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A Finite Element Method for Numerical Solution of Parabolic Diffusion-Reaction Equation

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ABSTRACT

This study considers the Finite Element Method (FEM), a well-conversant numerical method, used to evaluate approximate solutions of 2D higher-order non-homogeneous Diffusion-Reaction (DR) equation with more accuracy. In this paper, regular and irregular geometrical shapes are available for the FEM and this method is capable to provide more accurate solutions. Our present research also focuses on the acceptance of the FEM by utilizing absolute error analysis. This work includes two examples and their approximate results are portrayed both graphically and in a tabular form which is sufficient to ensure the validity and efficiency of the FEM.

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1 Introduction

In modern life, different types of problems in form of real-world, scientific, biological, or industrial problems can be represented mathematically with the help of differential equations and this is a great challenge for scientists and researchers to find more efficient solutions to these problems. For the numerical analysis of differential equations, frequently used methods are the Finite Difference Method [1], the Galerkin and Modified Galerkin Methods [2–4], the Shooting Method [5], the Sub-domain Least Square Method [6], and the Decomposition Method [7]. But all these methods are not applicable to obtain the numerical solutions at particular grid points. Moreover, the computational cost to obtain higher accuracy from numerical solutions is unbearable.

The two-dimensional parabolic PDEs with nonlocal boundary conditions and dirichlet boundary conditions have been studied in many papers. The numerical solution of partial differential equations was derived by using Finite Difference Methods in [1]. A Diffusion-Reaction system in human-environment disease modeling was described in [8]. A numerical method for the diffusion equation with non-local boundary specifications was introduced in [9]. The existence and uniqueness of solutions to the two-dimensional equation subject to the mass specification in a conductor region are discussed in [10]. The smoothing of the Crank-Nicolson numerical

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scheme based on Pade‘ approximation to the matrix exponential for two-dimensional parabolic PDEs with non-local boundary conditions was discussed in [11]. In [12], the Finite Element Method for time fractional partial differential equations was discussed and the existence and uniqueness of the solutions were proved by using the Lax-Milgram Lemma. A comparative study between the Finite Element Method and the Second-Order Central Difference Method (SCDM) for two-dimensional Elliptic Partial Differential Equations was introduced in [13].

In [14], Galerkin Finite Element Method (GFEM) was operated to decipher the nonlinear parabolic PDEs having robin boundary condition. The authors also ensured the stability of the numerical scheme and included a correlative study between analytic and numerical results to proclaim the efficiency and reliability of GFEM. In [15–17], a numerical technique was derived from GFEM for finding the most accurate numerical solution of Diffusion-Reaction equations: Burger's equation, Fisher's equation, Newell-Whitehead-Segel equation, and Burgers-Huxley equation. Due to several applications of the fractional-order Bagley-Torvik equation in our present life, a new numerical scheme was proposed in [18] and it has been proved that its accuracy is more sustainable. Using the numerical scheme, GFEM, the famous FitzHugh-Nagumo equation was solved and another renowned Newell-Whitehead equation was solved to verify the constancy of the algorithm in [19]. The formulation and solution procedure of the FEM was demonstrated in [20–22] to find numerical solutions of Convection-Diffusion-Reaction (CDR) equations as well as parabolic PDEs. In [1, 21], FitzHugh-Nagumo equation and Fisher's equation with stable and unstable geometrical shapes were considered and evaluated numerical solutions to make a comparison with the exact solution. However, the paper [22] disclosed the convergence and stability analysis for nonlinear parabolic PDEs.

It is very rare to use FEM to solve the Diffusion-Reaction (DR) equation, although it gives the most accurate results which almost correspond with the theoretical results. That's why in this paper, we are interested in the 2D general DR model with dirichlet boundary conditions in the following form:

$$\begin{cases} \mu(x,y)\dfrac{\partial U}{\partial t} = \alpha_1\dfrac{\partial^2 U}{\partial x^2} + \alpha_2\dfrac{\partial^2 U}{\partial y^2} + f(U(t,x,y)); \\ t\in(0,T],\ (x,y)\in\Omega\equiv[a,b]\times[c,d] \\ U(0,x,y)=U_0(x,y),\ (x,y)\in\Omega\equiv[a,b]\times[c,d] \\ U(t,a,y)=U_a(t,y),\ U(t,b,y)=U_b(t,y),\ t>0,\ y\in\partial\Omega \\ U(t,x,c)=U_c(t,x),\ U(t,x,d)=U_d(t,x),\ t>0,\ x\in\partial\Omega. \end{cases} \tag{1.1}$$

In the above two dimensional system (1.1), $U(t,x,y)$ represents heat, diffusion and so on, $\alpha_1\frac{\partial^2 U}{\partial x^2} + \alpha_2\frac{\partial^2 U}{\partial y^2}$ stands for the diffusion term where α_1 and α_2 are the diffusion coefficients, and $f(U(t,x,y))$ represents the reaction term. Here, $U_a(t,y)$, $U_b(t,y)$ are the functions of spatial variable, y and time, t, and $U_c(t,x)$, $U_d(t,x)$ are the functions of spatial variable, x and time, t. The initial condition, $U_0(x,y)$ represents the function of spatial variables, x and y. Over the spatial variables x and y, the initial and terminal boundary points are a,b and c,d respectively. Moreover, the reaction function $f(U(t,x,y))$ is sufficiently smooth. In order to make our work easier throughout the paper, let introduce the notation $\mathcal{D}=\Omega\times(0,T]$, $T>0$, and $\Omega\equiv[a,b]\times[c,d]$ such that $(t,x,y)\in\mathcal{D}$.

This study is embodied as follows: in Section 2, a weak formulation of the FEM has been executed for the 2D general Diffusion-Reaction (DR) model (1.1), considered as governing equation of this paper. Afterwards, weak formulation has been implemented in Section 3 with numerical analysis of 2D boundary value problems (3.2) and (3.5). A comparative study between theoretical and numerical results is also included here. Moreover, this section exhibits absolute error maps and tabular results of the numerical experiments. Finally, in the last Section 4 of this paper, we conclude remarks and include some general discussion.

2 Formulation of FEM for DR Equation

In this section, weak formulation of FEM for DR equation has been derived, which describes the spread of population in two space. Reaction means interaction and diffusion indicates the uniform distribution by the movement of the substance's from a higher concentration to a lower one and vice versa. In this section, we execute the weak formulation of FEM for the classical DR equation in two dimensional space. Before starting the procedure, we should have the fundamental idea regarding element, nodes and basis, shape or interpolation functions. For applying the FEM to solve any boundary value problem, at first we need to divide the domain of the problem into a finite number of sub-domains. Each sub-domains is known as element. Moreover, the starting and ending points of elements are referred as nodes and each node of the element is approximated by some piecewise polynomials, known as basis, shape or interpolation functions.

For getting accurate results and making the process easier, we may allow linear shape functions instead of using quadratic and other shape functions. Hence, the preferable shape functions in natural coordinate (η) are

$$P_1(\eta) = \frac{(1-\eta)}{2},\ P_2(\eta) = \frac{(1+\eta)}{2},\ \eta \in [-1, 1]. \tag{2.1}$$

For weak formulation of the model (1.1), let the trial solution be

$$\tilde{U}(t, x, y) = \sum_{j=1}^{n} a_j(t)\psi_j(x)\psi_j(y). \tag{2.2}$$

where the parameter a_j is a function of t, $\psi_j(x)$ and $\psi_j(y)$ are shape or coordinate functions over the spatial domain x and y.

Consequently, we obtain the following matrix after simplification and derive the usual matrix form as

$$\frac{da_j(t)}{dt}C_{i,j} + K_{i,j}a_j(t) = F_i(t) \tag{2.3}$$

Frequently, $C_{i,j}$ is referred to as the capacity or heat capacity integral and also called as capacity matrix.

The nodal values U_{j+1} may be obtained by using row-column operation and it is more relevant to use initial values, obtained from initial condition for the very first approximation.

3 Test Examples

In this section, we will discuss about two dimensional space PDEs. This discussion and numerical results ensure the acceptance and accuracy of the FEM by identifying a good matching between the exact and approximate solutions at different time steps. In this work, we have used MATLAB programming to originate the numerical solutions of these initial boundary value problems. The *Error* is computed by the following formula

$$E = |U_j^{exact} - N_j^{FEM}|.$$

Example 1. *Diffusion-Reaction equations narrate the conduct of a huge range of chemical and physical phenomena where diffusion of material stands against with the production of that material by some form of chemical and physical reaction and diffusion causes the substances to spread out over a surface in space and it is the molecular transport of mass, heat or momentum. These equations correspond to several phenomena and many other kinds of systems are recited by the same type of relation. Thus systems where heat (or fluid) is produced and diffuses away from the heat (or fluid) production site are narrated by the similar form of equation. This Diffusion-Reaction equation creates a great beneficial and vital effect in our modern life and in the field of science. During some decades, many numerical schemes are used to solve them but new methods are always attractive due to their satisfactory results. For this example, let the reaction term* $f(U(t, x, y)) = 0$ *in the DR model (1.1) and get a two dimensional parabolic PDE in the following form:*

$$\mu(x, y)\frac{\partial U}{\partial t} = \alpha_1\frac{\partial^2 U}{\partial x^2} + \alpha_2\frac{\partial^2 U}{\partial y^2};\ (t, x, y) \in \mathcal{D} \equiv \Omega \times (0, T];\quad T > 0,\ \Omega \equiv [0, 1] \times [0, 1] \tag{3.1}$$

Here, $U(t, x, y)$ *represents the unknown results, need to calculate by using numerical technique. For this experiment, consider that* $\mu = 1$, $\alpha_1 = \alpha_2 = 1$ *for the equation (3.1), which helps us to obtain (3.2).*

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2};\ (t, x, y) \in \mathcal{D} \equiv \Omega \times (0, T];\ T > 0 \tag{3.2}$$

Additionally, the initial and boundary conditions are demonstrated by equation (3.3) and (3.4) respectively:

$$U(0, x, y) = (1 - y)e^{x};\ (x, y) \in \Omega, \tag{3.3}$$

$$\begin{cases} U(t,0,y) = (1-y)e^{t}, \ \ U(t,1,y) = (1-y)e^{1+t};\ t>0 \\ U(t,x,0) = e^{x+t}, \ \ U(t,x,1) = 0;\ t>0. \end{cases} \tag{3.4}$$

The corresponding exact solution of the equation(3.2) is $U(t,x,y) = (1-y)e^{x+t}$.

Here, we have calculated the approximate solution of this boundary value problem by using the procedure of the weak formulation of FEM, described in Section 2 to ensure the validity of our present numerical scheme. At this stage, we consider the number of finite element is $n = 10$ and two linear shape functions represented by equation (2.1), to complete a compatible simplification. After that, we get a convenient matrix form which is as similar as equation (2.3) and here,

$$\begin{cases} K_{i,j} = A_{i,j} + B_{i,j} \\ A_{i,j} = \int\limits_e \int\limits_e \left[\frac{d\psi_i}{dx} \sum_{j=1}^{n} \frac{d\psi_j(x)}{dx} \psi_j(y) \right] dx \psi_i(y) dy \\ B_{i,j} = \int\limits_e \int\limits_e \left[\frac{d\psi_i}{dy} \sum_{j=1}^{n} \frac{d\psi_j(y)}{dy} \psi_j(x) \right] dy \psi_i(x) dx \\ C_{i,j} = \sum_{j=1}^{n} \int\limits_e \int\limits_e \psi_i(x)\psi_j(x)\psi_i(y)\psi_j(y) dx dy \\ F_i(t) = \int\limits_e \left[\frac{\partial \tilde{U}}{\partial x} \psi_i(x) \right]_e \psi_i(y) dy + \int\limits_e \left[\frac{\partial \tilde{U}}{\partial y} \psi_i(y) \right]_e \psi_i(x) dx \end{cases}$$

After doing this straight forward calculations, we find out the numerical solution of the equation (3.2) at various time steps in two spatial domain. Hence, the required results are tabulated in Table 1.

Table 1: Tabular exhibition of FEM and exact solution of equation (3.2).

x	y	$h = \Delta t = 0.0001$			$h = \Delta t = 0.001$			$h = \Delta t = 0.01$		
		FEM	Exact	Error	FEM	Exact	Error	FEM	Exact	Error
0.0000	0.0000	0.9999	1.0001	2.00×10^{-04}	0.9987	1.0010	2.30×10^{-03}	0.9866	1.0100	2.35×10^{-02}
0.1000	0.1000	0.9945	0.9948	2.00×10^{-04}	0.9933	0.9956	2.30×10^{-03}	0.9813	1.0047	2.34×10^{-02}
0.2000	0.2000	0.9770	0.9772	2.00×10^{-04}	0.9758	0.9781	2.30×10^{-03}	0.9640	0.9870	2.30×10^{-02}
0.3000	0.3000	0.9448	0.9450	2.00×10^{-04}	0.9436	0.9458	2.20×10^{-03}	0.9321	0.9544	2.23×10^{-02}
0.4000	0.4000	0.8950	0.8952	2.00×10^{-04}	0.8939	0.8960	2.10×10^{-03}	0.8830	0.9041	2.11×10^{-02}
0.5000	0.5000	0.8242	0.8244	2.00×10^{-04}	0.8232	0.8252	1.90×10^{-03}	0.8131	0.8326	1.95×10^{-02}
0.6000	0.6000	0.7287	0.7289	2.00×10^{-04}	0.7279	0.7296	1.70×10^{-03}	0.7189	0.7362	1.73×10^{-02}
0.7000	0.7000	0.6040	0.6042	1.00×10^{-04}	0.6033	0.6047	1.50×10^{-03}	0.5956	0.6102	1.46×10^{-02}
0.8000	0.8000	0.4451	0.4452	1.00×10^{-04}	0.4445	0.4456	1.00×10^{-03}	0.4394	0.4496	1.02×10^{-02}
0.9000	0.9000	0.2459	0.2460	8.30×10^{-05}	0.2454	0.2462	8.00×10^{-04}	0.2400	0.2484	8.41×10^{-03}
1.0000	1.0000	0.0000	0.0000	7.80×10^{-05}	0.0008	0.0000	8.00×10^{-04}	0.0079	0.0000	7.89×10^{-03}

From Table (1), it has been recognized that our introduced numerical scheme provides a better accuracy over two spatial domain at different time steps $h = \Delta t$. A good harmony can be observed between the characteristics of the approximate and exact solutions. The required data, applying the established formulation, is presented graphically in Figures 1 and 2. Analyzing these configurations, we are able to show the correspondence between these two solutions at different time steps $h = \Delta t$. Here, the error term can be neglected which declares the accuracy and acceptance of our introduced numerical scheme. However, for large time step, the error is not as much ignorable as for small time steps. To get transparent idea, let include three dimensional surface plot in Figures 3, and 5. Also a comparative analysis has been shown in Figures 4, and 6. From this comparative analysis, it's really hard to distinguish them. Hence, to overcome this tough situation, error map is represented over two spatial domain x and y. At long last, it ensures that this FEM is more applicable to solve two dimensional parabolic PDEs without any complexity. Also maintains a rapid convergence for the equation (3.2). Eventually, the Finite Element Method is schematic for this problem (3.2).

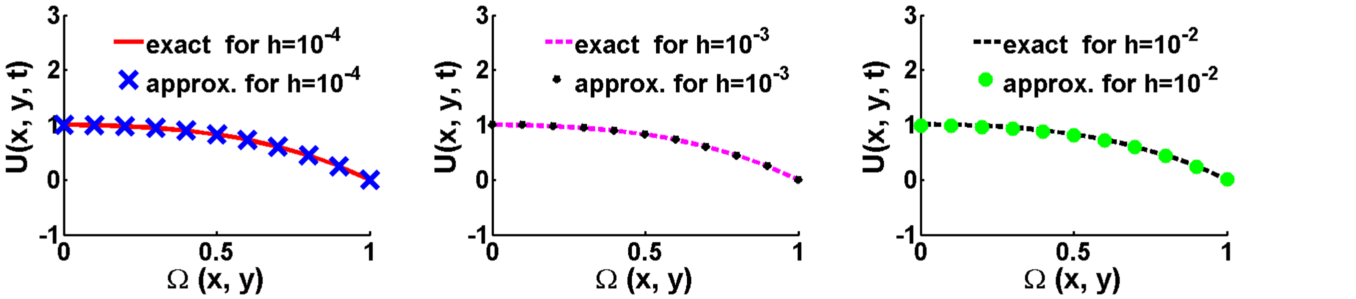

Figure 1: FEM and exact solution of equation (3.2) at $t = 0.0001, 0.001, 0.01$ respectively.

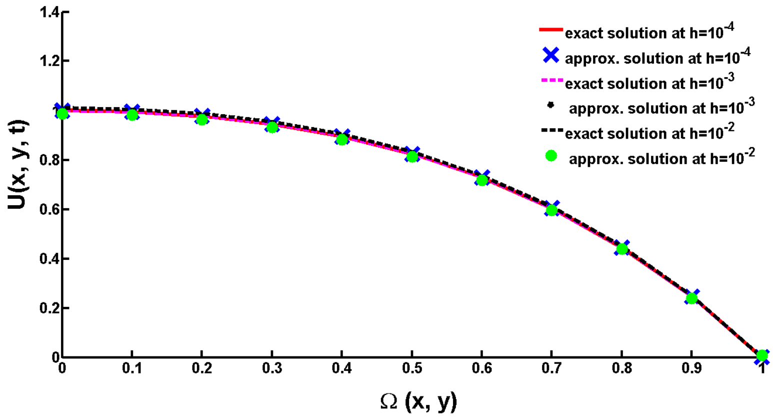

Figure 2: Correlative study between FEM and exact solution of equation (3.2) at $t = 0.0001, 0.001, 0.01$.

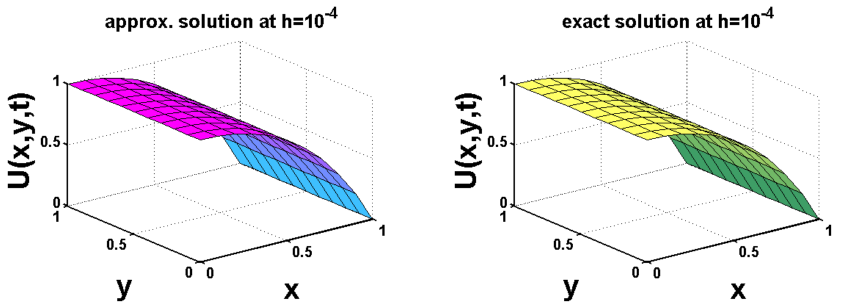

Figure 3: FEM and exact solution of equation (3.2) at $t = 0.0001$.

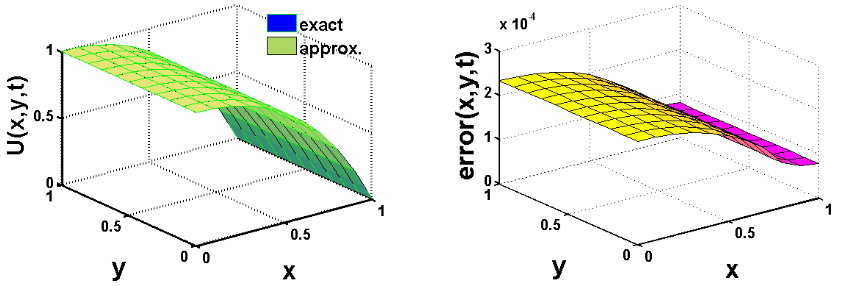

Figure 4: Comparative analysis of equation (3.2) and absolute error map at $t = 0.0001$.

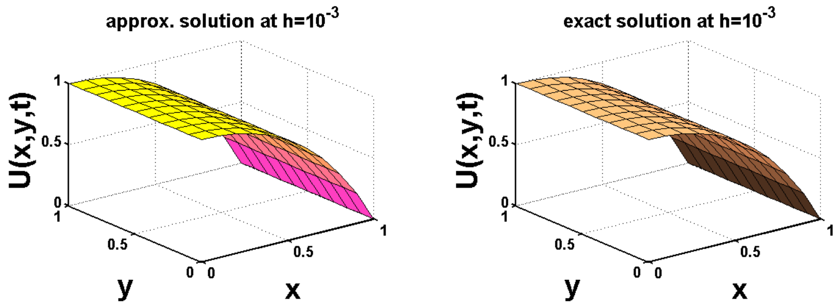

Figure 5: FEM and exact solution of equation (3.2) at $t = 0.001$.

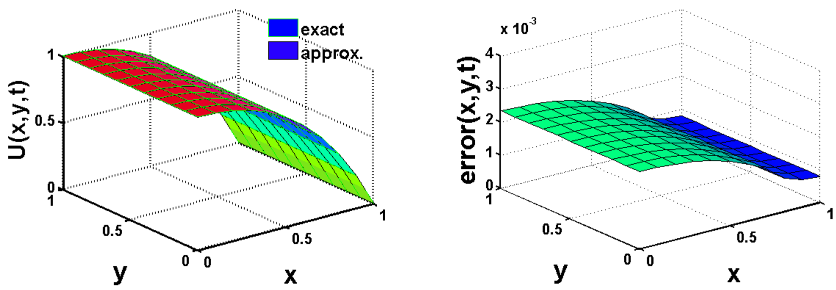

Figure 6: Comparative analysis of equation (3.2) and absolute error map at $t = 0.001$.

Example 2. *In the sake of Example 2, let introduce the reaction function $f(U(t, x, y)) = -e^{-t}(x^2 + y^2 + 4)$ in equation (3.2) and obtain a Diffusion-Reaction equation (3.5), is a mathematical model, shows consistency to different physical phenomena. This equation indicates the change over space and time of the concentration of one or more substances. This type of equation is naturally applied in chemistry. Nevertheless, this equation is also used to explain the dynamical processes of non-chemical nature. The Diffusion-Reaction equation is found in biology, physics, geology, and ecology. Eventually, this equation (3.5) takes the form of semi-linear parabolic partial differential equation. To get conceptual idea of physical phenomena and to prove the accuracy of various numerical methods, many authors are interested to solve two dimensional Diffusion-Reaction model. Moreover, we have considered (3.5), completed numerical analysis and demonstrated the acceptance of our introduced numerical scheme in this present research.*

$$\frac{\partial U}{\partial t} = \left[\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} - e^{-t}(x^2 + y^2 + 4)\right]; (t, x, y) \in \mathcal{D} \equiv \Omega \times (0, T], \quad T > 0, \ \Omega \equiv [0, 1] \times [0, 1]. \tag{3.5}$$

Subject to the initial condition

$$U(0, x, y) = x^2 + y^2 + 1, \ (x, y) \in \Omega, \tag{3.6}$$

and boundary conditions are given by equation (3.7)

$$\begin{cases} U(t, 0, y) = 1 + y^2 e^{-t}, \ U(t, 1, y) = 1 + (1 + y^2)e^{-t}, \ t > 0 \\ U(t, x, 0) = 1 + x^2 e^{-t}, \ U(t, x, 1) = 1 + (1 + x^2)e^{-t}, \ t > 0. \end{cases} \tag{3.7}$$

The reciprocal theoretical solution of the equation (3.5) is $U(t, x, y) = 1 + (x^2 + y^2)e^{-t}$, obtained from first-rated literature. As like Example 1, we follow similar weak formulation of FEM with 10 number of elements, two linear shape functions (2.1) to analyze the numerical solution of (3.5) and check the accuracy of the FEM. Consequently, the usual matrix form (2.3) is obtained with different coefficients. Afterwards, the computed solution of (3.5) is portrayed in Table 2, which indicates that the result tends to be unstable with the increment of $h = \Delta t$.

Table 2: Approximate and theoretical solution of (3.5).

x	y	$h = \Delta t = 0.0001$			$h = \Delta t = 0.001$			$h = \Delta t = 0.01$		
		FEM	Exact	Error	FEM	Exact	Error	FEM	Exact	Error
0.0000	0.0000	0.9999	1.0000	1.00×10^{-04}	0.9987	1.0000	1.30×10^{-03}	0.9870	1.0000	1.30×10^{-02}
0.1000	0.1000	1.0199	1.0200	1.00×10^{-04}	1.0187	1.0200	1.30×10^{-03}	1.0068	1.0198	1.30×10^{-02}
0.2000	0.2000	1.0799	1.0800	1.00×10^{-04}	1.0786	1.0799	1.30×10^{-03}	1.0660	1.0792	1.32×10^{-02}
0.3000	0.3000	1.1798	1.1800	1.00×10^{-04}	1.1785	1.1798	1.40×10^{-03}	1.1646	1.1782	1.36×10^{-02}
0.4000	0.4000	1.3198	1.3200	1.00×10^{-04}	1.3183	1.3197	1.40×10^{-03}	1.3028	1.3168	1.41×10^{-02}
0.5000	0.5000	1.4998	1.5000	1.00×10^{-04}	1.4980	1.4995	1.50×10^{-03}	1.4804	1.4950	1.47×10^{-02}
0.6000	0.6000	1.7198	1.7199	2.00×10^{-04}	1.7177	1.7193	1.60×10^{-03}	1.6974	1.7128	1.55×10^{-02}
0.7000	0.7000	1.9797	1.9799	2.00×10^{-04}	1.9774	1.9790	1.60×10^{-03}	1.5942	1.9702	1.61×10^{-02}
0.8000	0.8000	2.2797	2.2799	2.00×10^{-04}	2.2769	2.2787	1.80×10^{-03}	2.2491	2.2673	1.82×10^{-02}
0.9000	0.9000	2.6197	2.6198	2.00×10^{-04}	2.6169	2.6184	1.50×10^{-03}	2.5887	2.6039	1.52×10^{-02}
1.0000	1.0000	2.9995	2.9998	3.00×10^{-04}	2.9948	2.9980	3.20×10^{-03}	2.9480	2.9801	3.21×10^{-02}

Taking a view on the tabulated results from Table 2, we must say that an excellent accuracy is detected for several time steps. Figures 7 and 8, speak for the acceptance of our proposed method since the approximate solution almost coincides with the theoretical solution. Also Figures 9, 11, 13 stand for the three dimensional configuration of the the approximate and theoretical solution of equation (3.5) for different time steps. However, it's not so easy to realize the comparison between the approximate and theoretical solution by observing the two dimensional configuration . To confirm transparent idea, we comprise three dimensional surface plot of the solutions of equation (3.5) for several time steps represented by Figures 10, 12, 14, holding a comparison between approximate and theoretical solutions and absolute error map over the spatial domain x and y. Finally, after doing a diligent inspection, a good match is found between them with an ignorable error.

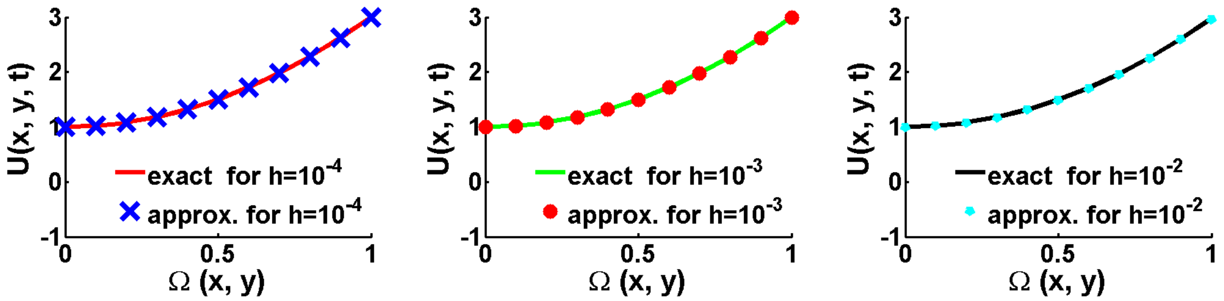

Figure 7: Approximate and theoretical solution of equation (3.5) at $t = 0.0001, 0.001, 0.01$ respectively.

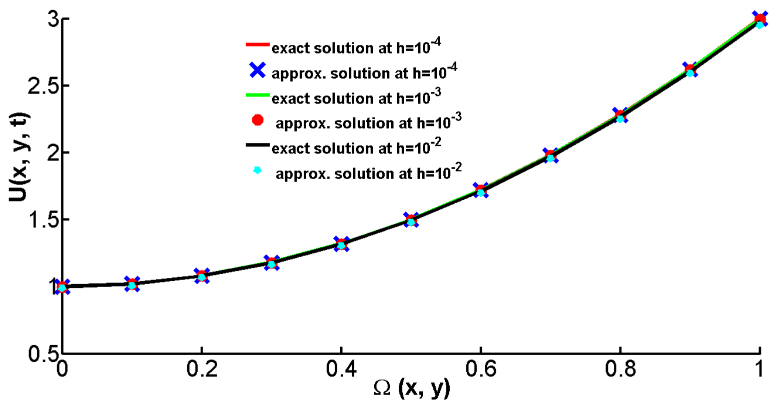

Figure 8: Analogy between approximate and theoretical solution of (3.5) at $t = 0.0001, 0.001, 0.01$.

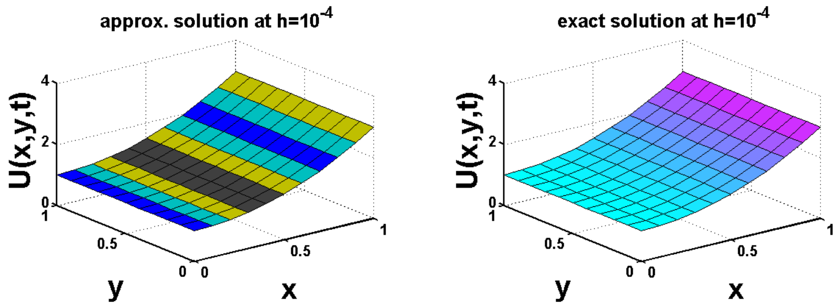

Figure 9: Approximate and theoretical solutions of (3.5) at $t = 0.0001$.

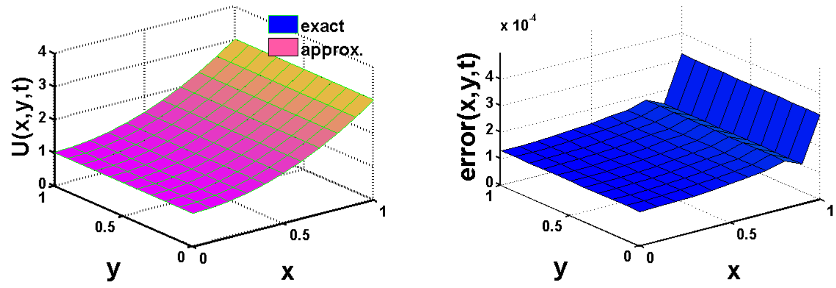

Figure 10: Comparative reading and absolute error map of (3.5) at $t = 0.0001$.

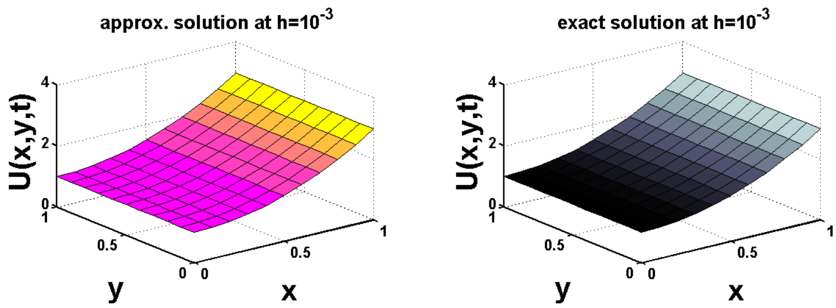

Figure 11: Approximate and theoretical solutions of (3.5) at $t = 0.001$.

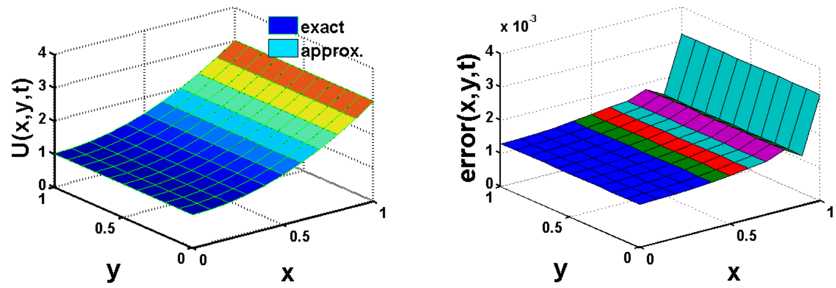

Figure 12: Comparative reading and absolute error map of (3.5) at $t = 0.001$.

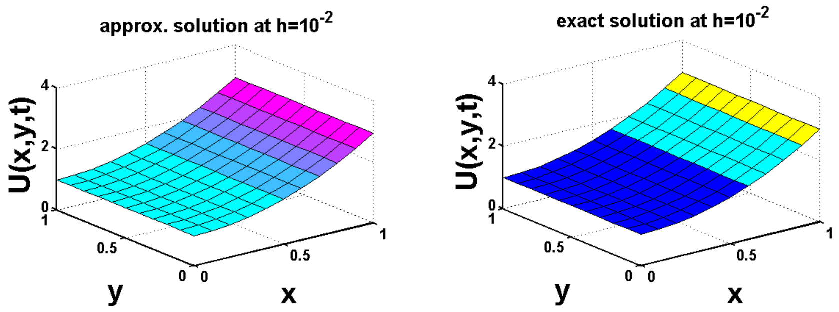

Figure 13: Approximate and theoretical solution of (3.5) at $t = 0.01$.

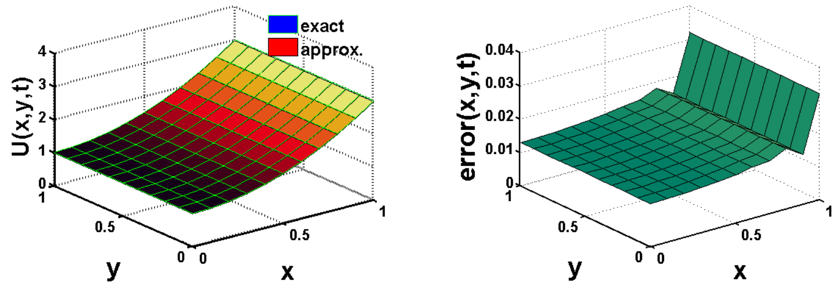

Figure 14: Comparative reading and absolute error map of (3.5) at $t = 0.01$.

Last but not the least, the numerical analysis of (3.5) discloses the efficiency and compliance of FEM to solve a two dimensional parabolic partial differential equation.

4 Conclusion

In this paper, we have procured the weak formulation of FEM for two dimensional parabolic partial differential equations. This work has disclosed two examples of DR model, where all approximate solutions of two examples converge rapidly to the respective exact solutions. This method is successful to provide approximate solution, which is good enough to accept by the researchers with an ignorable error by the analysis of absolute error map. A compatible match can be realized between the approximate and exact solution from the data structured in table and graphical presentation. Our scheme produces stable results and higher-order accuracy, which acts as an evidence for the acceptance of this scheme.

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