivity-preserving related work. Wade et al. [13, 14] and Siddique [25] have used the positivity preserving Padé schemes to construct smoothing schemes for parabolic partial differential equations

Definition 3.1: A numerical scheme is called positivity preserving if the graph of its stability function stays above x-axis and converges to zero monotonically. The (0, 2m-1) – Padé schemes are positivity-preserving schemes where m = 0, 1, 2, ... (0,1) – Padé, (0,3) – Padé, (0,5) – Padé, etc are all positivity-preserving Padé` schemes. The graphs of amplification symbols of (0,1) – Padé, (0,3) – Padé, (0,3) – Padé, (0,5) – Padé, (0,5) – Padé are shown in Figure 1.



Figure 1. Positivity preserving Padé`

(1,1) – Padé, (1,2) – Padé and (2,2) – Padé are nonpositivitypreserving Padé. The graphs of amplification symbols of

(1,1) – Padé, (1,2) – Padé and (2,2) – Padé are shown in Figure 2.



Figure 2. Non-positivity preserving Padé

The (n,m) – Padé approximation of e^{-kA} is approximated by $e^{-kA} \approx \{Q_m(kA)\}^{-1} P_n(-kA) \equiv R_{n,m}(kA),$ (3.1)

where k is the time step.

Approximating the matrix exponential e^{-kA} by (0,1) – Padé, denoted by $R_{0,1}(kA)$ to give

$$v_{n+1} = (I + kA)^{-1}v_n$$
(3.2)
which is the backward Euler's method.

(0,3) – Padé approximation to the matrix exponential e^{-kA} is

given by
$$v_{n+1} = \left(I + kA + \frac{1}{2}k^2A^2 + \frac{1}{6}k^3A^3\right)^{-1}v_n$$
 (3.3)

(0,5) – Padé approximation to the matrix exponential

 e^{-kA} is given by $v_{n+1} = \left(I + kA + \frac{1}{2}k^2A^2 + \frac{1}{6}k^3A^3 + \frac{1}{24}k^4A^4 + \frac{1}{120}k^5A^5\right)^{-1}v_n$ (3.4) 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-enditioning of the matrix *A* comes into picture.

Definition 3.2: The condition number of a matrix A denoted by cond(A) and is defined by

$$cond(A) = ||A|| ||A^{-1}||.$$
 (3.5)

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 to rewrite a rational function in simple terms. Gallopoulos and Saad [28] used (m, m) – Padé (diagonal Padé) and constructed parallel algorithms using the factorizations. Khaliq et al. [30] discussed diagonal and subdiagonal Padé approximations in factored and partial fraction forms. They have used the partial fraction forms of diagonal and subdiagonal Padé approximations to construct following efficient parallel algorithm.

Algorithm: (Homogeneous Case)

Step 1. For $i = 1, 2, ..., q_1 + q_2$, solve $(kA - c_iI) = v_i = v_s$ in parallel.

Step 2. Compute

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

We have used this algorithm for the implementation of our Padé schemes. Maple is used to compute the poles and weights of Padé approximants. The poles and weights for (0,3) – Padé are as follows:

$$c_1 = -1.5960716379833, w_1 = 1.475686517795720,$$

 $c_2 = -0.7019641810083 - 1.807339494452i$
 $w_2 = -0.7378432588979 + 0.365017840801i$

For (0,3) – Padé, we have $q_1 = q_2 = 1$ and the algorithm solve

 $(kA - c_1I)y_1 = v_s$ and $(kA - c_2I)y_2 = v_s$ and compute

 $v_{s+1} = w_1 y_1 + 2 \operatorname{Re}(w_2 y_2)$ for $s = 0, 1, 2, \dots$

Algorithm: (Inhomogeneous Case)

Step 1. For $i = 1, 2, ..., q_1 + q_2$, solve

$$(kA - c_i I)y_i = w_i v_s + \sum_{j=1}^m k w_{ij} f(t_s + \tau_j k)$$
 for y_i .

Step 2. Compute

 $v_{s+1} = \sum_{i=1}^{q_1} y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \operatorname{Re} y_i$

We have used this algorithm for the implementation of our Pade` schemes. Poles and weights of Padé approximants are computed by using Maple. For (0,3) – Padé, we have

 $q_1 = q_2 = 1$. The poles and weights for (0,3) – Padé are as follows:

 $c_1 = -1.5960716379833, w_1 = 1.475686517795720,$

 $c_2 = -0.7019641810083 - 1.807339494452i$

 $w_2 = -0.7378432588979 + 0.365017840801i$

 $w_{11} = 0.25964745169791, w_{21} = 0.66492666056455,$

 $w_{12} = -0.3128364277412 + 0.472314917248i$

 $w_{22} = 0.3505493716099 - 0.049419054571i$

and the algorithm looks like

$$v_{s+1} = y_1 + 2 \operatorname{Re} y_2$$
 for $s = 0, 1, 2, \dots$

where

 $(kA - c_1I)y_1 = w_1v_s + kw_{11}f(t_s + \tau_1k) + kw_{12}f(t_s + \tau_2k)$ and

 $(kA - c_2I)y_2 = w_2v_s + kw_{21}f(t_s + \tau_1k) + kw_{22}f(t_s + \tau_2k)$ For the numerical experiments, we have implemented first and third order positivity-preserving schemes.

4. NUMERICAL EXPERIMENTS

In this section we present the performance of positivity preserving Padé schemes by implementing these schemes to solve three problems from literature. Twizell et al. [15], Ishak [16] and many others considered these problems as test problems. We have considered both homogeneous and inhomogeneous problems. All positivity-preserving Padé schemes are implemented by using partial fraction decomposition techniques described earlier. We present graphs of the exact and numerical solutions for different parameter values.

Problem 1 (Twizell et al. [15] and Ishak [16])

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

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

in which u = u(x, y, t), with Dirichlet time-dependent boundary conditions on the boundary $\partial \Omega$ of the square Ω defined by the lines x = 0, y = 0, x = 1, y = 1, given by

$$u(0, y, t) = e^{(y+2t)}, \quad 0 \le t \le T, \quad 0 \le y \le 1,$$

$$u(1, y, t) = e^{(1+y+2t)}, \quad 0 \le t \le T, \quad 0 \le y \le 1,$$

$$u(x, 0, t) = e^{(x+2t)}, \quad 0 \le t \le T, \quad 0 \le x \le 1,$$

$$u(x, 1, t) = e^{(1+x+2t)}, \quad 0 \le t \le T, \quad 0 \le x \le 1,$$

and nonlocal boundary condition

11

$$\int_{0}^{1} \int_{0}^{1} u(x, y, t) dx dy = (e - 1)^{2} e^{2t}$$

with initial conditions $u(x, y, 0) = e^{(x+y)}$. Theoretical solution is given by $u(x, y, t) = e^{(x+y+2t)}$.

Table 1. Exact and Num. Sol. for (0, 1) – Padé

х	у	Num. Sol	Ext. Sol.	Errors
0.0	0.0	7.38905610	7.38905610	0.0000e+000
0.1	0.1	9.04041689	9.02501350	1.7038e-003
0.2	0.2	11.06951484	11.02317638	4.1861e-003
0.3	0.3	13.54531347	13.46373804	6.0224e-003
0.4	0.4	16.55780082	16.44464677	6.8339e-003
0.5	0.5	20.21997846	20.08553692	6.6489e-003
0.6	0.6	24.67258833	24.53253020	5.6767e-003
0.7	0.7	30.09034598	29.96410005	4.1956e-003
0.8	0.8	36.69004490	36.59823444	2.5023e-003
0.9	0.9	44.74237856	44.70118449	9.2069e-004
1.0	1.0	54.59815003	54.59815003	0.0000e+000



Figure 3. Graph of (0, 1) – Padé

Table 1 and Figure 3 show the numerical and exact solution for Padé (0, 1), whereas the corresponding Padé (0, 3) results are shown in Table 2 and Figure 4.

Table 2. Exact and Num. Sol. for (0, 3) – Padé

х	у	Num. Sol	Ext. Sol.	Errors
0.0	0.0	7.38905610	7.38905610	0.0000e+000
0.1	0.1	9.02278044	9.02501350	2.4749e-004
0.2	0.2	11.02453679	11.02317638	1.2340e-004
0.3	0.3	13.46680327	13.46373804	2.2761e-004
0.4	0.4	16.44870004	16.44464677	2.4642e-004
0.5	0.5	20.09092511	20.08553692	2.6819e-004
0.6	0.6	24.53979277	24.53253020	2.9595e-004
0.7	0.7	29.97228128	29.96410005	2.7296e-004
0.8	0.8	36.60187800	36.59823444	9.9545e-005
0.9	0.9	44.68687430	44.70118449	3.2023e-004
1.0	1.0	54.59815003	54.59815003	0.0000e+000



Figure 4. Graph of (0, 3) – Padé

Problem 2. (Ishak [16]) Consider the two-dimensional diffusion problem

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

subject to the initial condition

$$u(x, y, 0) = (1 - y)e^x$$
, $0 \le x \le 1$, $0 \le y \le 1$

and the boundary conditions

$u(0, y, t) = (1 - y)e^t,$	$0 \le t \le 1$,	$0 \le y \le 1$
$u(1, y, t) = (1 - y)e^{1+t},$	$0 \le t \le 1$,	$0 \le y \le 1$,
$u(x,0,t) = e^{x+t},$	$0 \le t \le 1$,	$0 \le x \le 1,$
u(x,1,t)=0,	$0 \le t \le 1$,	$0 \le x \le 1,$

and nonlocal boundary condition

$$\int_0^1 \int_0^{x(1-x)} u(x, y, t) dx dy = 2(11-4e)e^t, \quad 0 \le x \le 1, 0 \le y \le 1.$$

The exact solution is given by $u(x, y, t) = (1 - y)e^{x+t}$

Table 3. Exact and Num. Sol. for (0, 1) – Padé

Х	у	Num. Sol	Ext. Sol.	Errors
0.0	0.0	2.71828183	2.71828183	0.0000e+000
0.1	0.1	2.63778350	2.70374942	2.4274e-002
0.2	0.2	2.59254212	2.65609354	2.2808e-002
0.3	0.3	2.50819548	2.56850767	2.1110e-002
0.4	0.4	2.37679262	2.43311998	1.9229e-002
0.5	0.5	2.18935112	2.24084454	1.7144e-002
0.6	0.6	1.93566543	1.98121297	1.4790e-002
0.7	0.7	1.60411458	1.64218422	1.2057e-002
0.8	0.8	1.18144246	1.20992949	8.7990e-003
0.9	0.9	0.65250663	0.66858944	4.8449e-003
1.0	1.0	0.00000000	0.0000e+000	0.0000e+000

Table4. Exact and Num. Sol. for (0, 3) – Padé

х	у	Num. Sol	Ext. Sol.	Errors
0.0	0.0	2.71828183	2.71828183	0.0000e+000
0.1	0.1	2.70355558	2.70374942	1.9384e-004
0.2	0.2	2.65617813	2.65609354	8.4596e-005
0.3	0.3	2.56868615	2.56850767	1.7849e-004
0.4	0.4	2.43330126	2.43311998	1.8128e-004
0.5	0.5	2.24100360	2.24084454	1.5906e-004
0.6	0.6	1.98134861	1.98121297	1.3564e-004
0.7	0.7	1.64228952	1.64218422	1.0530e-004
0.8	0.8	1.20998105	1.20992949	5.1554e-005
0.9	0.9	0.66857060	0.66858944	1.8847e-005
1.0	1.0	0.00000000	0.0000e+000	0.0000e+000

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Figure 5. Graph of (0, 1) – Padé



Figure 6. Graph of (0, 3) – Padé

Problem 3. Consider the two-dimensional nonhomogeneous diffusion problem

$$\frac{\partial u}{\partial t} = \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - e^{-t} (x^2 + y^2 + 4) \right); 0 < x, y < 1, t > 0$$

The problem has nonsmooth data with the initial condition $u(0, x, y) = 1 + x^2 + y^2$ and the

boundary conditions

$$u(0, y, t) = 1 + y^2 e^{-t}, \quad 0 \le t \le 1, \quad 0 \le y \le 1,$$

$$u(1, y, t) = 1 + (1 + y^2)e^{-t}, \quad 0 \le t \le 1, \quad 0 \le y \le 1,$$

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

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

and nonlocal boundary condition

$$\int_{0}^{11} \int_{0}^{1} u(x, y, t) dx dy = 1 + \frac{2}{3} e^{-t}, \quad 0 \le x \le 1, 0 \le y \le 1$$

The exact solution is $u(t, x, y) = 1 + e^{-t}(x^2 + y^2)$. Table 3 and Figure 5 shows the numerical and exact solutions using Padé (0, 1), and the corresponding Padé (0, 3) results are shown in Table 4 and Figure 6.

Table 5. Exact and Num. Sol. using (0, 1) – Padé

х	у	Num. Sol	Ext. Sol.	Errors
0.0	0.0	1.00000000	1.00000000	0.0000e+000
0.1	0.1	1.00738402	1.00735759	2.6235e-005
0.2	0.2	1.02953533	1.02943036	1.0196e-004
0.3	0.3	1.06645182	1.06621830	2.1897e-004
0.4	0.4	1.11813036	1.11772142	3.6573e-004
0.5	0.5	1.18456735	1.18393972	5.2983e-004
0.6	0.6	1.26575934	1.26487320	7.0009e-004
0.7	0.7	1.36170370	1.36052185	8.6792e-004
0.8	0.8	1.47239930	1.47088568	1.0280e-003
0.9	0.9	1.59784805	1.59596469	1.1787e-003
1.0	1.0	1.73575888	1.73575888	0.0000e+000



Figure 7. Graph of (0, 1) – Padé

Table 6. Exact and Num. Sol. for diffusion problem using(0, 3) - Padé

х	у	Num. Sol	Ext. Sol.	Errors
0.0	0.0	1.00000000	1.00000000	0.0000e+000
0.1	0.1	1.00735759	1.00735759	1.7413e-009
0.2	0.2	1.02943035	1.02943036	4.6097e-009
0.3	0.3	1.06621829	1.06621830	1.0956e-008
0.4	0.4	1.11772141	1.11772142	1.2258e-008
0.5	0.5	1.18393971	1.18393972	1.1614e-008
0.6	0.6	1.26487319	1.26487320	8.7720e-009
0.7	0.7	1.36052188	1.36052185	1.9439e-008
0.8	0.8	1.47088594	1.47088568	1.7066e-007
0.9	0.9	1.59596524	1.59596469	3.4276e-007
1.0	1.0	1.73575888	1.73575888	0.0000e+000



Figure 8. Graph of (0, 3) – Padé

5. CONCLUSIONS

In this work, we presented the positivity-preserving Padé numerical schemes and implementation of these schemes on two dimensional diffusion equations with nonlocal boundary conditions on four boundaries. We considered two test problems taken from the literature. To verify the accuracy of these schemes, the absolute relative errors between the exact and numerical solutions are computed. Numerical results show that these schemes are efficient and provide very accurate results.

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