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Fourth Order Positively Smoothed Padé Schemes for Parabolic Partial Differential Equations with Nonlocal Boundary Conditions

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Abstract

Parabolic partial differential equation with nonlocal boundary conditions arise in modeling of various physical phenomena in areas such as chemical diffusion, thermoelasticity, heat conduction process, control theory and medicine science. This paper deals with the successful implementation of the positively smoothed Pade` schemes (PSP) to two-dimensional parabolic partial differential equations with nonlocal boundary conditions. We considered both Homogeneous and Inhomogeneous cases. The numerical results show that these numerical schemes are quite accurate.

Keywords: Fourth order positively smoothed Pade schemes, parabolic partial differential equations, nonlocal boundary conditions

1. Introduction

Parabolic partial differential equations (PDEs) with nonlocal boundary conditions arise in the mathematical modeling of important applications in sciences [6, 7, 8, 9, 22]. In the past two decades, a number of numerical methods [1, 7, 10, 17, 18, 19, 23] for the numerical solution of parabolic PDEs with nonlocal boundary conditions have been developed. Twizell et al. [1] reported that some of these methods (explicit methods) suffer stability restrictions. In this paper we consider the implementation of both homogeneous positively smoothed Padé (PSP(*m*)) and inhomogeneous positively smoothed Padé (IPSP(*m*)) schemes for the numerical solution of two-dimensional parabolic PDEs with nonlocal boundary conditions. The PSP(*m*) and IPSP(*m*), numerical schemes of order 2*m* (where *m* is a positive integer), have recently been developed by Wade et al. [4, 5] and applied to various examples from financial mathematics, especially pricing options with nonsmooth payoffs. This is the first application of the PSP(*m*) and IPSP(*m*) schemes for the numerical solution of parabolic PDEs with nonlocal boundary conditions and are based on a combination of positivity preserving Padé [4] and diagonal Padé approximants. We will give a brief description of Padé approximants in the next section.

2. Padé Approximants

If $P_n(x)$ and $Q_m(x)$ are polynomials of degree n and m respectively, then "$\dfrac{P_n(x)}{Q_m(x)}$ is a Padé approximation to a function $f(x)$" means that

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

In [1], the Padé approximant $R_{n,m}(z)$ to the exponential function $f(z)=e^{-z}$ is defined as follows:
Let

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

where

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

and

$$Q_m(z)=\sum_{j=0}^{m}\frac{(n+m-j)!m!}{(m+n)!j!(n-j)!}(z)^n \tag{2.4}$$

Satisfying $R_{n,m}(z)=e^{-z}+O(|z|^{n+m+1})$ as $|z|\to 0$, (2.5)

We will call $R_{n,m}(z)$ an (n,m) – Padé scheme of order $(n+m)$. When $n=m$, the (m,m) – Padé approximants are known as diagonal Padé approximants and are denoted by $R_{m,m}(z)$.

The positivity preserving Padé schemes are a relatively 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 and the concept of positivity has emerged prominently because it has been found to be an important factor in controlling spurious oscillations. The concept of using positivity-preserving Padé schemes has been discussed in a number of papers [3, 14, 15, 20, 21].

Definition: A numerical scheme is called a *positivity preserving scheme* if the graph of its stability function stays above the *x*-axis and approaches zero monotonically.
The $(0,2m-1)$ – Padé are positivity-preserving schemes. For $m=1,2,3,\ldots$, we have $(0,1)$ – Padé, $(0,3)$ – Padé, $(0,5)$ – Padé, … as positivity-preserving schemes.

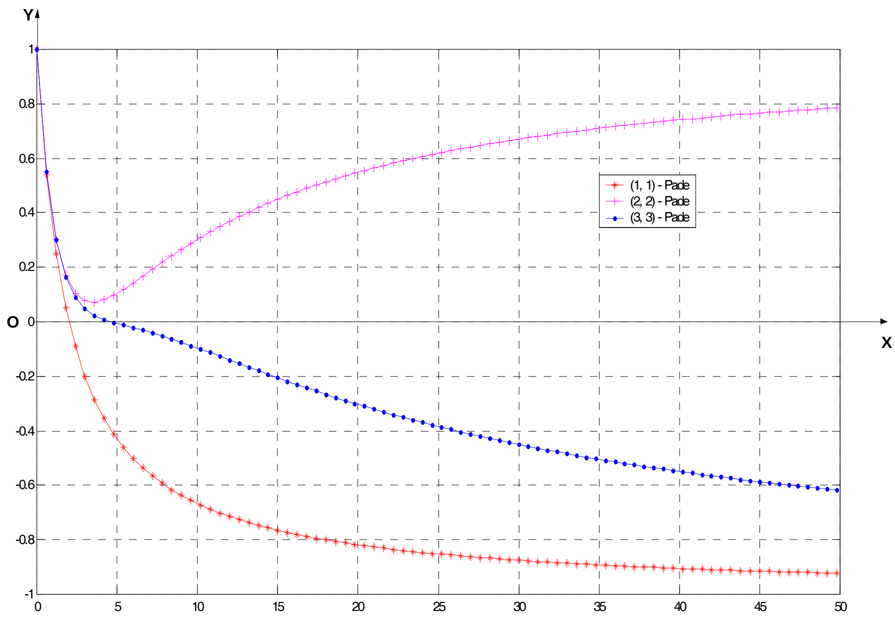

Figure 1. Amplification symbols of the first three diagonal Padé approximants of exp(-z).

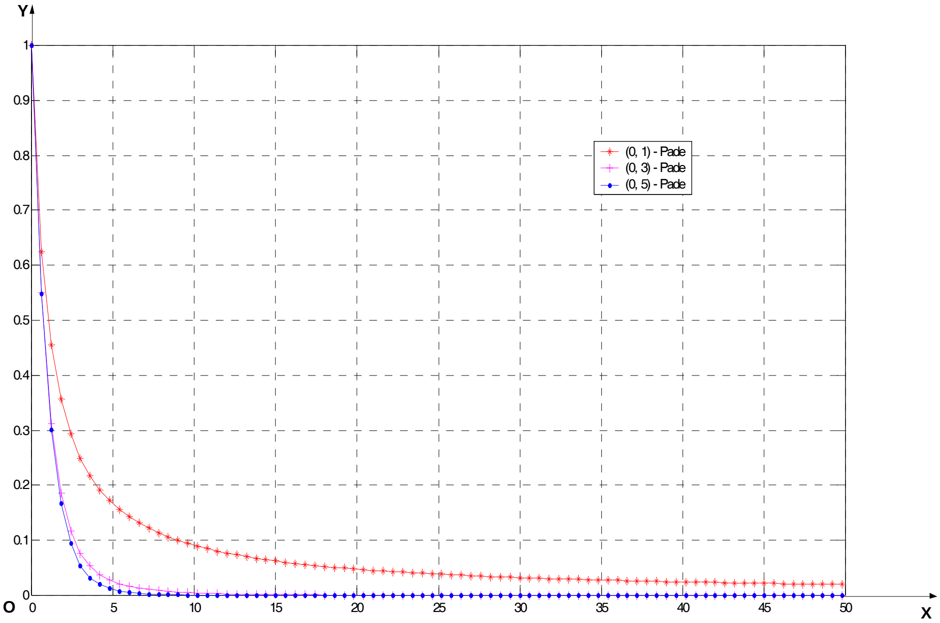

Figure 2. Amplification symbols of three positivity-preserving Padé i. e. (0, 1) – Padé, (0, 3) – Padé and (0, 5) – Padé.

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

$$e^{-kA} \approx \{Q_m(kA)\}^{-1} P_n(-kA) \equiv R_{n,m}(kA) \tag{2.6}$$

where k is the time step and A is a tridiagonal matrix.

The approximation of the matrix exponential e^{-kA} by the $(2,2)-$Padé, denoted by $R_{2,2}(kA)$ yields the method

$$v_{n+1} = \left(I + \tfrac{1}{2}kA + \tfrac{1}{2}k^2A^2\right)^{-1}\left(I - \tfrac{1}{2}kA + \tfrac{1}{2}k^2A^2\right)v_n \tag{2.7}$$

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

$$v_{n+1} = \left(I + kA + \tfrac{1}{2}k^2A^2 + \tfrac{1}{6}k^3A^3\right)^{-1} v_n \tag{2.8}$$

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-conditioning of the matrix A comes into picture. The condition number of a matrix A denoted by $cond(A)$ and is defined by

$$cond(A) = \|A\| \|A^{-1}\|. \tag{2.9}$$

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.

Techniques that employ partial fraction decomposition of rational functions handle this difficulty very effectively. Gallopoulos and Saad [11] have used (m, m) – Padé (diagonal Padé) and constructed parallel algorithms using the factorizations. Khaliq et al. [2] has used the 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 algorithm.

Algorithm for homogeneous case:

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

Step 2. Compute ($m < n$)

$$v_{n+1} = \sum_{i=1}^{q_1} w_i y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \mathrm{Re}(w_i y_i) \tag{2.10}$$

Step 3. Compute ($m = n$)

$$v_{n+1} = (-1)^m v_s + \sum_{i=1}^{q_1} w_i y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \mathrm{Re}(w_i y_i) \tag{2.11}$$

Algorithm for inhomogeneous case:

Step 1. For $i = 1, 2, \ldots, q_1 + q_2$, solve $(kA - c_i I) y_i = w_i v_s + \sum_{j=1}^{m^*} k w_{i\,j} f(t_s + \tau_j k)$ for y_i.

Step 2. Compute ($m < n$)

$$v_{n+1} = \sum_{i=1}^{q_1} y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \mathrm{Re}(y_i) \tag{2.12}$$

Step 2. Compute ($m = n$)

$$v_{n+1} = (-1)^m v_s + \sum_{i=1}^{q_1} y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \mathrm{Re}(y_i) \tag{2.13}$$

Using partial fraction decomposition technique, we can write $R_{0,3}(kA)$ and $R_{2,2}(kA)$ respectively as

$$v_{n+1} = [w_1(kA - c_1 I)^{-1} + 2\,\mathrm{Re}\, w_2\left(kA - c_2 I\right)^{-1}]v_n \tag{2.14}$$

$$v_{n+1} = [I + 2\,\mathrm{Re}\, w\left(kA - cI\right)^{-1}]v_n \tag{2.15}$$

In the next section, we will give a brief description of PSP (m) and IPSP (m) numerical schemes.

3. Positively Smoothed Pade Schemes

The PSP(m) and IPSP(m) numerical schemes are designed by Wade et al. [4, 5] to take advantage of the positivity-preserving Padé schemes. These numerical schemes use two steps of positivity-preserving Padé followed by the diagonal Padé schemes. For example for m = 2, we have PSP(2) and IPSP(2) schemes of order 4 which use two steps of the (0, 3) – Padé followed by the (2,2) – Padé schemes. We present PSP(m) scheme followed by the IPSP(m) scheme.

Homogeneous Case: PSP(m)

Wade et al. [4] introduced Positively Smoothed Padé (PSP(m)) schemes for homogeneous parabolic partial differential equations. The PSP(m) numerical schemes are of order 2m. For $0 < k \le k_0$ and nonnegative integer n, let $t_n = nk$ and $\{v_n\}_{n=0}^{\infty}$ be the numerical approximations for $\{u(t_n)\}_{n=0}^{\infty}$ with $v_0 = v$. Let m be a positive integer, and p the number of special starting steps. The family of PSP(m) schemes [4] is as follows:

$$v_{n+1} = \begin{cases} R_{0,\,2m-1}(kA)v_n & 0 \le n < p; \\ R_{m,\,m}\,(kA)v_n & n > p. \end{cases} \tag{3.1}$$

For simplicity of notation, r_s is utilized for the starting scheme $R_{0,\,2m-1}(kA)$ and r_m for the main scheme $R_{m,\,m}$. The particular value of p which works best is not known. But in [4] numerical experiments as well as convergence results show that p is never required to be larger than 2 in the PSP family.

For m = 2, we have PSP(2) numerical scheme as follows:

$$v_{n+1} = \begin{cases} R_{0,\,3}(kA)v_n & 0 \le n \le 2; \\ R_{2,2}\,(kA)v_n & n > 2. \end{cases} \tag{3.2}$$

$$v_{n+1} = \begin{cases} \left[w_1 (kA - c_1 I)^{-1} + 2\,\mathrm{Re}\, w_2 \left(kA - cI\right)^{-1} \right] v_n & 0 \le n \le 2; \\ \left[I + 2\,\mathrm{Re}\, w \left(kA - cI\right)^{-1} \right] v_n & n > 2. \end{cases} \tag{3.3}$$

where

$c_1 = -1.59607163798332152311285414 3997$ (Real Pole)

$c_2 = -0.70196418100833923844359729 2801 - 1.80733949445202185357645984296\,i$

$w_1 = 1.47568651779572071651904657 51319$

$w_2 = -0.73784325889786035825952328 7566 + 0.36501784080102847244443762 9792i$

PSP(2) scheme uses 2 steps of $(0,3)-$Padé scheme followed by $(2,2)-$ Padé scheme. Using this smoothing criteria a second order scheme PSP(2) can be written as:

1. First two time steps of $(0,3)-$ Padé scheme

$$v_1 = \left[w_1 (kA - c_1 I)^{-1} + 2\,\mathrm{Re}\, w_2 \left(kA - cI\right)^{-1} \right] v_0$$

$$v_2 = \left[w_1 (kA - c_1 I)^{-1} + 2\,\mathrm{Re}\, w_2 \left(kA - cI\right)^{-1} \right] v_1$$

2. Remaining time steps of $(2,2)-$ Padé scheme

$$v_{n+1} = \left[I + 2\,\mathrm{Re}\, w \left(kA - cI\right)^{-1} \right] v_n, \qquad n > 2.$$

First two time steps of $(0,3)-$ Padé scheme are sufficient to capture the spurious oscillations of $(2,2)-$ Padé scheme in PSP(2) scheme.

Inhomogeneous Case: IPSP(*m*)

Wade et al. [5] also developed positively smoothed Pade schemes for inhomogeneous parabolic partial differential equations and used the notation **(IPSP).** The family of IPSP (m) schemes is as follows:

$$v_{n+1} = \begin{cases} R_{0,\,2m-1}(kA) v_n + k \sum_{i=1}^{m} P_i(kA)\, f(t_n + \tau_i k) & 0 \le n < p; \\ R_{m,\,m}(kA) v_n + k \sum_{i=1}^{m} P_i(kA)\, f(t_n + \tau_i k) & n > p. \end{cases} \tag{3.4}$$

The formula to obtain P_i in [5] is

$$\sum_{i=1}^{s} \tau_i^l P_i(z) = \frac{l!}{(-z)^{l+1}} \left(r(z) - \sum_{j=0}^{l} \frac{(-z)^j}{j!} \right), \quad l = 0,1,2,\ldots,s-1. \tag{3.5}$$

where $r = R_{0,\,2m-1}$ or $R_{m,\,m}$ respectively.

For m = 2, we have IPSP(2) numerical scheme as follows:

IPSP(2) scheme uses 2 steps of $(0,3)-$Padé scheme followed by $(2,2)-$ Padé scheme. Using this smoothing criteria a second order scheme IPSP(2) can be written as:

1. First two time steps of $(0,3)-$ Padé scheme

$$v_{s+1} = y_1 + 2R(y_2)$$

where

$(kA - c_1 I)\, y_1 = w_1 v_s + k w_{11} f(t_s + \tau_1 k) + k w_{12} f(t_s + \tau_2 k)$ and

$$(kA - c_2 I)\, y_2 = w_2 v_s + k w_{21} f(t_s + \tau_1 k) + k w_{22} f(t_s + \tau_2 k)$$

$$\mathrm{c}_1 = -1.596071637983321523112854143 9$$
$$\mathrm{c}_2 = -0.70196418100833923844359729280 1 - 1.80733949445202185357645984296\mathrm{i}$$
$$\mathrm{w}_1 = 1.4756865177957207165190465751 3$$
$$\mathrm{w}_2 = -0.737843258897860358259523287 57 + 0.36501784080102847244443762979\mathrm{i}$$

$$\mathrm{w}_{11} = 0.25964745169791, \quad \mathrm{w}_{12} = -0.3128364277412 + 0.472314917248\mathrm{i}$$
$$\mathrm{w}_{21} = 0.66492666056455, \quad \mathrm{w}_{22} = \ 0.3505493716099 - 0.494190545719\mathrm{i}$$

$$\tau_1 = \frac{3-\sqrt{3}}{6} \text{ and } \tau_2 = \frac{3+\sqrt{3}}{6}.$$

2. Remaining time steps of $(2,2)-$ Padé scheme

$$v_{s+1} = v_s + 2R(y)$$

where

$$(kA - cI)\, y_1 = w v_s + k w_{11} f(t_s + \tau_1 k) + k w_{12} f(t_s + \tau_2 k)$$

$$c = -3 - 1.732050807568877i, \; w = -6 + 10.39230484541327i$$

$w_{11} = -0.86602540378 + 3.232050807569i,\ w_{12} = 0.86602540378 + 0.23205080757i$

In the next section, we will demonstrate the implementation of PSP(2) and IPSP(2) (both schemes are of order 4) on model problems taken from the literature.

4. Numerical Experiments

We consider two model problems from the literature [1, 13, 16], for which exact solutions are known. We apply PSP (2) and IPSP (2) to these model problems. The errors between the exact and numerical solutions are shown in the tables for each problem. The graphs of numerical and smoothed solutions are also shown.

Problem 1. (Ishak [13])

Consider the two-dimensional diffusion problem

$$\frac{\partial u}{\partial t} = \alpha\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right); \qquad 0 < x, y < 1, \qquad t > 0 \tag{4.1}$$

subject to the initial condition

$$u(x, y, 0) = (1-y)e^x, \quad 0 \le x \le 1,\ 0 \le y \le 1 \tag{4.2}$$

and the boundary conditions

$$\begin{aligned} u(0, y, t) &= (1-y)e^t, && 0 \le t \le 1, \quad 0 \le y \le 1, \\ u(1, y, t) &= (1-y)e^{1+t}, && 0 \le t \le 1, \quad 0 \le y \le 1, \\ u(x, 0, t) &= e^{x+t}, && 0 \le t \le 1, \quad 0 \le x \le 1, \\ u(x, 1, t) &= 0, && 0 \le t \le 1, \quad 0 \le x \le 1, \end{aligned} \tag{4.3}$$

and nonlocal boundary condition

$$\int_0^1 \int_0^{x(1-x)} u(x, y, t)\,dx\,dy = 2(11-4e)e^t, \quad 0 \le x \le 1, 0 \le y \le 1. \tag{4.4}$$

The exact solution is given by

$$u(x, y, t) = (1-y)e^{x+t} \tag{4.5}$$

Table 1. Exact and PSP(2) solutions of two-dimensional Diffusion Problem

x	y	Exact Solution	PSP(2)	Abs. Rel. Error
0.0	0.0	2.71828183	2.71828183	0.0000e+000
0.1	0.1	2.70374942	2.70375192	2.4977e-006
0.2	0.2	2.65609354	2.65609807	4.5307e-006
0.3	0.3	2.56850767	2.56851445	6.7828e-006
0.4	0.4	2.43311998	2.43312813	8.1475e-006
0.5	0.5	2.24084454	2.24085289	8.3525e-006
0.6	0.6	1.98121297	1.98122030	7.3253e-006
0.7	0.7	1.64218422	1.64218962	5.3975e-006
0.8	0.8	1.20992949	1.20993254	3.0498e-006
0.9	0.9	0.66858944	0.66859040	9.5485e-007
1.0	1.0	0.00000000	0.00000000	0.0000e+000

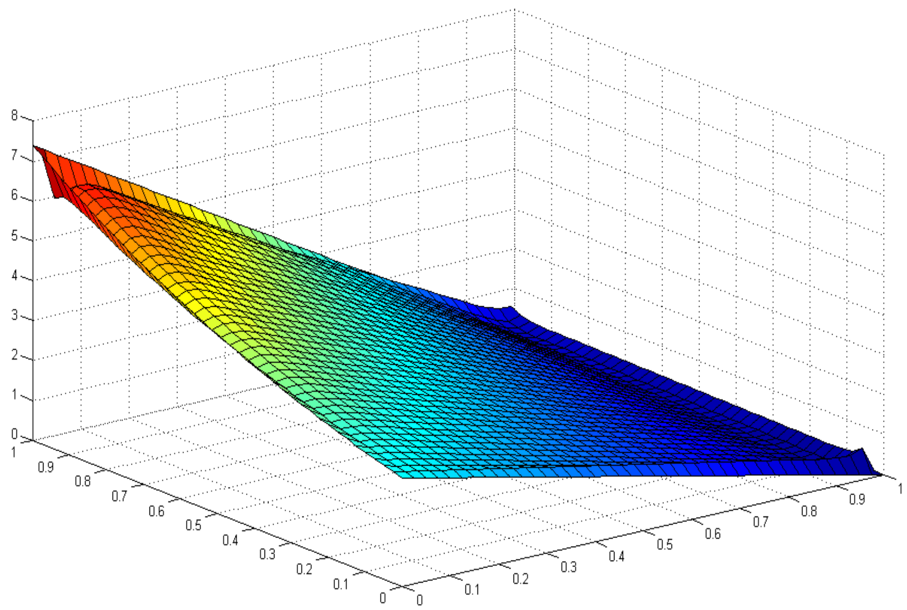

Figure 1. Numerical Solution of (2, 2) – Padé

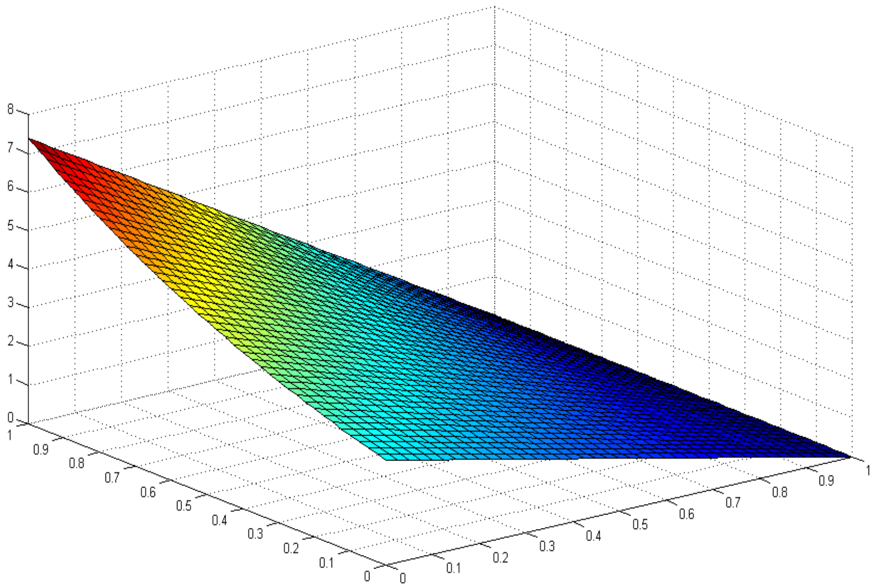

Figure 2. Smoothing of (2, 2) – Padé using PSP(2) smoothing technique

Problem 2

Consider the two-dimensional inhomogeneous diffusion problem

$$\frac{\partial u}{\partial t}=\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}-e^{-t}\left(x^2+y^2+4\right)\right),\quad t>0,\quad 0<x,y<1 \tag{4.6}$$

The problem has nonsmooth data with initial condition

$$u(x,y,0)=1 \tag{4.7}$$

and the boundary conditions

$$\begin{aligned}
&u(0,y,t)=1+y^2e^{-t}, && 0\le t\le 1,\quad 0\le y\le 1,\\
&u(1,y,t)=1+(1+y^2)e^{-t}, && 0\le t\le 1,\quad 0\le y\le 1,\\
&u(x,0,t)=1+x^2e^{-t}, && 0\le t\le 1,\quad 0\le x\le 1,\\
&u(x,1,t)=1+(1+x^2)e^{-t}, && 0\le t\le 1,\quad 0\le x\le 1,
\end{aligned} \tag{4.8}$$

and nonlocal boundary condition

$$\int_0^1\int_0^1 u(x,y,t)dxdy = 1+\frac{2}{3}e^{-t}\ . \qquad (4.9)$$

The exact solution is $u(x,y,t) = 1 + e^{-t}(x^2+y^2)$. (4.10)

Table 2. Exact and IPSP(2) solutions of the Inhomogeneous Diffusion Problem

x	y	Exact Solution	IPSP(2)	Abs. Rel. Error
0.0	0.0	1.000000000000	1.000000000000	0.0000e+000
0.1	0.1	1.007357588823	1.007357544940	4.3563e-008
0.2	0.2	1.029430355294	1.029430344090	1.0884e-008
0.3	0.3	1.066218299411	1.066218275375	2.2543e-008
0.4	0.4	1.117721421175	1.117721395910	2.2604e-008
0.5	0.5	1.183939720586	1.183939704400	1.3671e-008
0.6	0.6	1.264873197643	1.264873162720	2.7610e-008
0.7	0.7	1.360521852348	1.360521824917	2.0162e-008
0.8	0.8	1.470885684699	1.470885931022	1.6747e-007
0.9	0.9	1.595964694698	1.595965248352	3.4691e-007
1.0	1.0	1.735758882343	1.735758882343	0.0000e+000

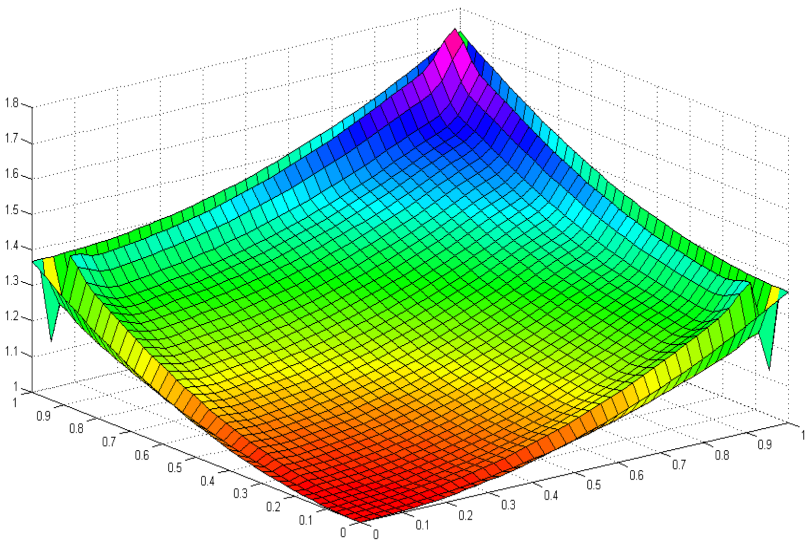

Figure 3. Numerical Solution of (2, 2) – Padé

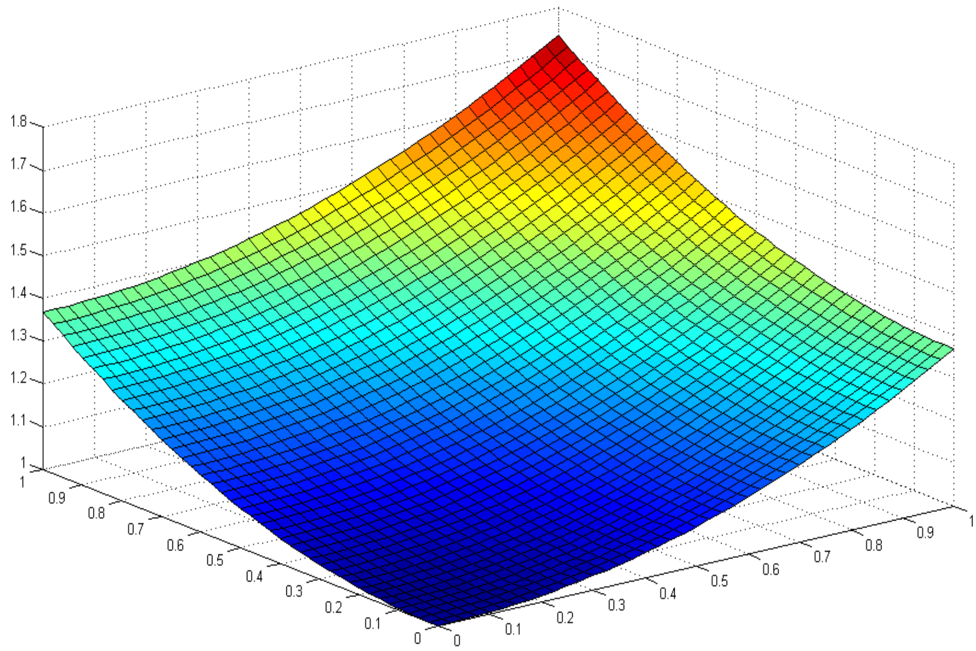

Figure 4. Smoothing of (2, 2) – Padé by PSP(2) smoothing technique

In order to verify numerically whether the PSP (2) scheme leads to higher accuracy, we can evaluate the numerical solution. Tables 1 and 2 show the exact solution, the numerical results of PSP (2) scheme, and the error between the exact and numerical solutions for various values of x and y, when t =1. The graph of Padé – (2, 2) shows spurious oscillations, which are captured by PSP (2) scheme.

5. Conclusions

In this work, we have employed PSP (2) and IPSP (2) numerical schemes of order 4 for the solutions of two dimensional diffusion equations with nonlocal boundary conditions on four boundaries. The problems considered consist of both homogenous and inhomogeneous cases. To verify the accuracy of these schemes for parabolic problems with nonlocal boundary conditions, the errors between the exact and numerical solutions are computed. Numerical results show that the PSP

(2) and IPSP (2) schemes are efficient and provide very accurate results. We have demonstrated with time evolution graphs computational performance for the two model problems. These numerical schemes have promise due to their efficient implementation in solving higher degree of polynomial matrices that arise with Padé schemes as well as the potential to implement in parallel.

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