Numerical Computation of Two-dimensional Diffusion Equation with Nonlocal Boundary Conditions

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Abstract— **The diffusion equations with nonlocal boundary conditions arise in the mathematical modeling of many physical phenomena. In this paper, we present Padé schemes for the numerical solution of two-dimensional (both homogeneous and inhomogeneous) diffusion equations subject to nonlocal boundary conditions. These numerical schemes are based on $(1,2)-$ Padé and $(0,3)-$ Padé approximations to the matrix exponentials arising from the method of lines semidiscretization approach. Numerical solutions for two model problems with known theoretical solutions are obtained. The numerical results prove the accuracy of these schemes.**

***Index Terms*— Diffusion Equations, Nonlocal boundary conditions, Padé schemes, Parabolic Problems.**

I. INTRODUCTION

The study of mathematical models for many important applications such as chemical diffusion, heat conduction processes, population dynamics, thermoelasticity, medical science, electrochemistry and control theory give rise the two-dimensional parabolic partial differential equation with nonlocal boundary conditions [1 – 13, 20]. The two-dimensional parabolic partial differential equations with nonlocal boundary conditions and Dirichlet boundary conditions have been studied in many papers [1, 11, 16]. In this paper we will develop two third order new schemes for the numerical solution of two-dimensional diffusion problem with nonlocal boundary conditions. We will use the method of lines semidiscretization approach to transform the model partial differential equation (PDE) into a system of first order, linear, ordinary differential equations (ODEs). The solution of this system of ODEs satisfies a certain recurrence relation involving matrix exponential terms. The approximation of matrix exponential by $(1,2)-$Padé and (0, 3) – Padé yields the new Padé schemes. We will use the partial fraction decomposition techniques for (1,2) – Padé and (0, 3) – Padé approximants [19] to construct the new efficient numerical schemes.

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II. NUMERICAL PRELIMINARIES

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

$$u_t = \Delta u; \qquad 0 < x, y < 1, \qquad t > 0 \tag{2.1}$$

Initial conditions are assumed to be of the form

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

while the Dirichlet time-dependent boundary conditions are

$$\begin{aligned} u(0,y,t) &= \psi_0(y,t), && 0 \le t \le T, \quad 0 \le y \le 1, \\ u(1,y,t) &= \psi_1(y,t), && 0 \le t \le T, \quad 0 \le y \le 1, \\ u(x,0,t) &= \varphi_0(x)\gamma(t), && 0 \le t \le T, \quad 0 \le x \le 1, \\ u(x,1,t) &= \varphi_1(x,t), && 0 \le t \le T, \quad 0 \le x \le 1, \end{aligned} \tag{2.2}$$

with $f, \psi_o, \psi_1, \varphi_o$ and φ_1 known functions.

The function $\gamma(t)$ is to be determined. Nonlocal boundary condition is

$$\int_0^1\int_0^1 u(x,y,t)dxdy = \alpha(t), \qquad (x,y) \in \Omega \cup \partial\Omega, \tag{2.3}$$

where α is known function.

We divide both intervals $0 \le x \le L$ and $0 \le y \le L$ into $N+1$ equal subintervals with space mesh $h = \dfrac{L}{N+1}$, $x_i = ih$, $y_j = jh$ and the time t is discretized in steps of length k. At each time step $t = t_n = nk, n = 0,1,2,\ldots$ and we will have a square mesh with N^2 points within the square and $N+2$ equally spaced points on each side of the boundary. To approximate the solution $u(x,y,t)$ of (4.1) at each point (x_i, y_j, t_l) where $i, j = 1,2,\ldots,N$ and $l = 0,1,2,\ldots$. Replacing the spatial derivatives in (4.1) by their second order central difference approximation leads to a system of N^2 first order, linear, ordinary differential equations of the form

$$\frac{dv}{dt} = Av + \beta(t), \qquad t > 0, \quad v(x,y,0) = f(x,y) \tag{2.4}$$

where A is a matrix f order N^2 and can be split into block diagonal matrices A_1 and A_2 given by

$$A_1 = [a_{ij}], \quad i = j = 1,2,3,\ldots,N.$$

where

$$a_{ij} = \begin{cases} A_1^* & if\ i = j \\ 0 & if\ i \ne j \end{cases}$$

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

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$A_1^* = [a_{mn}],\quad i = j = 1,2,3,\ldots,N.$

where

$$a_{mn} = \begin{cases} -2 & if\ m = n \\ 1 & if\ m = n-1\ or\ m = n+1 \\ 0 & otherwise \end{cases}$$

and

$$A_2 = \frac{1}{h^2}[a_{lk}],\quad l = k = 1,2,3,\ldots,N.$$

where

$$a_{lk} = \begin{cases} -2I & if\ l = k \\ I & if\ l = k-1\ or\ l = k+1 \end{cases}$$

and I is the identity matrix of order N.

Solving the system (2.4) subject to the initial condition $v(x,y,0) = f(x,y)$ yields [21],

$$v(t) = e^{tA}.f + \int_0^1 e^{(t-s)A}.\beta(s)\,ds,\quad t \geq 0$$

and agrees with

$$v(t+k) = e^{kA}.v(t) + \int_t^{t+k} e^{(t+k-s)A}.\beta(s)\,ds,\ t = 0,k,2k,\ldots \quad (2.5)$$

Approximating the quadrature in (2.5) by the trapezoidal rule yields

$$v(t+k) = e^{kA}.v(t) + \tfrac{k}{2}[\beta(t+k) + e^{kA}\beta(t)],\ t = 0,k,2k,\ldots \quad (2.6)$$

and may takes the form as

$$v_{n+1} = e^{kA}[v_n + \beta(t_n)] + \frac{k}{2}\beta(t_{n+1}) \quad (2.7)$$

III. Numerical Schemes

For $n > m$, the approximation of the matrix exponential e^{-kA} by the (n,m) – Padé, denoted by $R_{n,m}(kA)$ yields L_0 – stable Padé numerical schemes (see for details G. D Smith [18]). The approximation of the matrix exponential e^{-kA} by the $(1,2)$ – Padé, denoted by $R_{1,2}(kA)$ yields a third order numerical scheme

$$v_{n+1} = \left(I - \tfrac{1}{3}kA\right)\left(I + \tfrac{2}{3}kA + \tfrac{1}{6}k^2A^2\right)^{-1}[v_n + \beta(t_n)] + \frac{k}{2}\beta(t_{n+1}). \quad (3.1)$$

The approximation of the matrix exponential e^{-kA} by the $(0,3)$ – Padé`, denoted by $R_{0,3}(kA)$ yields the third order scheme

$$v_{n+1} = \left(I + kA + \tfrac{1}{2}k^2A^2 + \tfrac{1}{6}k^3A^3\right)^{-1}\left(v_n + \beta_n\right) + \frac{k}{2}\beta_{n+1} \quad (3.2)$$

The both schemes involve higher powers of the tridiagonal matrix A bring illconditioning into picture, which may cause computational difficulties and make the scheme computationally less efficient.

To avoid illconditioning, we will use the partial fraction decomposition techniques introduced by Khaliq et al [19] to (3.1) and (3.2), Following Wade et. al. [14], we obtain new numerical schemes for $(1,2)$ – Padé and $(0,3)$ – Padé as follows:

(1,2) – Padé numerical scheme

$$v_{n+1} = 2\,\mathrm{Re}\,w(kA - cI)^{-1}\left(v_n + \beta_n\right) + \frac{k}{2}\beta_{n+1}. \quad (3.3)$$

where $w = -1 + 3.535533905932738\,i$,
$c = -2 - 1.414213562373095\,i$.

(0, 3) – Padé numerical scheme

$$v_{n+1} = \left[w_1(kA - c_1I)^{-1} + 2\,\mathrm{Re}\,w_2(kA - c_2I)^{-1}\right]\left(v_n + \beta(t_n)\right) + \tfrac{k}{2}\beta(t_{n+1}) \quad (3.4)$$

where

$c_1 = -1.596071637983321523112854143997$

$c_2 = -0.70196418100833923844359729280014 - 1.80733949445202185357645984296640\,i$

$w_1 = 1.4756865177957207165190465751319$

$w_2 = -0.7378432588978603582595232875659 + 0.3650178408010284724444376297915\,i$

Extension to Inhomogeneous Problem

By adding a forcing function $f(x,y,t)$ on right hand side of (2.1), we will have inhomogeneous problem. Following [15], the $(1,2)$ – Padé and $(0,3)$ – Padé numerical schemes for inhomogeneous problem are as follows:

(1, 2) – Padé Scheme (Inhomogeneous case)

$$v_{n+1} = 2R(y)\left(v_n + \beta_n\right) + \frac{k}{2}\beta_{n+1} \quad (3.5)$$

where

$$\left(kA - c_1I\right)y = w_1v_n + kw_{11}f(t_n + \tau_1k) + kw_{12}f(t_n + \tau_2k)$$

and

$c_1 = -2.+1.41421356237309504880168872421\,i$

w_1=-1.-3.53553390593273762200422181052 i

w_{11}=-.18301270189221932338186158538 -1.3194792168823420489501653808 i

w_{12}=0.68301270189221932338186158538 -0.094734345490752999851523343427i

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

(0, 3) – Padé Scheme (Inhomogeneous case)

$$v_{n+1} = [y_1 + 2R(y_2)]\left(v_n + \beta_n\right) + \frac{k}{2}\beta_{n+1} \quad (3.6)$$

where

$$\left(kA - c_1I\right)y_1 = w_1v_n + kw_{11}f(t_n + \tau_1k) + kw_{12}f(t_n + \tau_2k)$$

and

$$\left(kA - c_2I\right)y_2 = w_2v_n + kw_{21}f(t_n + \tau_1k) + kw_{22}f(t_n + \tau_2k)$$

$c_1 = -1.596071637983321523112854143997$

$c_2 = -0.70196418100833923844359729280014 - 1.80733949445202185357645984296640\,i$

$w_1 = 1.4756865177957207165190465751319$

$w_2 = -0.73784325889786035825952328756592 + 0.36501784080102847244443762979145\,i$

$w_{11} = 0.25964745169791,\ w_{21} = 0.66492666056455,$
$w_{12} = -0.3128364277412 + 0.472314917248i$
$w_{22} = \ 0.3505493716099 - 0.494190545719i$
$\tau_1 = \frac{3-\sqrt{3}}{6}$ and $\tau_2 = \frac{3+\sqrt{3}}{6}$.

The presence of an integral term in a boundary condition immensely complicates the application of standard numerical techniques. The accuracy of the quadrature must be compatible with the discretization of the differential equation. Cannon et. al. [11] used second order composite trapezoidal rule, whereas Dehghan, M. [2] used fourth order Simpson's third rule for their fourth order scheme. Noye et. al. [22] used Simpson closed rule and Twizell et. al. [16] used trapezoidal rule to approximate the nonlocal boundary condition (2.3). Following Twizell et. al. [16], we have used Trapezoidal rule to handle the nonlocal boundary condition.

IV. Numerical Results

In this section we demonstrate the performance of (1, 2) – Padé and (0, 3) – Padé. Following [3, 10, 15], we took $h = \frac{1}{20}$, $k = \frac{1}{2400}$ such that p was kept constant i.e. $p = \frac{k}{h^2} = \frac{1}{6}$. We consider three test problems taken from the literature. The exact solutions are known for these problems and are used to test the accuracy of these numerical schemes. The absolute relative errors between the exact and numerical solutions are shown in the tables and the graphs of numerical and exact solutions are also shown.

A. *Problem 1.* ***(Twizell et al. [16] , Ishak [17], Siddique [23,24])***

We consider the two-dimensional diffusion equation

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

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

$$\begin{aligned} u(0, y, t) &= e^{(y+2t)}, \quad 0 \le t \le T, \quad 0 \le y \le 1, \\ u(1, y, t) &= e^{(1+y+2t)}, \quad 0 \le t \le T, \quad 0 \le y \le 1, \\ u(x, 0, t) &= e^{(x+2t)}, \quad 0 \le t \le T, \quad 0 \le x \le 1, \\ u(x, 1, t) &= e^{(1+x+2t)}, \quad 0 \le t \le T, \quad 0 \le x \le 1, \end{aligned} \qquad (4.2)$$

and nonlocal boundary condition

$$\int_0^1\int_0^1 u(x, y, t)\,dxdy = (e-1)^2 e^{2t} \qquad (4.3)$$

with initial conditions $u(x, y, 0) = e^{(x+y)}$. (4.4)

Theoretical solution is give by $u(x, y, t) = e^{(x+y+2t)}$. (4.5)

Here the PDE (4.1) subject to (4.2), (4.3) and (4.4) is solved numerically using (1, 2)–Padé and (0, 3)–Padé and schemes. The numerical results for (1, 2)–Padé and (0, 3)–Padé schemes are computed. Following [11, 16, 22], the discretization parameters h and k are given the values $h = \frac{1}{20}$, $k = \frac{1}{2400}$. The absolute relative errors for the problems are tabulated in Table 1 which shows that these schemes gave accurate results. The numerical solutions of (1, 2)–Padé, (0, 3)–Padé and theoretical solution are graphically shown in Figure 1, Figure 2 and Figure 3 respectively.

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

x	y	Exact Sol.	(1, 2) – Padé	(0, 3) – Padé
0.1	0.1	9.02501350	7.2911e-006	7.2921e-006
0.2	0.2	11.02317638	1.7967e-005	1.7967e-005
0.3	0.3	13.46373804	2.5890e-005	2.5890e-005
0.4	0.4	16.44464677	2.9399e-005	2.9399e-005
0.5	0.5	20.08553692	2.8601e-005	2.8601e-005
0.6	0.6	24.53253020	2.4402e-005	2.4402e-005
0.7	0.7	29.96410005	1.8015e-005	1.8015e-005
0.8	0.8	36.59823444	1.0727e-005	1.0727e-005
0.9	0.9	44.70118449	3.9316e-006	3.9328e-006

Twizell et. al. [16] have introduced a parallel algorithm based on (1, 2) – Padé approximation to the matrix exponential. The parallel algorithm is implemented on problem 1 for $h = \frac{1}{20}, k = \frac{1}{2400}$. The following table is presented in [16].

Table 2. Comparing Absolute Relative Error $h = \frac{1}{20}, k = \frac{1}{2400}$

x	y	Exact Sol.	(1, 2) – Padé Parallel Alg	(1.5) FTCS
0.1	0.1	9.02501350	3.3993 e-004	3.4000e-003
0.2	0.2	11.02317638	3.2676 e-004	2.2000e-004
0.3	0.3	13.46373804	2.6002 e-004	4.2000e-004
0.4	0.4	16.44464677	1.8408 e-004	1.5000e-004
0.5	0.5	20.08553692	1.1595 e-004	3.2000e-004
0.6	0.6	24.53253020	6.3782 e-005	4.2000e-004
0.7	0.7	29.96410005	2.9338 e-005	4.4000e-004
0.8	0.8	36.59823444	5.1982 e-006	3.5000e-004
0.9	0.9	44.70118449	3.3960 e-006	1.6000e-004

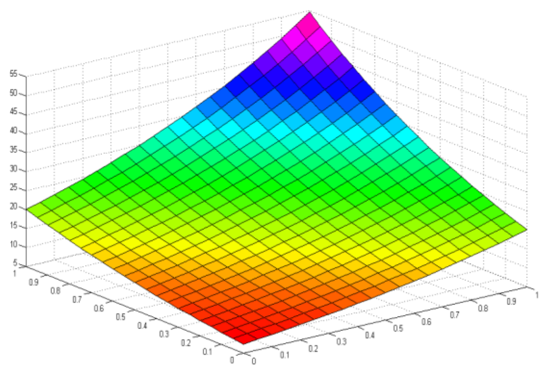

Figure 1. Graph of (0, 3) – Padé numerical scheme

Comparing the numerical results of Table 1 and 2, we see that (1, 2) – Padé and (0, 3) – Padé gave more accurate results to those computed using parallel algorithm based on (1, 2) – Padé [16] and (1, 5) FTCS explicit scheme [22].

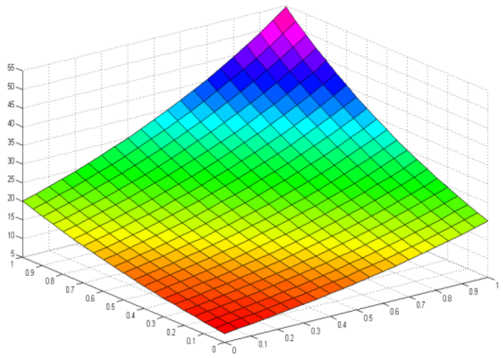

Figure 2. Graph of (1, 2) – Padé numerical scheme

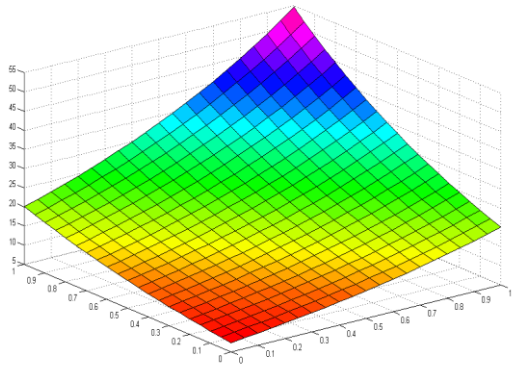

Figure 3. Graph of theoretical solution

B. ***Problem 2***. *(Ishak [17], Siddique [23, 24])*

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

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}; \qquad 0<x,y<1, \qquad t>0 \tag{4.6}$$

subject to the initial condition

$$u(x,y,0)=(1-y)e^{x}, \quad 0\le x\le 1,\ 0\le y\le 1 \tag{4.7}$$

And the boundary conditions

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

Table 3. Comparing Absolute Relative Errors $h=\dfrac{1}{20}, k=\dfrac{1}{2400}$

x	y	Exact Sol.	(1, 2) –Padé	(0, 3) –Padé
0.1	0.1	2.703749421552	2.5200e-006	2.5203e-006
0.2	0.2	2.656093538189	6.5980e-006	6.5980e-006
0.3	0.3	2.568507667333	1.0448e-005	1.0448e-005
0.4	0.4	2.433119980107	1.3310e-005	1.3310e-005
0.5	0.5	2.240844535169	1.4786e-005	1.4786e-005
0.6	0.6	1.981212969758	1.4698e-005	1.4698e-005
0.7	0.7	1.642184217518	1.3035e-005	1.3035e-005
0.8	0.8	1.209929492883	9.9070e-006	9.9070e-006
0.9	0.9	0.668589444228	5.4944e-006	5.4946e-006

and nonlocal boundary condition

$$\int_0^1\int_0^{x(1-x)} u(x,y,t)\,dxdy=2(11-4e)e^{t},\ 0\le x\le 1,\ 0\le y\le 1. \tag{4.9}$$

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

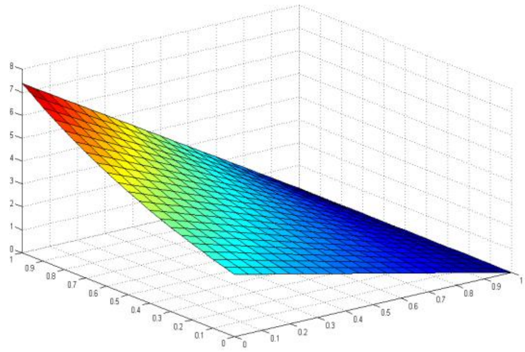

Figure 4. Graph of (0, 3) – Padé numerical scheme

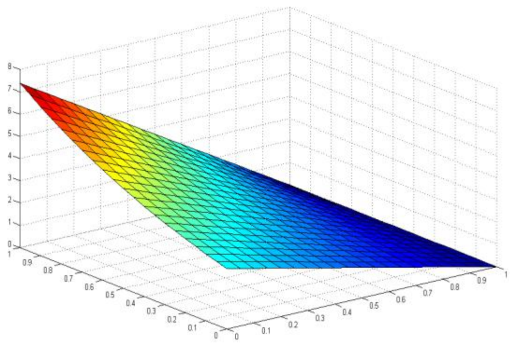

Figure 5. Graph of (1, 2) – Padé numerical scheme

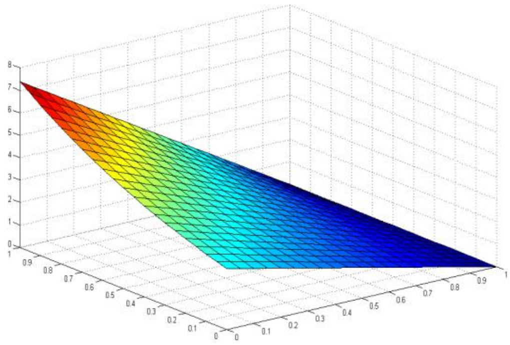

Figure 6. Graph of Theoretical Solution

C. *Problem 3*. ***(Siddique [23, 24]) Consider the two-dimensional nonhomogeneous diffusion problem***

$$\frac{\partial u}{\partial t}=\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}-e^{-t}(x^2+y^2+4)\right],\ t>0,\ \ 0<x,y<1. \quad , \tag{4.11}$$

The problem has nonsmooth data with the initial condition

$$u(0,x,y)=1+x^2+y^2 \tag{4.12}$$

and the boundary conditions

$$\begin{aligned} u(0,y,t)&=1+y^2e^{-t}, && 0\le t\le 1, \quad 0\le y\le 1,\\ u(1,y,t)&=1+(1+y^2)e^{-t}, && 0\le t\le 1, \quad 0\le y\le 1,\\ u(x,0,t)&=1+x^2e^{-t}, && 0\le t\le 1, \quad 0\le x\le 1,\\ u(x,1,t)&=1+(1+x^2)e^{-t}, && 0\le t\le 1, \quad 0\le x\le 1, \end{aligned} \tag{4.13}$$

and nonlocal boundary condition

$$\int_0^1\int_0^1 u(x,y,t)dxdy=1+\tfrac{2}{3}e^{-t}, \quad 0\le x\le 1, 0\le y\le 1 \tag{4.14}$$

The exact solution is $u(t,x,y)=1+e^{-t}(x^2+y^2)$ (4.15)

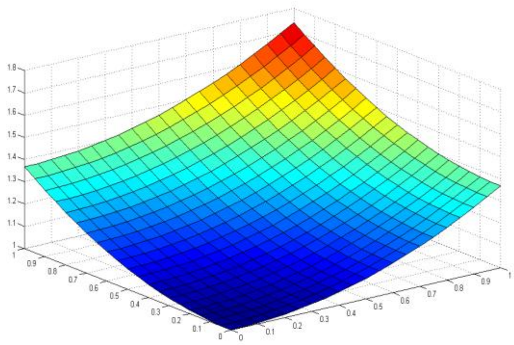

Figure 7.Graph of (0, 3) – Padé numerical scheme

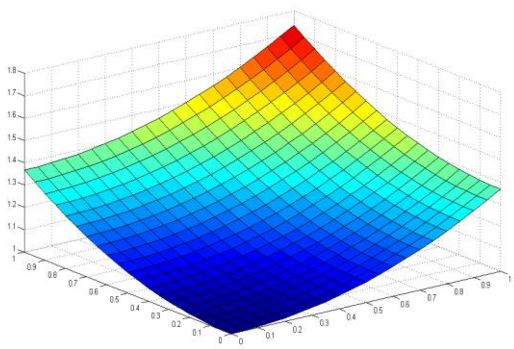

Figure 8. Graph of (1, 2) – Padé numerical scheme

Table 4. Comparing Absolute Relative Errors $h=\dfrac{1}{20}, k=\dfrac{1}{2400}$

x	y	Exact Sol.	(1, 2) – Padé	(0, 3) – Padé
0.1	0.1	1.00735759	1.4024e-012	3.3129e-012
0.2	0.2	1.02943036	1.4766e-012	4.3694e-012
0.3	0.3	1.06621830	1.4533e-012	4.2808e-012
0.4	0.4	1.11772142	1.4024e-012	4.1402e-012
0.5	0.5	1.18393972	1.3285e-012	3.9455e-012
0.6	0.6	1.26487320	1.2357e-012	3.6930e-012
0.7	0.7	1.36052185	1.1249e-012	3.3877e-012
0.8	0.8	1.47088568	9.9720e-013	2.8451e-012
0.9	0.9	1.59596469	1.2458e-011	1.7570e-010

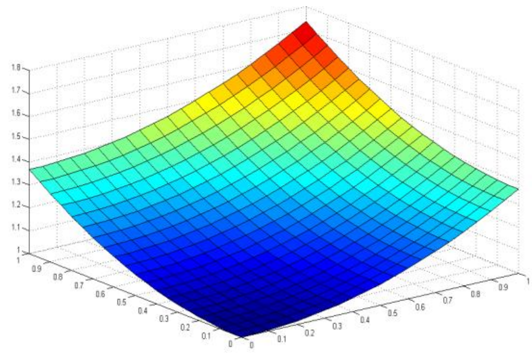

Figure 9. Graph of Theoretical solution

The absolute relative errors for problem 2 and 3 are tabulated in Table 3 and 4, which shows that (1, 2) – Padé and (0, 3) – Padé give superior results for problem 3, which is inhomogeneous diffusion equation with nonlocal boundary conditions.

V. CONCLUSION

In this work, we employed new Padé 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. The numerical results show that these Padé schemes are efficient and provide very accurate results.

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