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Orthogonal cubic spline collocation method for the Cahn–Hilliard equation

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Abstract

The Cahn–Hilliard equation plays an important role in the phase separation in a binary mixture. This is a fourth order nonlinear partial differential equation. In this paper, we study the behaviour of the solution by using orthogonal cubic spline collocation method and derive optimal order error estimates. We discuss some computational experiments by using monomial basis functions in the spatial direction and RADAU 5 time integrator. The method we present here is better in terms of stability, efficiency and conditioning of the resulting matrix. Since no integrals to be evaluated or approximated, it behaves better than finite element method.

Keywords: Cahn–Hilliard equation; Orthogonal cubic spline collocation method; Lyapunov functional; *A priori* bounds; Optimal error estimates; Monomial basis functions; RADAU 5

1. Introduction

We consider the one spatial dimensional Cahn–Hilliard equation:

$$\frac{\partial u}{\partial t} + \gamma \frac{\partial^4 u}{\partial x^4} = \frac{\partial^2 \phi(u)}{\partial x^2}, \quad (x,t) \in I \times (0,T] \tag{1.1}$$

with the initial condition

$$u(x,0) = u_0(x), \quad x \in I, \tag{1.2}$$

and boundary conditions

$$\begin{aligned} &u(0,t) = u(1,t) = 0, \quad t \in (0,T], \\ &\frac{\partial^2 u}{\partial x^2}(0,t) = \frac{\partial^2 u}{\partial x^2}(1,t) = 0, \quad t \in (0,T], \end{aligned} \tag{1.3}$$

where $\gamma > 0$, $\phi(u) = \gamma_2 u^3 + \gamma_1 u^2 + \gamma_0 u$, $\gamma_2 > 0$, $I = (0,1)$ and $0 < T < \infty$.

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Eq. (1.1) arises in a variety of applications such as phase transition in material science. We refer the reader to [5] and the references there in. In this paper, we use second–order splitting procedure combined with orthogonal spline collocation method for Eq. (1.1) and derive optimal error estimates. Since this method is much superior to B-splines in terms of stability, efficiency and conditioning of the resulting matrix. Compared to finite element method (FEM) the calculation of the coefficients of the mass and stiffness matrices determining the approximate solution is very fast since no integrals need to be evaluated or approximated. We discuss numerical experiments using monomial basis functions and RADAU 5 time integrator.

Earlier, mixed methods in combination with orthogonal spline collocation methods used to fourth order evolution equations by Li et al. [9], Manickam et al. [12,13], Danumjaya and Pani [3]. In the context of Cahn–Hilliard equation, Elliott et al. [6] discussed a second order splitting combined with lumped mass finite element method and derived optimal error estimates.

We split Eq. (1.1) by setting $v = \gamma u_{xx} - \phi(u)$ then we obtain the following system:

$$u_t + v_{xx} = 0, \quad (x,t) \in I \times (0,T], \tag{1.4}$$

$$\gamma u_{xx} - v - \phi(u) = 0, \quad (x,t) \in I \times (0,T] \tag{1.5}$$

with initial condition

$$u(x,0) = u_0(x), \quad x \in I, \tag{1.6}$$

and the boundary conditions

$$\begin{aligned} u(0,t) = u(1,t) = 0, \quad t \in (0,T], \\ v(0,t) = v(1,t) = 0, \quad t \in (0,T]. \end{aligned} \tag{1.7}$$

We use orthogonal cubic spline collocation method for the system (1.4)–(1.7) in the spatial direction to compute the approximate solutions using monomial basis functions. Let $\{x_i\}_{i=1}^{N+1}$ denote a partition of $\bar{I} = [0,1]$ with

$$\begin{aligned} &0 = x_1 < x_2 < \cdots < x_{N+1} = 1, \\ &I_j = (x_j, x_{j+1}), \quad h_j = x_{j+1} - x_j, \qquad j = 1,2,3,\ldots,N \end{aligned}$$

and

$$h = \max_{1 \leqslant j \leqslant N} h_j.$$

Assume that the partition is quasi-uniform, i.e., there exists a finite positive constant σ such that

$$\max_{1 \leqslant j \leqslant N} \left(\frac{h}{h_j}\right) \leqslant \sigma.$$

We define a finite dimensional subspace $\mathscr{H}_3$ as

$$\mathscr{H}_3 = \{\chi \in C^1(\bar{I}) : \chi|_{\bar{I}_j} \in P_3,\ j = 1,2,\ldots,N \text{ and } \chi(0) = \chi(1) = 0\},$$

where P_3 denotes the set of all cubic polynomials. Let $\{\lambda_k\}_{k=1}^{2}$ denote the roots of the Legendre polynomial of degree 2 i.e., $\left(\lambda_1 = \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right), \lambda_2 = \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right)\right)$. These are the nodes of the 2-point Gaussian quadrature rule on the interval I with corresponding weights $w_k = 1/2$, $k = 1,2$. Now, we define the collocation point

$$\lambda_{jk} = x_j + h_j \lambda_k, \quad j = 1,2,\ldots,N, \ \ k = 1,2.$$

Below, we define discrete innerproduct and its induced norm. For any $\varphi, \psi \in C^0(\bar{I})$, the discrete innerproduct is defined as

$$\langle \varphi, \psi \rangle = \sum_{j=1}^{N} \langle \varphi, \psi \rangle_j,$$

where

$$\langle \varphi, \psi \rangle_j = \frac{h_j}{2} \sum_{k=1}^{2} \varphi(\lambda_{jk})\psi(\lambda_{jk}),$$

and its induced discrete norm by

$$|\varphi|_D = \langle \varphi, \varphi \rangle^{1/2}.$$

Lemma 1.1. *For* $w, z \in \mathscr{H}_3$,

$$-\langle w'', z \rangle = (w', z') + \frac{1}{1080} \sum_{j=1}^{N} w_j^{(3)} z_j^{(3)} h_j^5 = -\langle z'', w \rangle,$$

where $w_j^{(3)}$ (*respectively*, $z_j^{(3)}$), *is the third derivative of* w_j (*respectively*, z_j) *which is constant on each subinterval* I_j.
Note that when $z = w$ *with* $w \in \mathscr{H}_3$, *we have*

$$\|w'\|_{L^2}^2 \leqslant -\langle w'', w \rangle.$$

For a proof of Lemma 1.1, we refer to Douglas and Dupont [4].

The outline of the paper is as follows. In Section 1, we introduce some notations and preliminaries. Section 2 deals with continuous-time orthogonal cubic spline collocation method for the solution of (1.4)–(1.7). We establish optimal error estimates. Finally, Section 3 is devoted to numerical experiments. Here, we show that both theoretical order of convergence and numerically computed order of convergence are same.

Throughout this paper, C denotes a generic positive constant which is independent of the discretization parameter h which may have different values at different places.

2. Continuous-time orthogonal cubic spline collocation method

The continuous-time orthogonal cubic spline collocation approximation to the solution $\{u, v\}$ of (1.4,1.5) is a pair of differentiable maps $\{U, V\} : [0, T] \to \mathscr{H}_3 \times \mathscr{H}_3$ such that for $j = 1, 2, \ldots, N$ and $k = 1, 2$

$$U_t(\lambda_{jk}, t) + V_{xx}(\lambda_{jk}, t) = 0, \quad t \in (0, T], \tag{2.1}$$

$$\gamma U_{xx}(\lambda_{jk}, t) - V(\lambda_{jk}, t) - \phi(U(\lambda_{jk}, t)) = 0, \quad t \in (0, T] \tag{2.2}$$

with appropriate initial approximation $U(0) = U(x, 0)$, which we shall define later. The corresponding discrete Galerkin formulation is written as

$$\langle U_t, \chi \rangle + \langle V_{xx}, \chi \rangle = 0, \quad \chi \in \mathscr{H}_3, \tag{2.3}$$

$$\gamma \langle U_{xx}, \psi \rangle - \langle V, \psi \rangle - \langle \phi(U), \psi \rangle = 0, \quad \psi \in \mathscr{H}_3. \tag{2.4}$$

The consistent initial condition $V(0)$ can be determined from (2.4) by putting $t = 0$, i.e., $V(\cdot, 0)$ satisfies

$$\langle V(x, 0), \psi \rangle = \gamma \langle U_{xx}(x, 0), \psi \rangle - \langle \phi(U(x, 0)), \psi \rangle, \quad \psi \in \mathscr{H}_3. \tag{2.5}$$

Since $\mathscr{H}_3$ is a finite dimensional space, the problem (2.3,2.4) leads to a system of nonlinear differential algebraic equations (DAE's) of index one. The system is solvable [2,8], therefore, the unique solution exists locally. For global existence, i.e., existence of a unique solution on the interval $(0, \infty)$, we need the following *a priori* bounds.

Theorem 2.1. *Let* U *and* V *be the solutions of* (2.3,2.4). *Then there exists a positive constant* C *such that the following inequality holds*:

$$\|U\|_1 \leqslant C(\|U_0\|_2), \quad t > 0. \tag{2.6}$$

Moreover, for $t > 0$

$$\|U(t)\|_{L^\infty} \leqslant C(\|U_0\|_2). \tag{2.7}$$

Proof. We consider the Lyapunov functional

$$\mathscr{F}(U) = \frac{\gamma}{2}|U_x|_D^2 + \langle H(U), 1\rangle, \tag{2.8}$$

where $H'(\cdot) = \phi(\cdot)$. Differentiating (2.8) with respect to t, we obtain

$$\frac{\mathrm{d}\mathscr{F}(U)}{\mathrm{d}t} = \gamma\langle U_x, U_{xt}\rangle + \langle \phi(U), U_t\rangle. \tag{2.9}$$

Choosing $\psi = U_t$ in (2.4), we obtain the following expression:

$$-\gamma\langle U_{xx}, U_t\rangle + \langle V, U_t\rangle + \langle \phi(U), U_t\rangle = 0. \tag{2.10}$$

We note that from Lemma 1.1

$$-\langle U_{xx}, U_t\rangle = (U_x, U_{xt}) + \frac{1}{1080}\sum_{j=1}^{N} U_j^{(3)} U_{j,t}^{(3)} h_j^5, \tag{2.11}$$

and

$$\langle U_x, U_{xt}\rangle = (U_x, U_{xt}) - \frac{1}{720}\sum_{j=1}^{N} U_j^{(3)} U_{j,t}^{(3)} h_j^5. \tag{2.12}$$

Using Eqs. (2.11) and (2.12) we find that

$$-\gamma\langle U_{xx}, U_t\rangle = \gamma\langle U_x, U_{xt}\rangle + \frac{\gamma}{432}\sum_{j=1}^{N} U_j^{(3)} U_{j,t}^{(3)} h_j^5. \tag{2.13}$$

Substituting Eq. (2.13) in (2.10), we arrive at

$$\gamma\langle U_x, U_{xt}\rangle + \frac{\gamma}{432}\sum_{j=1}^{N} U_j^{(3)} U_{j,t}^{(3)} h_j^5 + \langle V, U_t\rangle + \langle \phi(U), U_t\rangle = 0. \tag{2.14}$$

Using Eq. (2.9) in (2.14), we obtain

$$\frac{\mathrm{d}\mathscr{F}(U)}{\mathrm{d}t} + \frac{\gamma}{432}\sum_{j=1}^{N} U_j^{(3)} U_{j,t}^{(3)} h_j^5 + \langle V, U_t\rangle = 0. \tag{2.15}$$

For completing the proof, we need to evaluate the estimate for $\langle V, U_t\rangle$. Setting $\chi = V$ in (2.3) implies that

$$\langle U_t, V\rangle + \langle V_{xx}, V\rangle = 0. \tag{2.16}$$

Substituting Eq. (2.16) in (2.15) and using Lemma 1.1 to obtain

$$\frac{\mathrm{d}\mathscr{F}(U)}{\mathrm{d}t} + \frac{\gamma}{864}\frac{\mathrm{d}}{\mathrm{d}t}\sum_{j=1}^{N} h_j^5 (U_j^{(3)})^2 + \frac{1}{1080}\sum_{j=1}^{N} (V_j^{(3)})^2 h_j^5 = -|V_x|_D^2. \tag{2.17}$$

Integrating the above Eq. (2.17), we get the following expression:

$$\mathscr{F}(U) + \frac{\gamma}{864}\sum_{j=1}^{N} h_j^5 (U_j^{(3)})^2 \leqslant \mathscr{F}(U_0) + \frac{\gamma}{864}\sum_{j=1}^{N} h_j^5 (U_j^{(3)}(0))^2. \tag{2.18}$$

Note that $|U_j^{(3)}(0)| \leqslant C\|U(0)\|_{W^{3,\infty}(I)}$ and using the inverse inequality (for a proof see [1])

$$\|\Phi\|_{W^{3,\infty}(I)} \leqslant Ch^{-3/2}\|\Phi\|_{H^2(I)},$$

we find that

$$\sum_{j=1}^{N} h_j^5 |U_j^{(3)}(0)|^2 \leqslant C\|U(0)\|_2. \tag{2.19}$$

Substituting (2.19) in (2.18) and using the definition of $\mathscr{F}(\cdot)$, we finally obtain

$$|U_x|_D^2 \leqslant C(\|U_0\|_2).$$

Using Poincaré inequality, we find that

$$\|U\|_1 \leqslant C|U|_1 \leqslant C(\|U_0\|_2).$$

An application of Sobolev imbedding theorem yields

$$\|U\|_{L^\infty} \leqslant C(\|U_0\|_2).$$

This completes the rest of the proof. □

2.1. Error estimates

For deriving optimal order error estimates, we construct the intermediate projections as differentiable maps $\{\widetilde{U}, \widetilde{V}\} : [0, T] \to \mathscr{H}_3 \times \mathscr{H}_3$ satisfying

$$\langle (v - \widetilde{V})_{xx}, \chi \rangle = 0, \quad \chi \in \mathscr{H}_3, \tag{2.20}$$

$$\gamma\langle (u - \widetilde{U})_{xx}, \psi \rangle = 0, \quad \psi \in \mathscr{H}_3. \tag{2.21}$$

Let $\eta = u - \widetilde{U}$ and $\rho = v - \widetilde{V}$, then the estimates for η and ρ can be easily estimated. For a proof see [14]. Below, we state the estimates for η and ρ without proof.

Lemma 2.1. *Let $u, v \in C^1(\bar{I})$ be such that $u, v \in H^6(I_j)$, $j = 1, 2, \ldots, N$. Further, let $\widetilde{U}$ and $\widetilde{V}$ be the solutions of (2.21) and (2.20), respectively. Then, for $t \in (0, T]$*

$$|\eta|_D + |\eta_t|_D \leqslant \|\eta\|_{L^\infty(I)} + \|\eta_t\|_{L^\infty(I)} \leqslant Ch^4(\|u\|_{H^6(I)} + \|u_t\|_{H^6(I)}), \tag{2.22}$$

and

$$|\rho|_D + |\rho_t|_D \leqslant \|\rho\|_{L^\infty(I)} + \|\rho_t\|_{L^\infty(I)} \leqslant Ch^4(\|v\|_{H^6(I)} + \|v_t\|_{H^6(I)}). \tag{2.23}$$

We now split the error $e_1 = u - U$ and $e_2 = v - V$ as

$$e_1 = (u - \widetilde{U}) - (U - \widetilde{U}) = \eta - \theta,$$

and

$$e_2 = (v - \widetilde{V}) - (V - \widetilde{V}) = \rho - \xi.$$

We now state and prove the optimal error estimates.

Theorem 2.2. *Let $u \in L^\infty(H^8)$, $u_t \in L^2(H^8)$, $u_0 \in H^8(I)$ and let U, V be the solutions of (2.3) and (2.4). Assume that $U(0) = \widetilde{U}(0)$, then the following estimate holds:*

$$\|u - U\|_{L^\infty(L^2)} + \|v - V\|_{L^\infty(L^2)} \leqslant Ch^4\left(\|u_0\|_{H^8} + \|u\|_{L^\infty(H^8)} + \|u_t\|_{L^2(H^8)}\right). \tag{2.24}$$

Proof. We know the estimates of η, ρ from Lemma 2.1 and for completing the proof, we need to estimate θ and ξ. We take the discrete innerproduct between (1.4) and (1.5) by χ and ψ, respectively and the resulting equations, we subtract from (2.3) and (2.4), respectively and using (2.20) and (2.21), we obtain

$$\langle \theta_t, \chi \rangle + \langle \xi_{xx}, \chi \rangle = \langle \eta_t, \chi \rangle, \quad \chi \in \mathscr{H}_3 \tag{2.25}$$

$$\gamma\langle \theta_{xx}, \psi \rangle - \langle \xi, \psi \rangle = \langle \phi(U) - \phi(u), \psi \rangle + \langle \rho, \psi \rangle, \quad \psi \in \mathscr{H}_3. \tag{2.26}$$

Setting $\chi = \theta$ and $\psi = \xi$ in (2.25) and (2.26), respectively, we obtain

$$\langle \theta_t, \theta \rangle + \langle \xi_{xx}, \theta \rangle = \langle \eta_t, \theta \rangle, \tag{2.27}$$

$$\gamma \langle \theta_{xx}, \xi \rangle - |\xi|_D^2 = \langle \phi(U) - \phi(u), \xi \rangle + \langle \rho, \xi \rangle. \tag{2.28}$$

Multiplying Eq. (2.27) by γ, using Lemma 1.1 for second term on the left hand side and the resulting equation we subtract from (2.28), we arrive at

$$\frac{\gamma}{2} \frac{\mathrm{d}}{\mathrm{d}t} |\theta|_D^2 + |\xi|_D^2 = \gamma \langle \eta_t, \theta \rangle - \langle \phi(U) - \phi(u), \xi \rangle - \langle \rho, \xi \rangle. \tag{2.29}$$

We evaluate the nonlinear term

$$\begin{aligned} |\langle \phi(U) - \phi(u), \xi \rangle| &= |\langle \gamma_2 (U^3 - u^3) + \gamma_1 (U^2 - u^2) + \gamma_0 (U - u), \xi \rangle \\ &= |\langle \gamma_2 ((U - u)(U^2 + Uu + u^2)) + \gamma_1 (U - u)(U + u) + \gamma_0 (U - u), \xi \rangle|. \end{aligned} \tag{2.30}$$

Using the boundedness of $\|u\|_{L^\infty}$ and $\|U\|_{L^\infty}$, the above Eq. (2.30) implies that

$$|\langle \phi(U) - \phi(u), \xi \rangle| \leqslant C |\langle \eta - \theta, \xi \rangle|.$$

Using Cauchy–Schwarz inequality and Young's inequality, we find that

$$|\langle \phi(U) - \phi(u), \xi \rangle| \leqslant C(|\eta|_D^2 + |\theta|_D^2) + \frac{1}{4} |\xi|_D^2. \tag{2.31}$$

Substituting Eq. (2.31) in (2.29) and again using the Cauchy–Schwarz inequality, Young's inequality, we obtain

$$\frac{\gamma}{2} \frac{\mathrm{d}}{\mathrm{d}t} |\theta|_D^2 + \frac{1}{2} |\xi|_D^2 \leqslant C(|\eta|_D^2 + |\eta_t|_D^2 + |\rho|^2) + C|\theta|_D^2. \tag{2.32}$$

Integrating (2.32) with respect to t, it gives the following expression:

$$\gamma |\theta|_D^2 + \int_0^t |\xi|_D^2 \, \mathrm{d}\tau \leqslant C(|\theta(0)|_D^2 + \int_0^t (|\eta|_D^2 + |\eta_t|_D^2 + |\rho|^2) \, \mathrm{d}\tau) + \int_0^t |\theta|_D^2 \, \mathrm{d}\tau. \tag{2.33}$$

If $U(0) = \widetilde{U}(0)$ then $\theta(0) = 0$ and using the Gronwall's inequality, we obtain the estimate for $|\theta|_{L^\infty(L^2)}$. For completing the proof, we need to estimate $|\xi|_{L^\infty(L^2)}$. We now differentiate Eq. (2.26) with respect to t, we obtain

$$\gamma \langle \theta_{txx}, \psi \rangle - \langle \xi_t, \psi \rangle = \langle (\phi(U) - \phi(u))_t, \psi \rangle + \langle \rho_t, \psi \rangle. \tag{2.34}$$

Setting $\chi = \theta_t$ and $\psi = \xi$ in (2.25) and (2.34) respectively, we obtain

$$|\theta_t|_D^2 + \langle \xi_{xx}, \theta_t \rangle = \langle \eta_t, \theta_t \rangle \tag{2.35}$$

$$\gamma \langle \theta_{txx}, \xi \rangle - \frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} |\xi|_D^2 = \langle (\phi(U) - \phi(u))_t, \xi \rangle + \langle \rho_t, \xi \rangle. \tag{2.36}$$

Using Lemma 1.1 in (2.36), multiplying Eq. (2.35) by γ and subtract the resulting equation from (2.36), we arrive at

$$\gamma |\theta_t|_D^2 + \frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} |\xi|_D^2 = \gamma \langle \eta_t, \theta_t \rangle - \langle (\phi(U) - \phi(u))_t, \xi \rangle - \langle \rho_t, \xi \rangle. \tag{2.37}$$

Using Cauchy–Schwarz inequality in (2.37), we obtain

$$\gamma |\theta_t|_D^2 + \frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} |\xi|_D^2 \leqslant \gamma |\eta_t|_D |\theta_t|_D + (|(\phi(U) - \phi(u))_t|_D + |\rho_t|_D) |\xi|_D. \tag{2.38}$$

We evaluate the nonlinear term

$$|(\phi(U) - \phi(u))_t|_D = |\phi'(U) U_t - \phi'(u) u_t|_D. \tag{2.39}$$

Using the boundedness of $\|u\|_{L^\infty}$ and $\|U\|_{L^\infty}$ in (2.39), we find that

$$|(\phi(U)-\phi(u))_t|_D \leqslant C|(\theta-\eta)_t|_D \leqslant C(|\theta_t|_D+|\eta_t|_D). \tag{2.40}$$

Substituting (2.40) in (2.38) and using Young's inequality, we obtain

$$\gamma|\theta_t|_D^2+\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\xi|_D^2 \leqslant C(\gamma)(|\eta_t|_D^2+|\rho_t|_D^2+|\xi|_D^2)+\frac{\gamma}{2}|\theta_t|_D^2+\epsilon|\theta_t|_D^2. \tag{2.41}$$

Integrating (2.41) with respect to t, we get the following expression:

$$(\gamma-2\epsilon)\int_0^t|\theta_t|_D^2\,\mathrm{d}\tau+|\xi|_D^2 \leqslant |\xi(0)|_D^2+C\int_0^t(|\eta_t|_D^2+|\rho_t|_D^2)\,\mathrm{d}\tau+C\int_0^t|\xi|_D^2\,\mathrm{d}\tau. \tag{2.42}$$

In order to estimate $|\xi(0)|_D$, we take $t=0$ in (2.26) and using $\theta(0)=0$, we find

$$|\xi(0)|_D \leqslant |\rho(0)|_D \leqslant Ch^4\|v_0\|_{H^6} \leqslant Ch^4\|u_0\|_{H^8}.$$

Choose ϵ appropriately so that $(\gamma-2\epsilon)>0$ and substituting the estimate $|\xi|_{L^2(L^2)}$ in (2.42), we finally obtain the estimate for $|\xi|_{L^\infty(L^2)}$. This completes the proof. □

3. Numerical experiments

In this section, we use orthogonal cubic spline collocation method to approximate the problem (1.4)–(1.7) and we discuss some numerical results. The approximate solution is defined as a pair of differentiable maps $\{U,V\}:[0,T]\to\mathscr{H}_3\times\mathscr{H}_3$ satisfying (2.1) and (2.2). As in Robinson and Fairweather [14], we use the monomial basis functions to represent U and V, respectively, as

$$U(x,t)=\sum_{l=1}^{4}U_{j,l}(t)\frac{(x-x_j)^{l-1}}{(l-1)!},\quad x\in\bar{I}_j \tag{3.1}$$

and

$$V(x,t)=\sum_{l=1}^{4}V_{j,l}(t)\frac{(x-x_j)^{l-1}}{(l-1)!},\quad x\in\bar{I}_j, \tag{3.2}$$

where,

$$\begin{aligned}&U_{j,1}(t)=U(x_j,t),U_{j,2}(t)=U_x(x_j,t),\\&U_{j,3}(t)=U_{xx}(x_j,t),U_{j,4}(t)=U_{xxx}(x_j,t),\end{aligned}\qquad j=1,2,\ldots,N, \tag{3.3}$$

and similarly for $V_{j,l}$. In order to accommodate the boundary conditions, we define

$$\begin{aligned}&U_{N+1,1}(t)=U(x_{N+1},t),V_{N+1,1}(t)=V(x_{N+1},t),\\&U_{N+1,2}(t)=U_x(x_{N+1},t),V_{N+1,2}(t)=V_x(x_{N+1},t).\end{aligned} \tag{3.4}$$

Using (3.1) and (3.2) in (2.1) and (2.2), we obtain the following system of differential algebraic equations (DAEs):

$$\sum_{l=1}^{4}\dot{U}_{j,l}\frac{(h_j\lambda_k)^{l-1}}{(l-1)!}=-(V_{j,3}+h_j\lambda_kV_{j,4}), \tag{3.5}$$

$$\gamma(U_{j,3}+h_j\lambda_kU_{j,4})-\sum_{l=1}^{4}V_{j,l}\frac{(h_j\lambda_k)^{l-1}}{(l-1)!}-\phi\left(\sum_{l=1}^{4}U_{j,l}\frac{(h_j\lambda_k)^{l-1}}{(l-1)!}\right)=0, \tag{3.6}$$

for $j=1,2,\ldots,N$, $k=1,2$, where $\dot{U}_{j,l}(t)=\frac{\mathrm{d}}{\mathrm{d}t}U_{j,l}(t)$. For computation, we take $\phi(\chi)=\frac{1}{3}\chi^3-\chi$. The C^0 and C^1 continuity conditions on U and V require that for $j=1,2,\ldots,N$

$$\begin{aligned} U_{j+1,1} &= U_{j,1} + h_j U_{j,2} + \frac{h_j^2}{2!} U_{j,3} + \frac{h_j^3}{3!} U_{j,4}, \\ V_{j+1,1} &= V_{j,1} + h_j V_{j,2} + \frac{h_j^2}{2!} V_{j,3} + \frac{h_j^3}{3!} V_{j,4}, \\ U_{j+1,2} &= U_{j,2} + h_j U_{j,3} + \frac{h_j^2}{2!} U_{j,4}, \\ V_{j+1,2} &= V_{j,2} + h_j V_{j,3} + \frac{h_j^2}{2!} V_{j,4}. \end{aligned} \tag{3.7}$$

The boundary conditions (1.7), in view of (3.4) yields

$$\begin{aligned} &U_{1,1} = 0, U_{N+1,1} = 0, \\ &V_{1,1} = 0, V_{N+1,1} = 0. \end{aligned} \tag{3.8}$$

Rewriting Eqs. (3.5)–(3.8) in matrix form, we obtain

$$\mathbf{M}\mathbf{W}' = \mathbf{F}(t, \mathbf{W}), \tag{3.9}$$

which is of order $8N + 4$ with

$$\mathbf{W} = [\mathbf{W}_1^{1\mathrm{T}}, \mathbf{W}_1^{2\mathrm{T}}, \mathbf{W}_2^{1\mathrm{T}}, \mathbf{W}_2^{2\mathrm{T}}, \ldots, \mathbf{W}_N^{1\,\mathrm{T}}, \mathbf{W}_N^{2\,\mathrm{T}}, \mathbf{W}_{N+1}^{1\,\mathrm{T}}]^{\mathrm{T}},$$

where

$$\begin{aligned} &\mathbf{W}_j^1 = [U_{j,1}, V_{j,1}, U_{j,2}, V_{j,2}]^{\mathrm{T}}, \quad \mathbf{W}_j^2 = [U_{j,3}, V_{j,3}, U_{j,4}, V_{j,4}]^{\mathrm{T}}, \qquad j = 1, \ldots, N, \\ &\mathbf{W}_{N+1}^1 = [U_{N+1,1}, V_{N+1,1}, U_{N+1,2}, V_{N+1,2}]^{\mathrm{T}}, \end{aligned}$$

and the singular constant mass matrix $\mathbf{M}$ is of the form

$$\mathbf{M} = \begin{bmatrix} \mathbf{0}_{24} & & & & & & & \\ \mathbf{A}_1 & \mathbf{B}_1 & & & & & & \\ & \mathbf{0}_{44} & & & & & & \\ & & \mathbf{A}_2 & \mathbf{B}_2 & & & & \\ & & & \mathbf{0}_{44} & & & & \\ & & & & \ddots & & & \\ & & & & & \mathbf{A}_N & \mathbf{B}_N & \mathbf{0}_{44} \\ & & & & & & \mathbf{0}_{44} & \mathbf{0}_{44} \\ & & & & & & & \mathbf{0}_{24} \end{bmatrix}. \tag{3.10}$$

Here $\mathbf{A}_j$ and $\mathbf{B}_j$ are 4×4 matrices corresponding to the coefficients of the derivative terms in (3.5) and (3.6) and are of the form

$$\mathbf{A}_j = \begin{bmatrix} 1 & 0 & h_j\lambda_1 & 0 \\ 1 & 0 & h_j\lambda_2 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{B}_j = \begin{bmatrix} \frac{(h_j\lambda_1)^2}{2!} & 0 & \frac{(h_j\lambda_1)^3}{3!} & 0 \\ \frac{(h_j\lambda_2)^2}{2!} & 0 & \frac{(h_j\lambda_2)^3}{3!} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

and 0_{24} and 0_{44} are 2×4 and 4×4 zero matrices, respectively. The initial value $\mathbf{W(0)}$ is found from the intermediate projection (2.21) at $t = 0$ and the consistency condition (2.5). Since $U(0) = \widetilde{U}(0)$ from the assumption of the Theorem 2.2, it follows from (2.21) that:

$$U_{xx}(\lambda_{jk},0)=u_{0xx}(\lambda_{jk}),\quad j=1,\ldots,N,\ \ k=1,2.$$

Now along with the continuity conditions at the interior nodal points x_j and the boundary conditions, we obtain a linear system of $4N+2$ equations

$$\mathbf{RU}=\mathbf{U}_0, \tag{3.11}$$

where $\mathbf{R}$ is $(4N+2)\times(4N+2)$ block diagonal nonsingular matrix of the form

$$\mathbf{R}=\begin{bmatrix} \mathbf{I_1} & & & & & \\ \mathbf{X}_1\mathbf{Y}_1 & \mathbf{0}_{22} & & & & \\ \mathbf{C}_1\mathbf{D}_1 & \mathbf{I}_{22} & & & & \\ & \mathbf{X}_2\mathbf{Y}_2 & \mathbf{0}_{22} & & & \\ & \mathbf{C}_2\mathbf{D}_2 & \mathbf{I}_{22} & & & \\ & & & \ddots & & \\ & & & & \mathbf{X}_N\mathbf{X}_N & \mathbf{0}_{22} \\ & & & & \mathbf{C}_N\mathbf{D}_N & \mathbf{I}_{22} \\ & & & & & \mathbf{I_1} \end{bmatrix}.$$

Here,

$$\mathbf{X}_j=\begin{bmatrix}0&0\\0&0\end{bmatrix},\quad \mathbf{Y}_j=\begin{bmatrix}1&h_j\lambda_1\\1&h_j\lambda_2\end{bmatrix},\quad \mathbf{C}_j=\begin{bmatrix}-1&-h_j\\0&-1\end{bmatrix},\quad \mathbf{D}_j=\begin{bmatrix}-\frac{h_j^2}{2!}&-\frac{h_j^3}{3!}\\-h_j&-\frac{h_j^2}{2!}\end{bmatrix}.$$

I_{22} is the identity matrix of order 2×2, $\mathbf{0}_{22}$ is the zero matrix of order 2×2 and $\mathbf{I_1}=(1,0)$. Further, the vectors $\mathbf{U_0}$ and $\mathbf{U}$ are of the form

$$\mathbf{U}_0=[0,u_{0xx}(\lambda_{11}),u_{0xx}(\lambda_{12}),0,0,u_{0xx}(\lambda_{21}),u_{0xx}(\lambda_{22}),\ldots,u_{0xx}(\lambda_{N1}),u_{0xx}(\lambda_{N2}),0,0,0]^{\mathrm{T}}$$

and

$$\mathbf{U}=[\mathbf{U}_1,\mathbf{U}_2,\ldots,\mathbf{U}_N,\mathbf{U}_{N+1}]^{\mathrm{T}}\in R^{4N+2}$$

with $\mathbf{U}_j=[U_{j,1},U_{j,2},U_{j,3},U_{j,4}]$, $j=1,\ldots,N$ and $\mathbf{U}_{N+1}=[U_{N+1,1},U_{N+1,2}]$. Similarly for $V(x,0)$, we obtain from (2.5)

$$V(\lambda_{jk},0)=\gamma U_{xx}(\lambda_{jk},0)-\phi(U(\lambda_{jk},0)),\quad j=1,\ldots,N,\ \ k=1,2.$$

Along with continuity and boundary conditions yield a system of $4N+2$ equations

$$\widetilde{\mathbf{R}}\mathbf{V}=\mathbf{V}_0, \tag{3.12}$$

where

$$\begin{aligned}\mathbf{V}_0=\Bigg[&0,\gamma(U_{1,3}+h_1\lambda_1U_{1,4})-\frac{1}{3}\left(U_{1,1}+h_1\lambda_1U_{1,2}+\frac{(h_1\lambda_1)^2}{2}U_{1,3}+\frac{(h_1\lambda_1)^3}{6}U_{1,4}\right)^3\\&-\left(U_{1,1}+h_1\lambda_1U_{1,2}+\frac{(h_1\lambda_1)^2}{2}U_{1,3}+\frac{(h_1\lambda_1)^3}{6}U_{1,4}\right),\gamma(U_{1,3}+h_1\lambda_2U_{1,4})\\&-\frac{1}{3}\left(U_{1,1}+h_1\lambda_2U_{1,2}+\frac{(h_1\lambda_2)^2}{2}U_{1,3}+\frac{(h_1\lambda_2)^3}{6}U_{1,4}\right)^3\\&-\left(U_{1,1}+h_1\lambda_2U_{1,2}+\frac{(h_1\lambda_2)^2}{2}U_{1,3}+\frac{(h_1\lambda_2)^3}{6}U_{1,4}\right),0,0,\gamma(U_{2,3}+h_2\lambda_1U_{2,4})\end{aligned}$$

$$
\begin{aligned}
&-\frac{1}{3}\left(U_{2,1}+h_2\lambda_1U_{2,2}+\frac{(h_2\lambda_1)^2}{2}U_{2,3}+\frac{(h_2\lambda_1)^3}{6}U_{2,4}\right)^3\\
&-\left(U_{2,1}+h_2\lambda_1U_{2,2}+\frac{(h_2\lambda_1)^2}{2}U_{2,3}+\frac{(h_2\lambda_1)^3}{6}U_{2,4}\right),\gamma(U_{2,3}+h_2\lambda_2U_{2,4})\\
&-\frac{1}{3}\left(U_{2,1}+h_2\lambda_2U_{2,2}+\frac{(h_2\lambda_2)^2}{2}U_{2,3}+\frac{(h_2\lambda_2)^3}{6}U_{2,4}\right)^3\\
&-\left(U_{2,1}+h_2\lambda_2U_{2,2}+\frac{(h_2\lambda_2)^2}{2}U_{2,3}+\frac{(h_2\lambda_2)^3}{6}U_{2,4}\right),0,0,\ldots,\gamma(U_{N,3}+h_N\lambda_1U_{N,4})\\
&-\frac{1}{3}\left(U_{N,1}+h_N\lambda_1U_{N,2}+\frac{(h_N\lambda_1)^2}{2}U_{N,3}+\frac{(h_N\lambda_1)^3}{6}U_{N,4}\right)^3\\
&-\left(U_{N,1}+h_N\lambda_1U_{N,2}+\frac{(h_N\lambda_1)^2}{2}U_{N,3}+\frac{(h_N\lambda_1)^3}{6}U_{N,4}\right),\gamma(U_{N,3}+h_N\lambda_2U_{N,4})\\
&-\frac{1}{3}\left(U_{N,1}+h_N\lambda_2U_{N,2}+\frac{(h_N\lambda_2)^2}{2}U_{N,3}+\frac{(h_N\lambda_2)^3}{6}U_{N,4}\right)^3\\
&\left.-\left(U_{N,1}+h_N\lambda_2U_{N,2}+\frac{(h_N\lambda_2)^2}{2}U_{N,3}+\frac{(h_N\lambda_2)^3}{6}U_{N,4}\right),0,0,0\right]^{\mathrm{T}},
\end{aligned}
$$

and all the submatrices in $\widetilde{\mathbf{R}}$ are similar to $\mathbf{R}$ in (3.11) except for

$$
\mathbf{X}_j=\begin{bmatrix}1 & h_j\lambda_1\\ 1 & h_j\lambda_2\end{bmatrix},\quad \mathbf{Y}_j=\begin{bmatrix}\frac{(h_j\lambda_1)^2}{2!} & \frac{(h_j\lambda_1)^3}{3!}\\ \frac{(h_j\lambda_2)^2}{2!} & \frac{(h_j\lambda_2)^3}{3!}\end{bmatrix}.
$$

We have solved the Cahn–Hilliard equation mainly to validate the theoretical results. For this purpose, we have used the software packages that are freely available from the web sites.

For the solution of almost block diagonal linear systems (3.11) and (3.12), we have employed the code ABDPACK [10,11]. This code has been especially developed for the solution of the system which arises from the orthogonal spline collocation methods using the monomial basis functions.

Note that the *index* of the system (3.5) and (3.6) is one. We have used RADAU 5, a software package that is based on a three stage implicit Runge–Kutta scheme of RADAU-IIA (see [7]). This numerical scheme is self starting and *stiffly accurate*. The solution obtained using RADAU 5 has order of convergence five in every component. RADAU 5 can also solve DAEs of index upto 3.

Now we describe the numerical experiments that has been conducted for the Cahn–Hilliard equation. For computational convenience, we have considered the space in x direction as $[-1,1]$ instead of $[0,1]$. The numerical experiments are carried out for (1.4)–(1.7) with $\phi(u)=\frac{1}{3}u^3-u$ and using the initial function

$$u(x,0)=-\sin(\pi^2x),\quad x\in(-1,1). \tag{3.13}$$

We divide the domain into $N_i=10,20,40,80$ with each of equal intervals h_i, where

$$h_i=\frac{2}{N_i},\quad i=1,\ldots,4.$$

For computational convenience, we assume $U=U_h$ and $V=V_h$. We note that the exact solution of Cahn–Hilliard equation is not known and we replace it by numerical solution U_h with $N=160$ and treat this U_h as our exact solution. The order of convergence for the numerical method has been computed by the formula

Table 1
The order of convergence for $U_h(x,t)$ at $t = 0.05$

i	N_i	$\|U_h - U_{h_i}\|_{L^2}$	Order	$\|U_h - U_{h_i}\|_{L^\infty}$	Order
1	10	0.1199346780776978E−01		0.2265095710754395E−02	
2	20	0.1012027263641357E−02	3.5669	0.1476407051086426E−03	3.9394
3	40	0.6222724914550781E−04	4.0236	0.9857118129730225E−05	3.9048
4	80	0.3695487976074219E−05	4.0737	0.6016343832015991E−06	4.0342

Table 2
The order of convergence for $V_h(x,t)$ at $t = 0.05$

i	N_i	$\|V_h - V_{h_i}\|_{L^2}$	Order	$\|V_h - V_{h_i}\|_{L^\infty}$	Order
1	10	0.1743271946907043E−02		0.1607790589332581E−02	
2	20	0.1445934176445007E−03	3.5917	0.9499490261077881E−04	4.0811
3	40	0.9037554264068604E−05	3.9999	0.6260350346565247E−05	3.9235
4	80	0.5289912223815918E−06	4.0946	0.3650784492492676E−06	4.1000

$$\text{order} = \frac{\log\left[\frac{\|U_h - U_{h_i}\|_{L^j}}{\|U_h - U_{h_{i+1}}\|_{L^j}}\right]}{\log(2)}, \quad i = 1, 2, \;\; j = 2, \infty, \tag{3.14}$$

where U_{h_i} is the numerical solution with step size h_i and $h_{i+1} = \frac{h_i}{2}$.

All the codes have been written in FORTRAN with double precision. The experiments have been conducted with the following parameter values for RADAU 5: RTOL $= 10^{-6}$, ATOL $= 10^{-5}$ and the initial step size $k = 10^{-5}$. RADAU 5 uses the variable step size method. The maximum step size used in all calculations is

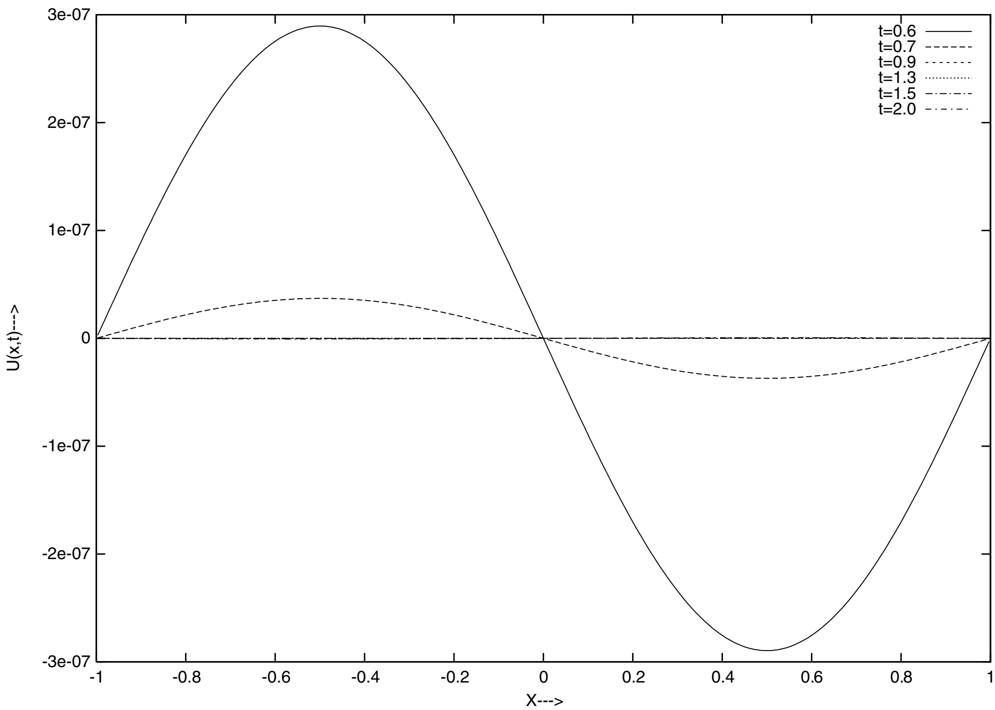

Fig. 1. The profile of $U(x,t)$ for $\gamma = 0.3$.

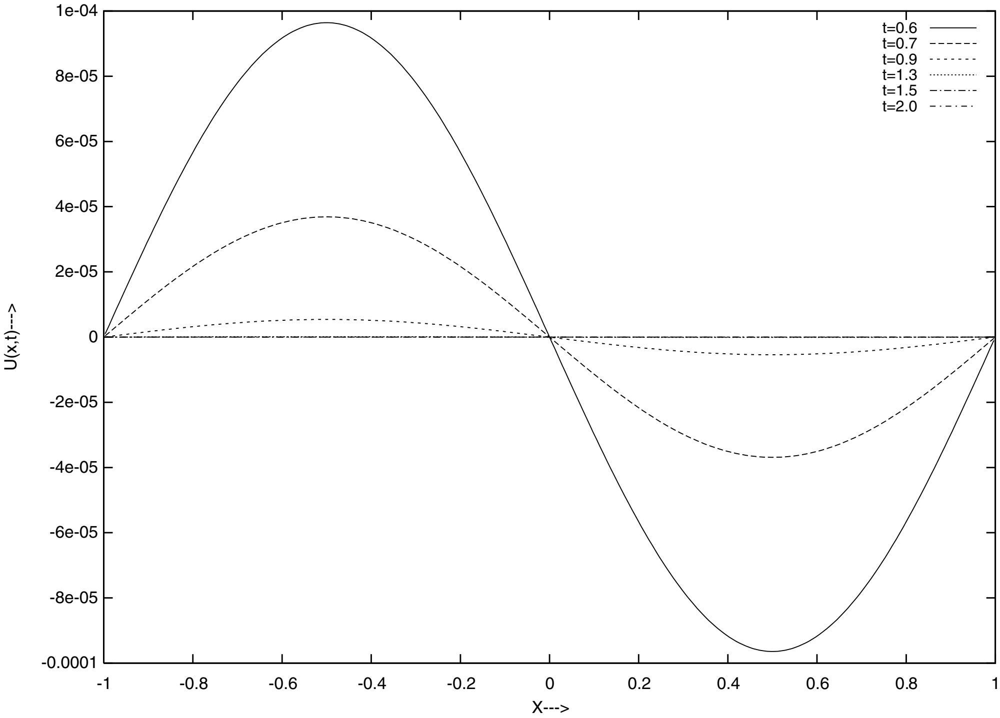

Fig. 2. The profile of $U(x,t)$ for $\gamma = 0.2$.

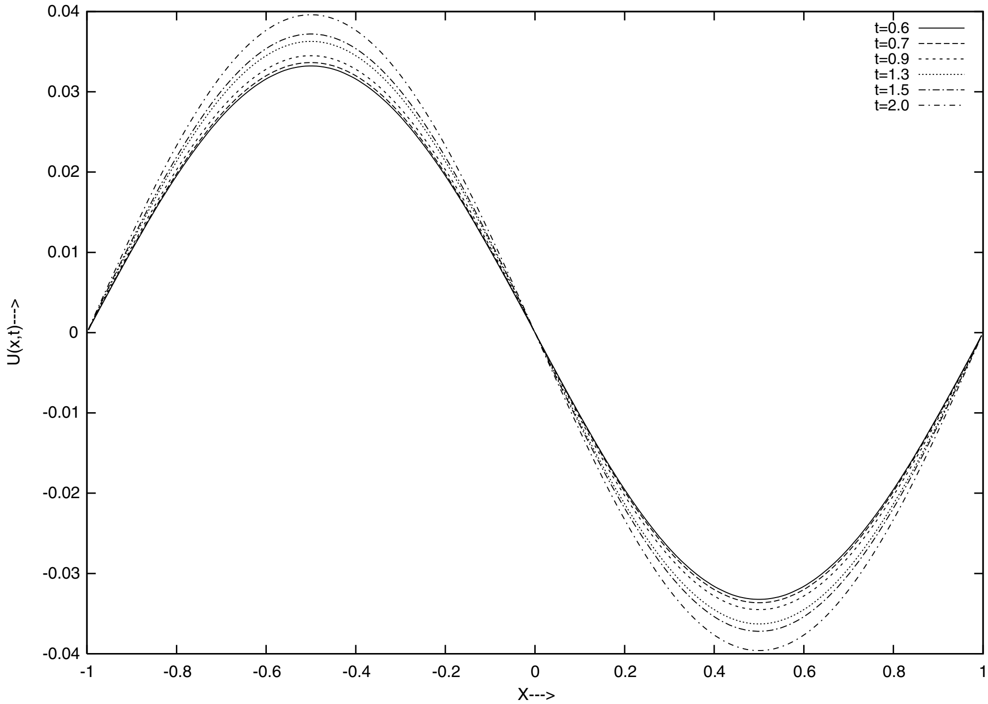

Fig. 3. The profile of $U(x,t)$ for $\gamma = 0.1$.

$k_{\max} = 0.087880501$. The numerical solution is carried out for several h_i with $\gamma = 0.02$. In the following Tables 1 and 2, we observe that the order of convergence estimated numerically is approximately equal to 4. This

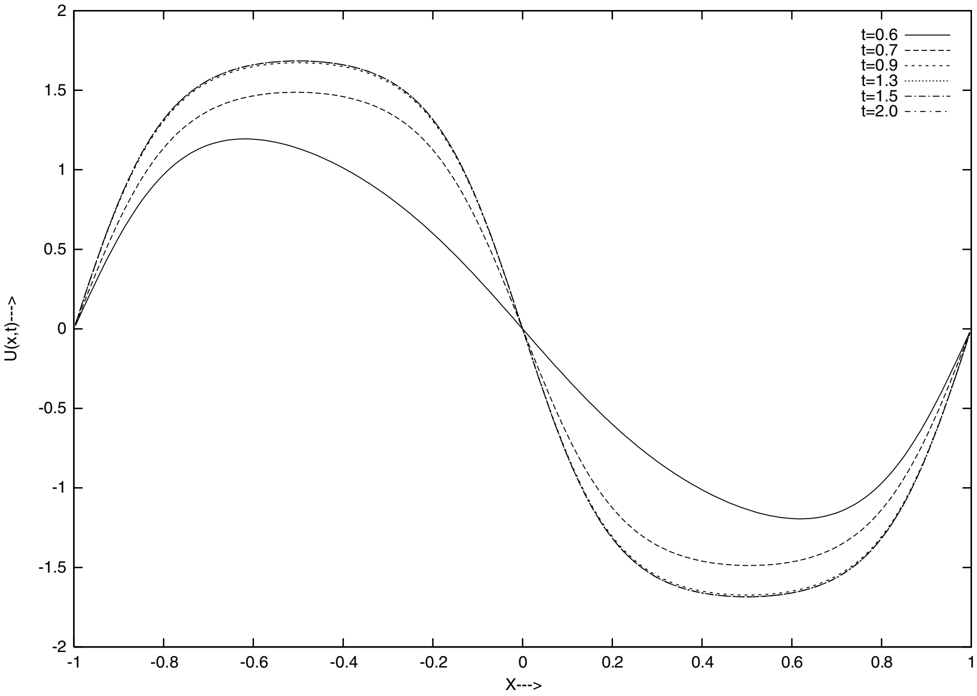

Fig. 4. The profile of $U(x,t)$ for $\gamma = 0.02$.

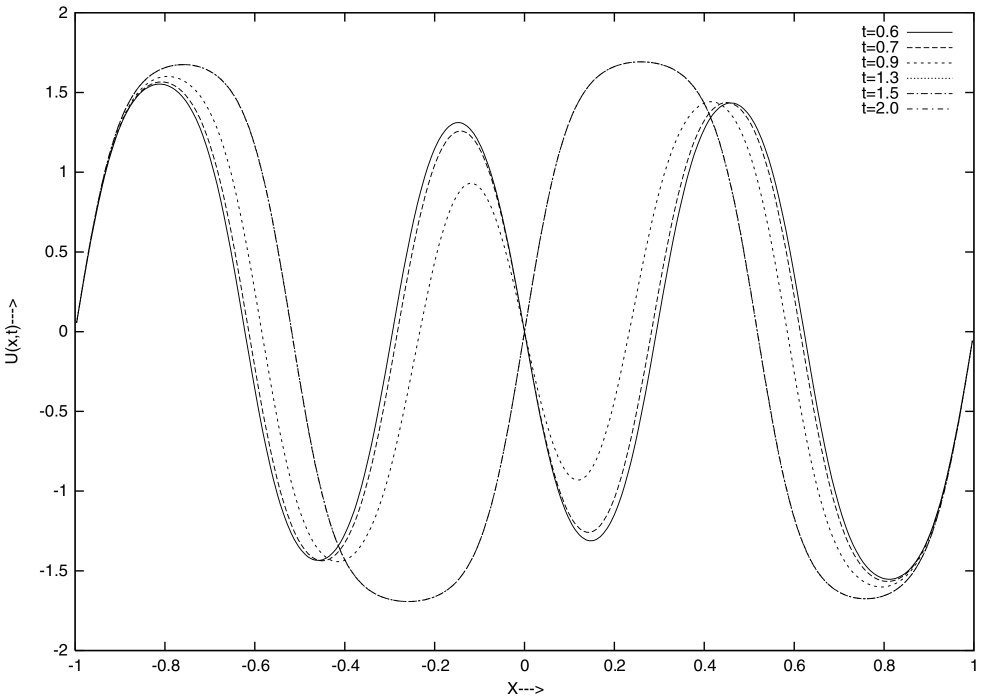

Fig. 5. The profile of $U(x,t)$ for $\gamma = 0.005$.

confirms the theoretical order of convergence found in Theorem 2.2 and hence is equivalent to the numerically computed order of convergence.

For the initial condition (3.13), we show the Figs. 1–5 of computed solutions of U at various time level.

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