Galerkin-Chebyshev Pseudo Spectral Method and a Split Step New Approach for a Class of Two dimensional Semi-linear Parabolic Equations of Second Order

F. Talay Akyildiz[1], K. Vajravelu [2] [†]

[1]Department of Mathematics and Statistics, Faculty of Science, Al-Imam University, Riyadh, Saudi Arabia

[2]Department of Mathematics, University of Central Florida, Orlando, Florida 32816, USA

Abstract

In this paper, we use a time splitting method with higher-order accuracy for the solutions (in space variables) of a class of two-dimensional semi-linear parabolic equations. Galerkin-Chebyshev pseudo spectral method is used for discretization of the spatial derivatives, and implicit Euler method is used for temporal discretization. In addition, we use this novel method to solve the well-known semi-linear Poisson-Boltzmann (PB) model equation and obtain solutions with higher-order accuracy. Furthermore, we compare the results obtained by our method for the semi-linear parabolic equation with the available analytical results in the literature for some special cases, and found excellent agreement. Furthermore, our new technique is also applicable for three-dimensional problems.

1 Introduction

Consider a class of semi-linear parabolic equations of the form

$$\frac{\partial u}{\partial t} = k(t)\Delta u + f(u)g(t) + h(x,y,t), in\ \Omega_t = (a,b) \times (c,d) \times (t_0,T), \tag{1}$$

with the initial condition

$$u(x,y,0) = a(x,y)\ on\ \Omega = (a,b) \times (c,d), \tag{2}$$

[†]K. Vajravelu.
Email address: kuppalapalle.vajravelu@ucf.edu

and the Dirichlet boundary conditions

$$
\begin{aligned}
u(a,y,t) &= \omega_1(x,y), u(b,y,t) = \omega_2(x,y), \\
u(x,c,t) &= \omega_3(x,y), u(x,d,t) = \omega_4(x,y),
\end{aligned}
\tag{3}
$$

where $k(t), a(x,y), \{\omega_i\}_{i=1}^4$ are all known functions, $0 < C_0 \le k(t) \le C_1, h(x,y,t) \le C_2 1/f(u), g(t) \in L^1$. It is not difficult to see that under usual change of independent and dependent variables, the above equation can be reduced to

$$
\frac{\partial u^*}{\partial t} = k^*(t)\Delta u^* + f(u^*)g^*(t) + h^*(x^*,y^*,t), in\ \Omega_t^* = (-1,-1) \times (-1,-1) \times (t_0,T),
\tag{4}
$$

with

$$
u^*(x^*,y^*,0) = a^*(x^*,y^*)\ on\ \Omega^* \text{and}\ u^*|_{\partial\Omega^*} = 0\ on\ (t_0,T).
\tag{5}
$$

There are many studies dealing with the numerical solution of this type of the equation; considering the finite difference, for example, Tian and Ge [1] and Mohebbi and Deghan [2]; and considering finite element method, for example, Lasis and Suli [3], very recently, two grid finite element methods were developed by Chen and Liu [4]. Related to the spectral method, there are some studies listed in Liu et al. [5]. We note that in all these studies, especially with spectral methods, the authors used explicit method, which is necessary for the temporal variable, which has stability problem for large time.

In this study, we use implicit method for temporal variables, and obtain the solution to semi-linear Poisson-Boltzmann (PB) equation, which is commonly used to characterize electrostatic interactions. Solving numerically the semi-linear PB equation is very challenging due to various factors of the PB model, such as complex geometry of protein structures, singular source terms, strong nonlinearity of ionic effects, systems with distributed mobile charges. These are vital for the study of a protein system immersed in an ionic solvent environment (see details see Geng and Zhao [6]).

Efficiency and accuracy are two major concerns in obtaining numerical solutions of the Poisson-Boltzmann equation, for applications in chemistry and biophysics. Developments in boundary element methods, interface methods, adaptive methods, finite element methods, and other approaches for the Poisson-Boltzmann equation are outlined in the review article by Lu et al. [7]. More recently, Deng et al. [8] used the discontinuous Galerkin method and obtained numerical solution for three-dimensional semi-linear PB equation using the regularization formulation technique.

The goal of this work is to introduce Galerkin-Chebyshev pseudo spectral method for two-dimensional semi-linear parabolic equations of second order in the form of Eqs.(4) and (5). The proposed method is built based on an operator splitting or time splitting framework. In this method, the nonlinear subsystem of the semi-linear partial differential equation can be analytically integrated in time and then linear part of the semi-linear equation can be integrated easily in time. Then the Galerkin-Chebyshev spectral method is used for discretization of the spatial derivatives. Literature review reveals that no such work exists; this gives us enough motivation for the present report. The details of the proposed time splitting pseudo spectral Chebyshev method is discussed in Section 2. Numerical validations of our results (of a benchmark example) with the available analytical results in the literature will be considered in Section 3. Finally, this work ends with a conclusions section.

2 Galerkin-Chebyshev spectral method and operator splitting

Consider a uniform grid partition in time with an increment Δt and denote $t_n = n\Delta t$. A first order time splitting scheme of Geng and Zhao [6], and Deng et al. [8] will be employed to update Eq.(4) in the subinterval $[t_n, t_{n+1}]$,

omitting star, we get

$$\frac{\partial \chi}{\partial t} = f(\chi)g(t) \text{ with } \chi(x,y,t_n) = u(x,y,t_n), t \in [t_n, t_{n+1}], \tag{6}$$

$$\frac{\partial \phi}{\partial t} = k(t)(\alpha^2 \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}) + h(x,y,t), \text{ with } \phi(x,y,t_n) = \chi(x,y,t_{n+1}), t \in [t_n, t_{n+1}] \tag{7}$$

where $\alpha = (\frac{d-c}{a-b})^2$, (aspect ratio). We then have $u(x,y,t_{n+1}) = \phi(x,y,t_{n+1})$. Since, Eq. (6) separable differential equation, and $1/f(\chi)$ and $g(t)$ are integrable

$$X(t) = \int \frac{\partial \chi}{f(\chi)} = \int g(t)dt = G(t). \tag{8}$$

Evaluating the expression both at t_n to t_{n+1}, we get

$$X(t_{n+1}) - X(t_n) = G(t_{n+1}) - G(t_n). \tag{9}$$

For example, for the well-known nonlinear Poisson-Boltzmann, we have $g(t) = 1, h(x,y,t) = 0$ and $f(\chi) = -k^2 \sinh(\chi)$(see for details Refs. [6]and [8]). In this case, following the same line as in Refs. [6] and [8], we have analytical solution as

$$X(x,y,t_{n+1}) = \ln\left[\frac{\cosh(\frac{1}{2}k^2\Delta t) + exp(-\chi(x,y,t_n))\sinh(\frac{1}{2}k^2\Delta t)}{\sin(\frac{1}{2}k^2\Delta t) + exp(-\chi(x,y,t_n))\cosh(\frac{1}{2}k^2\Delta t)}\right]. \tag{10}$$

2.1 Galerkin-Chebyshev spectral method

Let us denote $T_n(y)$ as the nth degree Chebyshev polynomial and

$$P_N = Span\{T_0(y), T_1(y), \ldots, T_N(y)\}, V_N = \{v \in P_N : v(\mp) = 0\}. \tag{11}$$

Now, the standard Chebyshev-Galerkin approximation to equations (6) and (7) is nothing but finding $X_N : [t_n, t_{n+1}] \to V_N^2$ and $\phi_N : [t_n, t_{n+1}] \to V_N^2$ such that

$$(X(t_{n+1}) - X(t_n), v)_w - (G(t_{n+1}) - G(t_n), v)_w = 0, \forall v \in V_N^2, t_n \le t \le t_{n+1}, \tag{12}$$

and

$$(\partial_t \phi_N, v)_w + k(t)(\Delta \phi_N, v)_w + (h(x,y,t,v)_w = 0, \forall v \in V_N^2, t_n \le t \le t_{n+1}, \tag{13}$$
$$(\phi_N(x,y,t_0) - \phi_0, v)_w = 0, \forall v \in V_N^2,$$

where inner product is defined in $L_w^2(\Omega)$ as $(u,v)_w = \int_\Omega uvwdxdy, w = (1-x^2)^{-1/2}(1-y^2)^{-1/2}$, $\|u\|_w = \|u\|_{L_w^2} = (u,u)_w^{1/2}$.

We need the following lemma for our algorithm and proof of Lemma 1 can be found in Shen et al. [9]

Lemma 1. *For Dirichlet boundary conditions, we consider*

$$\theta_k(y) = T_k(y) - T_{k+2}(y), k = 0.., n-2, \tag{14}$$

then, we have,

$$a_{kj} = -(\theta_j''(y), \theta_k(y))_w = \begin{cases} 2\pi(k+1)(k+2) & j = k \\ 4\pi(k+1), & j = k+2, k+4, \ldots \\ 0, & j > k \text{ or } j+k \text{ odd} \end{cases} \tag{15}$$

and

$$b_{kj} = -(\theta_j(y), \theta_k(y))_w = \begin{cases} \frac{(c_k+1)}{2}\pi & j = k, c_0 = 2, c_i = 1, i > 1 \\ -\frac{\pi}{2}, & j = k-2 \text{ and } j = k+2 \\ 0, & \text{Otherwise.} \end{cases} \tag{16}$$

Therefore, $V_N^2 = \{\theta_k(x)\theta_j(y), j, k = 0, 1, \ldots, N-2\}$. Let us assume that

$$u^N(x, y, t) = \sum_{k,j=0}^{N-2} C_{kj}(t)\theta_k(x)\theta_j(y). \tag{17}$$

Then, for $t \in [t_n, t_{n+1}]$

$$X^N(x, y, t) = \sum_{k,j=0}^{N-2} D_{kj}(t)\theta_k(x)\theta_j(y) \text{ with } X^N(x, y, t_n) = u(x, y, t_n), \tag{18}$$

and

$$\phi^N(x, y, t) = \sum_{k,j=0}^{N-2} E_{kj}(t)\theta_k(x)\theta_j(y) \text{ with } \phi^N(x, y, t_n) = X^N(x, y, t_{n+1}). \tag{19}$$

Inserting (18), (19) into (12), (13) respectively, and using

$$v = \theta_l(x)\theta_s(y)l, s = 0, 1, 2, \ldots N-2.$$

We get

$$(X(t_{n+1}) - X(t_n), \theta_l(x)\theta_s(y))_w - (G(t_{n+1}) - G(t_n), \theta_l(x)\theta_s(y))_w = 0, t_n \leq t \leq t_{n+1} \tag{20}$$

and

$$(\partial_t \hat{\phi}_N, \theta_l(x)\theta_s(y))_w + k(t_n)(\Delta \hat{\phi}_N, \theta_l(x)\theta_s(y))_w = 0, t_n \leq t \leq t_{n+1} \tag{21}$$
$$(\hat{\phi}_N(x, y, t_0) - \hat{\phi}_0, \theta_l(x)\theta_s(y))_w = 0.$$

Then in the light of Lemma 1, we have

$$BD_{kj}(t_{n+1})B - BD_{kj}(t_n)B - (G(t_{n+1}) - G(t_n))\pi = 0, \tag{22}$$

$$B\frac{d}{dt}E_{kj}(t_{n+1})B - k(t_n)(BE_{kj}(t_{n+1})A^T + AE_{kj}(t_{n+1})B) = 0, \tag{23}$$

$$BC_{kj}(t_0)B = U_0, (U_0)_{kj} = (u_0, \theta_k(x)\theta_j(y))_w, \tag{24}$$

where $A = (a_{kj}), B = (b_{kj})k, j = 0, 1, 2, \ldots, N-2$.

We now present the following theorem for weighted L_w^2 estimate for the discrete problem without proof. We refer to Liu et al. [5] for details.

Theorem 2. *Let u and u^N be solution of (4) and (12)-(13) respectively, Assume $0 < C_0 \leq k(t) \leq C_1, h(x, y, t) \in L^\infty(\Omega_t), \int \frac{du}{f(u)} \in C^1$ and $u, u_t \in L^\infty((t_0, T), H_s^w(\Omega) \cap H_{0,w}^1(\Omega)), s \geq 1$. Then we have*

$$\|u^N - u\|_w \leq CN^{-s}(\|u\|_{L^\infty((t_0,T);H_s^w(\Omega))} + \|u_t\|_{L^\infty((t_0,T);H_s^w(\Omega))}), \text{ for } t \in [t_0, T], \tag{25}$$

where

$$H_w^s(\Omega) = \{u : \|u\|_{s,w} < \infty\}, \|u\|_{s,w} = \left(\sum_{|r| \leq s} \|D^r u\|_w^2\right)^{\frac{1}{2}}, |u|_{s,w} = \left(\sum_{|r| = s} \|D^r u\|_w^2\right)^{\frac{1}{2}}, \tag{26}$$

here, $D^r u = \frac{\partial^{|r|}}{\partial x^{r_1} \partial y'^2} u, r = (r_1, r_2)$ and $|r| = r_1 + r_2$. Now, we define the Bochner space $L^p((t_0, T); H_s^w(\Omega))$ endowed with the following norm

$$\|u\|_{L^p((t_0,T);H_s^w(\Omega))} = \begin{cases} \left(\int_{t_0}^T \|u\|_{s,w}^p dt\right)^{1/p}, & 1 \leq p < \infty \\ \text{ess sup}_{t \in (t_0,T)} \|u\|_{s,w}, & p = \infty. \end{cases} \tag{27}$$

Let $H_{0,w}^1 = \{u \in H_w^1 : u(\partial\Omega) = 0\}$. The $L_w^2(\Omega)$ orthogonal projection $P_N^0 : H_{0,w}^1(\Omega) \to V_N^2$ is defined by

$$(P_N^0 u - u, \theta)_w = 0, \forall \theta \in V_N^2. \tag{28}$$

3 Numerical results

In this section, we present numerical examples to demonstrate the convergence and accuracy of the new method. Throughout this section, we use uniform grid for temporal discretization, $\Delta t = t_{n+1} - t_n$, $k+1$ is the time-step and the number of grid-points in the interval $[t_n, t_{n+1}]$.

3.1 Test Problem 1: Poisson-Boltzmann equation

We first briefly drive the model, the net electric charge density,ρ_e, in the EDL (electric double layer) can be related to the total potential field(Φ)by the Poisson equation

$$\bigtriangledown^2 \Phi = -\frac{\rho_e}{\varepsilon}, \tag{29}$$

where ε is the permittivity of the solution. The total electric field $\Phi = \Theta + \Psi$ is a linear superposition of the applied electric field generated by the electrodes,$\Theta(z)$, and the electric field due to the net charge distribution in the EDL, $\psi(x,y)$, for details Movahed [10]. Consider the above equation with the standard electrokinetic model in Refs. [10, 11]: Assume two dimensional, then RHS becomes a function of two variables,x and y. Substituting$\Phi = \Theta + \Psi$, we see that Eq.(18) can be separated very easily into the following two equations

$$\bigtriangledown^2 \psi = -\frac{\rho_e}{\varepsilon}, \bigtriangledown^2 \Theta = 0. \tag{30}$$

Therefore, the net electric charge density is independent of the external electric field and is determined by ψ. According to the quasi-equilibrium conditions, the ion density variation in the EDL obeys the Boltzmann distribution. So, for a symmetric electrolyte of equal valence ($\mathbb{Z} = \mathbb{Z}^+ = -\mathbb{Z}^-$), then the first part in Eq.(30) can be expressed explicitly by the PB equation as follows

$$\bigtriangledown^2 \psi = \frac{1}{\varepsilon}\left[2en_0 \sinh\left(\frac{e\mathbb{Z}\psi}{k_b T_m}\right)\right], \tag{31}$$

where n_0 is the bulk number concentration of ions in the electrolyte solution, T_m is the absolute average temperature, k_b is the Boltzmann constant, and e is the elementary electronic charge. If use the dimensionless variables and parameters as in Refs. [10]- [11], we obtain the dimensionless nonlinear Poisson-Boltzman. We further assume electrical field two-dimensional, in a two dimensional Cartesian coordinates system equation becomes

$$\frac{\partial^2 \bar{\psi}}{\partial x^2} + \frac{\partial^2 \bar{\psi}}{\partial y^2} = K^2 \sinh(\bar{\psi}). \tag{32}$$

This equation subject to the following boundary conditions (These conditions are widely suggested)

$$i)\ \bar{\psi}(x,0) = \bar{\psi}(y,0) = \bar{\psi}(x,1) = \bar{\psi}(y,1) = \psi_0,$$

$$ii)\ \frac{\partial \bar{\psi}}{\partial x}\big|_{x=0} = 0, \frac{\partial \bar{\psi}}{\partial y}\big|_{y=0} = 0, \bar{\psi}(x,1) = \bar{\psi}(y,1) = \psi_0. \tag{33}$$

Direct application of spectral method, requires solving highly nonlinear algebraic system which is not possible to solve numerically for large number of base elements. This motivates the development of pseudo-transient continuation approaches for solving the nonlinear PB equation (for details see Refs. [12–15], the method authors used in this study are mainly finite difference and finite element methods. Basically, a pseudo-transient variation is introduced to convert Eq.(32) from the time-independent form to a time-dependent form

$$\frac{\partial \bar{\psi}}{\partial t} = \frac{\partial^2 \bar{\psi}}{\partial x^2} + \frac{\partial^2 \bar{\psi}}{\partial y^2} - K^2 \sinh(\bar{\psi}). \tag{34}$$

We need now an initial solution, this could be the electrostatic potential obtained from a linearized PB equation or trivially $\bar{\psi} = 0$. We then numerically integrate Eq.(34) for a sufficiently large time period. The solution of the original nonlinear PB Eq.(32) can be recovered eventually by the steady state solution of the pseudo-time dependent process from Eq.(34).
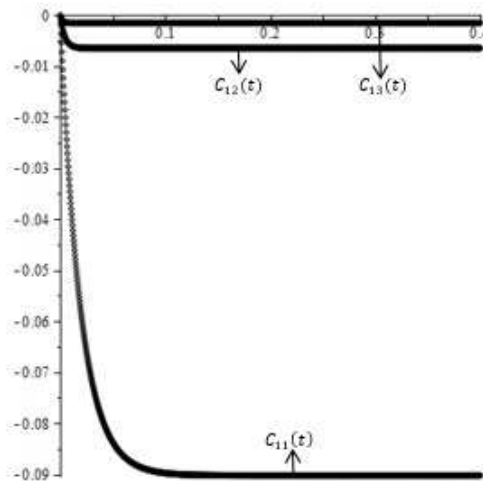

Fig. 1 First three approximation for time variable.

However, there exists a real difficulty involved in the numerical integration of the time dependent NPB equation (34). Generally speaking, since a long time integration is required to reach the steady state for Eq.(34), explicit time stepping methods are usually not efficient for pseudo-transient continuation approaches, see for example [12–15]. In the literature, semi-implicit time stepping methods [12, 13] are commonly used to solve time dependent NPB equation (34) so that a large time step could be used for a stable simulation. Nevertheless, a fully implicit time integration method has never been constructed for solving the classical nonlinear PB equation (34) by the method of Galerkin spectral method. Here we show that in Eqs.(12)-(13) and (10) that time splitting method enable us to use the implicit time integration. We first tested our algorithm for $\sinh(\bar{\psi}) \approx \bar{\psi}$ in which case Eq.(24) becomes linear and exact analytical solution is possible [6]. We found that L_w error less than 10^{-8} for $N = 10$ and $0 < t < 10$. Therefore, we expect similar error for nonlinear case. In Fig.1, we see

that steady state case has been easily obtained. Furthermore, we are only able to show on figure first three approximations, because the other approximations are very small to show on the figure, which shows the power of our approximations.

In Fig.2, we show the centerline electrostatic potential which shows the development of the profiles. We also show the three dimensional profile of electrostatic potential for $t = 2.5$. Figure 3 indicates the steady state solution, because any increase in the value of t, does not cause any change in the electrostatic potential.
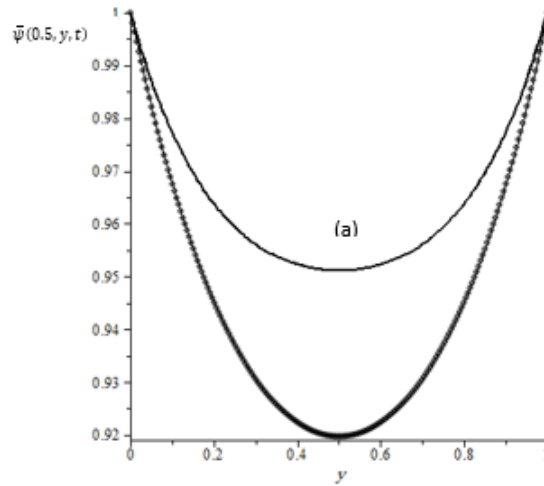
Fig. 2 Centerline electrostatic potential (a) t=0.05(line) (b) t=0.5(point) (c) t=2.5(polygon.)

Since the available experimental results for the Poisson-Boltzman equation are on $[0, a]$, we obtained our results on this region. However, we note here that, in order to apply Chebyshev-Galerkin spectral method, we first transformed the given region to $[-1, 1]$, then we obtain the solution. Finally we applied inverse transformation to the obtained solution in order to express the solution in the original region. We also note that integration of equation in Eq. (12), we use Gauss-Chebyshev quadrature method.
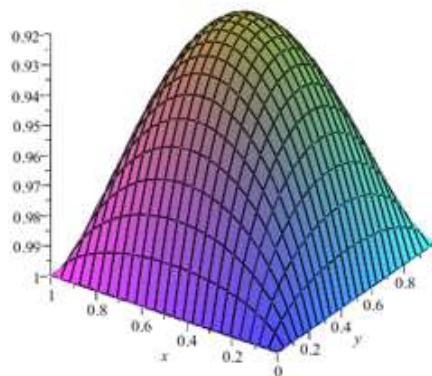
Fig. 3 Solution of NPB equation at t=2.5.

3.2   Test Problem 2

We consider in this case $k(t) = 1, a = c = 0, b = d = 1, \alpha^2 = 1, f(u) = \frac{1}{1+u^2} + h(x,y,t)$ and initial and boundary conditions

$$u(x,y,0) = \sin(\pi x)\sin(\pi y), \text{ on } \Omega = (0,1) \times (0,1), \tag{35}$$

$$u(-1,y,t) = u(1,y,t) = u(x,-1,t) = u(x,1,t) = 0, \text{ for } t > 0 \tag{36}$$

where the source function is chosen the such that exact solution is

$$u(x,y,t) = e^{-t}\sin(\pi x)\sin(\pi y). \tag{37}$$

In this case, according to our time splitting scheme, on $[t_n, t_{n+1}]$ we get

$$\frac{\partial \chi}{\partial t} = \frac{1}{(1+\chi^2)}, \text{ with } \chi(x,y,t_n) = u(x,y,t_n), t \in [t_n, t_{n+1}], \tag{38}$$

$$\frac{\partial \phi}{\partial t} = \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right) + h(x,y,t), \text{ with } \phi(x,y,t_n) = \chi(x,y,t_{n+1}), t \in [t_n, t_{n+1}], \tag{39}$$

where,

$$h(x,y,t) = \frac{-e^{-3t}(\sin(\pi x)\sin(\pi y))^3(1-2\pi^2) - e^{-t}\sin(\pi x)\sin(\pi y)(1-2\pi^2) - 1}{e^{-2t}(\sin(\pi x)\sin(\pi y))^2 + 1}.$$

Integration of equation (38) and using the Cardana formula, we get

$$\begin{aligned}
&\chi(x,y,t_{n+1}) - \chi(x,y,t_n) \\
&= \frac{1}{2}\left(12t_{n+1} + 4\sqrt{4+9(t_{n+1})^2}\right)^{\frac{1}{3}} - \frac{2}{\left(12t_{n+1} + 4\sqrt{4+9(t_{n+1})^2}\right)^{\frac{1}{3}}} \\
&\quad - \frac{1}{2}\left(12t_n + 4\sqrt{4+9(t_n)^2}\right)^{\frac{1}{3}} - \frac{2}{\left(12t_n + 4\sqrt{4+9(t_n)^2}\right)^{\frac{1}{3}}}.
\end{aligned} \tag{40}$$

Since we have solved nonlinear part analytically, we can apply implicit scheme for temporal discretization. Now, substituting (18) and (19) into (30) and (31), and applying the Chebyshev Galerkin method, we obtain simple expression temporal discretization which can be solved by implicit method as described earlier. Hence, we see that our method much more efficient than the usual spectral Galerkin method. Fig.4 shows the approximation for the $h(x,y,t)$ in terms of our base function in Eq.(14) for given fixed time. We see that the error is less than 10^{-4} except for the initial and end regions where $h(x,y,t)$ is not zero; whereas our base function satisfies the boundary condition zero at the end-point. Fig.5 shows the L_w error for different N.

4   Conclusions

In this paper, we presented a new technique to solve a class of semi-linear parabolic partial differential equations numerically. We combined Galerkin-Chebyhev pseudo spectral method with time splitting technique. This helped in reducing the problem to a linear parabolic partial differential equation in space variables. Then we could use the Galerkin-Chebyhev spectral method easily and this enabled us to use the implicit Euler method for temporal discretization. In this paper, we also studied two-dimensional problems. Furthermore, our new technique is applicable to three-dimensional problems. In a follow up paper, we shall analyse three-dimensional class of semi-linear parabolic partial differential equations and the associated error analyses.
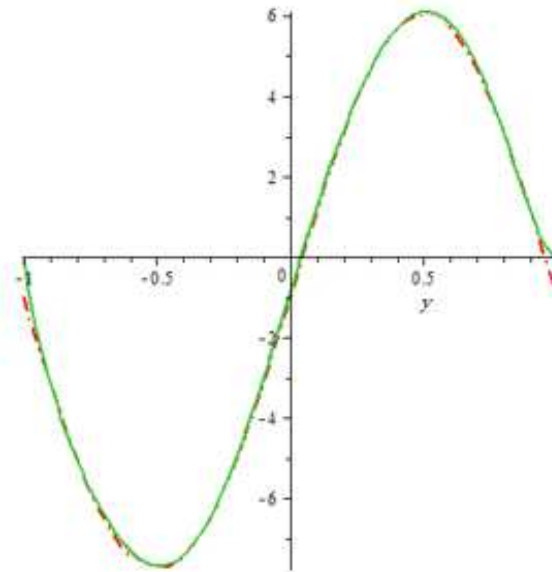
Fig. 4 Approximation to the Source function in terms of the base Function at t=1 for (N=8), Green line is the source function and red line(dotted line) approximation.
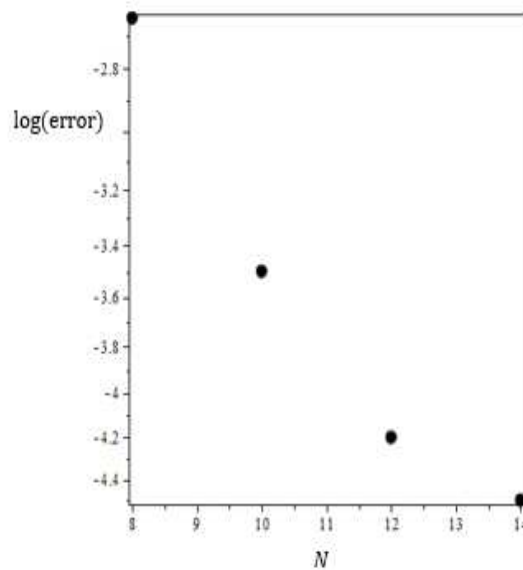
Fig. 5 L_w^2 error for test problem 2 at t=1.

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