Analysis of a scheme which preserves the dissipation and positivity of Gibbs' energy for a nonlinear parabolic equation with variable diffusion

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Abstract

In this work, we design and analyze a discrete model to approximate the solutions of a parabolic partial differential equation in multiple dimensions. The mathematical model considers a nonlinear reaction term and a space-dependent diffusion coefficient. The system has a Gibbs' free energy, we establish rigorously that it is non-negative under suitable conditions, and that it is dissipated with respect to time. The discrete model proposed in this work has also a discrete form of the Gibbs' free energy. Using a fixed-point theorem, we prove the existence of solutions for the numerical model under suitable assumptions on the regularity of the component functions. We prove that the scheme preserves the positivity and the dissipation of the discrete Gibbs' free energy. We establish theoretically that the discrete model is a second-order consistent scheme. We prove the stability of the method along with its quadratic convergence. Some simulations illustrating the capability of the scheme to preserve the dissipation of Gibb's energy are presented.

Keywords: nonlinear diffusion-reaction equation, dissipation of Gibbs' free energy, structure-preserving numerical model, stability and convergence analysis
2010 MSC: 65Mxx, 65Qxx

1. Introduction

There is a great diversity of physical problems modeled by ordinary of partial differential equations with applications in different fields of science and engineering [1]. Those models are usually very difficult to solve analytically and, in most of the cases, it is impossible to provide exact solutions for physically relevant initial-boundary conditions associated to those systems. In those cases, it is necessary to provide numerical models which approximate the solutions of those systems in a reliable way [2]. Moreover, in order to solve those problems numerically, it is important to take into account the qualitative properties of the underlying continuous physical system [3]. More precisely, it is highly desirable to design numerical schemes that reflect the qualitative behavior of the solutions for the original problem [4, 5]. In this sense, the qualitative properties of the numerical integrators are fundamental for the accuracy of the numerical simulations and the reliability of the predictions. Based on these ideas, a research field was started in 1990s for the numerical resolution of both ordinary and partial differential equations, in which the key idea has been to preserve essential properties of the solutions of the mathematical models [6, 7, 8]. Numerical models in this family of methods are called *structure-preserving* techniques, and this area has been a very fruitful avenue of research

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in the numerical analysis of differential equations. For example, some articles report on energy-conserving numerical schemes for the sine-Gordon equation [6], symplectic integrators for Hamiltonian problems [9], conservative and dissipative schemes for the solution of the nonlinear Schrödinger equation [10] and symplectic methods for the same system [11], just to mention some examples [12, 13, 14, 15, 16].

In this work, we consider a general reaction-diffusion equation in which the diffusion is presented in gradient form. The system considered here is spatially multidimensional with a non-constant diffusion coefficient and nonlinear reaction law. Various particular models from the physical sciences are generalized by the system investigated in this manuscript, including the well known Fisher–Kolmogorov–Petrovskii–Piscounov equation from population dynamics [17, 18], the Newell–Whitehead–Segel equation [19, 20, 21] and the Zeldovich equation from combustion theory [22]. We will consider initial conditions and homogeneous Dirichlet data on the boundary of a closed and bounded spatial domain. The initial-boundary-value problem studied here has associated a Gibbs' free energy functional [23], and we will show that this functional is dissipated with respect to time. Motivated by this fact, we propose a nonlinear, two-step, implicit finite-difference discretization to approximate the solutions of the nonlinear partial differential equation along with a discrete form of the Gibbs' free energy. In a first stage, we show theoretically that the numerical model is solvable by using a suitable fixed-point theorem [24], and we establish later that the discrete Gibbs' free energy is dissipated with respect to the discrete time. This feature of our numerical method establishes the structure-preserving nature of our discretization. Moreover, inspired by the proof of this last property, we employ a suitable form of the discrete energy method [25] to prove rigorously the stability and the convergence of our scheme. We show that, under suitable regularity assumptions on the solutions of the continuous model, the discrete model has a second-order consistency in both space and time. In addition, the finite-difference method is convergent of second order.

This manuscript is organized as follows. In Section 2, we present the initial-boundary-value problem governed by the nonlinear partial differential equation of interest. We also prove in this section that the Gibbs' free energy function of the continuous problem dissipates through time. In Section 3, we introduce the discrete nomenclature employed throughout this work, and present the finite-difference scheme to approximate the solution of the continuous problem. We prove the solubility of the numerical model using Brouwer's fixed-point theorem. Afterwards, we introduce a discrete form of the continuous Gibbs' free energy function, and we prove a discrete analogue of the theorem on the dissipation of energy of the continuous system. It is worth pointing out that the proof is carried out using a form of the energy method. Section 4 is devoted to studying the main numerical properties of the proposed numerical scheme. More concretely, we prove the properties of consistency of second order, stability and quadratic convergence of our numerical method. The unique solubility of our scheme will be proved therein, too. Some simulations will be provided in that section to illustrate the fact that the numerical model is capable to preserve the dissipation of Gibbs' free energy. This work will close summarizing the main conclusions of our study.

2. Preliminaries

We provide a fresh start by letting I_k represent the set $\{1, \ldots, k\}$, for each $k \in \mathbb{N}$. In addition, let us assume that $\overline{I}_k = I_k \cup \{0\}$, for each $k \in \mathbb{N}$. Throughout, we let $d \in \mathbb{N}$ be a number which physically represents the number of spatial dimensions. We define $a_i, b_i \in \mathbb{R}$ in such way that the inequality $a_i < b_i$ holds, for every $i \in I_d$. For the remainder of this work, we set $\boldsymbol{B} = \Pi_{i=1}^d (a_i, b_i) \subseteq \mathbb{R}^d$ and $\boldsymbol{B}_T = \Pi_{i=1}^d (a_i, b_i) \times (0, T)$, where $T \in \mathbb{R}^+$. Let $F : \mathbb{R} \to \mathbb{R}$ and $a, u_0 : \boldsymbol{B} \to \mathbb{R}$ be sufficiently smooth functions, and let us assume that a and u_0 are both strictly positive over all the spatial domain $\boldsymbol{B}$. In this work, we study the initial-boundary-value problem

$$\begin{aligned} &\frac{\partial u(x,t)}{\partial t} - \triangledown \cdot \left(a^2(x) \triangledown u(x,t) \right) + F'(u(x,t)) = 0, \quad \forall (x,t) \in \boldsymbol{B}_T, \\ &\text{such that } \begin{cases} u(x,0) = u_0(x), & \forall x \in \overline{\boldsymbol{B}}, \\ u(x,t) = 0, & \forall (x,t) \in \partial \boldsymbol{B} \times (0,T). \end{cases} \end{aligned} \tag{2.1}$$

Here, we assume that $x = (x_1, \ldots, x_d) \in \boldsymbol{B}$, and that $\triangledown$ represents the classical gradient operator on the spatial variables.

It is worth pointing out that the mathematical model (2.1) is a generalized form of the classical diffusion-reaction equation. In that case, $a^2(x)$ represents the variable diffusion coefficient, the partial derivative with respect to t is the local rate of change of the solution u, the term $\triangledown \cdot (a^2(x) \triangledown u(x,t))$ is the diffusion term, and $F'(u(x,t))$ is a nonlinear component representing the effect of reaction or sorption. Particular forms of this parabolic differential equation appear as several diffusive models, depending on the specific expressions of a and F. For example, if we consider that $a^2(x) = 1$ and $F'(u) = u(1 - u^2)$, then we obtain the Newell–Whitehead–Segel equation, or the amplitude equation which describes the thermal convection of a fluid [22]. If we consider $F'(u) = u^2(1-u)$ we would obtain the Zeldovich equation, common in combustion theory [26, 27]. In any case and under the assumptions imposed on this model, it is well known that the general system (2.1) possesses a Gibbs' free energy function given by

$$\mathcal{E}(t) = \int_{B} \left[\frac{1}{2} |a \triangledown u(x,t)|^2 + F(u(x,t)) \right] dx \quad \forall t \in [0,T]. \tag{2.2}$$

Moreover, we will check that this functional dissipates with time. However, we will provide firstly an equivalent expression for the Gibbs' free energy of the mathematical model (2.1).

Lemma 2.1 (Non-negativity of energy)**.** *The Gibbs' free energy function* (2.2) *can be rewritten equivalently as*

$$\mathcal{E}(t) = \frac{1}{2} \|a \triangledown u\|_{x,2}^2 + \langle F(u), 1 \rangle_x \tag{2.3}$$

for each $t \in [0,T]$. Moreover, if F is non-negative, then $\mathcal{E}(t) \geq 0$, for each $t \in (0,T)$. □

The next theorem is the analytical cornerstone for designing numerical models that preserves the dissipation of Gibbs' free energy for system (2.1). Its proof hinges on differentiating each term on the right-hand side of (2.2).

Theorem 2.2 (Dissipation of energy)**.** *If u satisfies the initial-boundary-value problem* (2.1)*, then the associated Gibbs' free energy is dissipated through time.*

Proof. By differentiating each term on the right-hand side of (2.2), we readily reach the next identities:

$$\frac{d}{dt}\frac{1}{2} \|a \triangledown u\|_{x,2}^2 = -\left\langle \triangledown \cdot \left(a^2(x) \triangledown u(x,t) \right), \frac{\partial u}{\partial t} \right\rangle_x, \quad \forall t \in (0,T), \tag{2.4}$$

$$\frac{d}{dt} \langle F(u), 1 \rangle_x = \left\langle F'(u), \frac{\partial u}{\partial t} \right\rangle_x, \quad \forall t \in (0,T). \tag{2.5}$$

Using these equations and the fact that u satisfies (2.1), it follows that

$$\begin{aligned} \mathcal{E}'(t) &= -\left\langle \triangledown \cdot \left(a^2(x) \triangledown u(x,t) \right), \frac{\partial u}{\partial t} \right\rangle_x + \left\langle F'(u), \frac{\partial u}{\partial t} \right\rangle_x \\ &= -\left\langle \frac{\partial u}{\partial t}, \frac{\partial u}{\partial t} \right\rangle_x = -\left\| \frac{\partial u}{\partial t} \right\|_{x,2}^2, \quad \forall t \in (0,T). \end{aligned} \tag{2.6}$$

It follows that $\mathcal{E}'(t) \leq 0$, for each $t \in (0,T)$. As a consequence, $\mathcal{E}(t) \leq \mathcal{E}(0)$, for all $t \in (0,T)$. We conclude that the Gibbs' free energy of the system (2.1) is dissipated throughout time, as desired. □

In the following section, we will propose an implicit numerical model to approximate the solutions of (2.1) along with a numerical approximation for the associated Gibbs' free energy function. In addition, we will prove the existence of numerical solutions using a fixed-point theorem. Our numerical technique will satisfy discrete versions of Theorem 2.2, along with the numerical properties of consistency, stability and convergence. It is important to mention that the uniqueness of solutions will be a consequence of the stability of the system.

3. Numerical method

For the remainder of this manuscript, let us assume that τ and h_i are positive step-sizes, for each $i \in I_d$. Moreover, for each $i \in I_d$, let $K = T/\tau$ and $M_i = (b_i - a_i)/h_i$, and suppose that those constants are all positive integers. Consider uniform partitions of the intervals $[a_i, b_i]$ and $[0,T]$, each one given

$$x_{i,j_i} = a_i + j_i h_i, \quad \forall i \in I_d, \forall j_i \in \overline{I}_{M_i}, \tag{3.1}$$

$$t_k = k\tau, \quad \forall k \in \overline{I}_K, \tag{3.2}$$

respectively. As it is usual in uniform discretizations for multi-dimensional finite-difference methods, we define the multi-index sets $J = \prod_{i=1}^{d} I_{M_i-1}$ and $\overline{J} = \prod_{i=1}^{d} \overline{I}_{M_i}$, and let ∂J represent the boundary of the multi-indexes $\overline{J}$. Let us agree that $x_j = (x_{1,j_1}, \dots, x_{d,j_d})$ for each multi-index $j = (j_1, \dots, j_d) \in \overline{J}$. In this manuscript, the notation U_j^k will represent a computational estimate for the exact value of $u_j^k = u(x_j, t_k)$, for each $(j,k) \in \overline{J} \times \overline{I}_K$.

For any grid function V, define the following discrete (difference) linear operators, for each $(j,k) \in J \times \overline{I}_{K-1}$:

$$\mu_t V_j^{k+1} = \frac{V_j^{k+1} + V_j^k}{2}, \tag{3.3}$$

$$\delta_t V_j^{k+1} = \frac{V_j^{k+1} - V_j^k}{\tau}, \tag{3.4}$$

$$\delta_{x_i} V_j^{k+1} = \frac{V_{j_1,\dots,j_{i-1},j_i,j_{i+1},\dots,j_{M_i}}^{k+1} - V_{j_1,\dots,j_{i-1},j_i-1,j_{i+1},\dots,j_{M_i}}^{k+1}}{h}, \quad \forall i \in I_d, \tag{3.5}$$

$$\delta_{V,t} F(V_j^{k+1}) = \begin{cases} \dfrac{F(V_j^{k+1}) - F(V_j^k)}{V_j^{k+1} - V_j^k}, & \text{if } V_j^{k+1} \neq V_j^k, \\ F'(V_j^k), & \text{if } V_j^{k+1} = V_j^k. \end{cases} \tag{3.6}$$

In addition, we introduce the vector $\nabla_h V_j^k = (\delta_{x_1} V_j^k, \delta_{x_2} V_j^k, \dots, \delta_{x_d} V_j^k)$. With this nomenclature, the discrete model to calculate the solution of the initial-boundary-value problem (2.1) on $\boldsymbol{B}_T$ is given by

$$\begin{gathered} \delta_t U_j^{k+1} - \nabla_h \cdot \left(a_{j-\frac{1}{2}}^2 \, \nabla_h \, \mu_t U_{j-1}^{k+1} \right) + \delta_{U,t} F(U_j^{k+1}) = 0, \quad \forall (j,k) \in J \times I_{K-1}, \\ \text{such that } \begin{cases} U_j^0 = u_0(x_j), & \forall j \in \overline{J}, \\ U_j^k = 0, & \forall (j,k) \in \partial J \times \overline{I}_K. \end{cases} \end{gathered} \tag{3.7}$$

Generally, notice that this scheme is an implicit nonlinear two-step method whose implementation will require the use of a fixed-point technique. Our first step in the theoretical analysis of the numerical scheme (3.7) is the determination on the existence of solutions. To that end, we will need to introduce some additional notation.

For the sequel, we will employ the computational parameters $h = (h_1, \dots, h_d)$ and $h_* = \prod_{i=1}^{d} h_i$, and introduce the spatial mesh $R_h = \{x_j\}_{j \in J} \subseteq \mathbb{R}^d$. Let $\mathcal{V}_h$ be the set of grid functions on R_h which are equal to zero on the boundary, considered as a vector space over the real numbers. For any $W \in \mathcal{V}_h$ and $j \in I$, let us agree that $V_j = V(x_j)$. Moreover, define the inner product $\langle \cdot, \cdot \rangle : \mathcal{V}_h \times \mathcal{V}_h \to \mathbb{R}$ and the norm $\| \cdot \|_1 : \mathcal{V}_h \to \mathbb{R}$, respectively, by

$$\langle U, V \rangle = h_* \sum_{j \in I} U_j V_j, \tag{3.8}$$

$$\|U\|_1 = h_* \sum_{j \in I} |U_j|, \tag{3.9}$$

for any $U, V \in \mathcal{V}_h$. We use $\| \cdot \|_2$ to represent the Euclidean norm induced by $\langle \cdot, \cdot \rangle$. In the following, we will represent the solutions of the finite-difference method (3.7) by $(U^k)_{k=0}^K$, where we convey that $U^k = (U_j^k)_{j \in J}$, for each $k \in \overline{I}_K$.

The following result will be crucial to prove the existence of solutions for the numerical model (3.7).

Lemma 3.1 (Brouwer's fixed-point theorem [28]). *Let $\mathcal{V}_{\mathbb{R}}$ be a finite-dimensional vector space, and $\langle \cdot, \cdot \rangle$ an inner product on $\mathcal{V}$. Suppose that $f : \mathcal{V}_{\mathbb{R}} \to \mathcal{V}_{\mathbb{R}}$ is continuous, and that there is some $\lambda > 0$ such that $\langle f(W), W \rangle \geq 0$, for each $W \in \mathcal{V}$ with $\|W\| = \lambda$. There exists some $W \in \mathcal{V}$ with $\|W\| \leq \lambda$, satisfying $f(W) = 0$.*

For each $W \in \mathcal{V}_h$ and $j \in J$, we will employ the following discrete operator:

$$\delta_{W,U,t} F_j^k(W) = \begin{cases} \dfrac{F(W_j) - F(U_j^k)}{W_j - U_j^k}, & \text{if } W_j \neq U_j^k, \\ F'(U_j^k), & \text{if } W_j = U_j^k. \end{cases} \tag{3.10}$$

Let us define the vector $\delta_{w,u,t} F^k(w) = (\delta_{w,u,t} F_j^k(w))_{j \in J}$. Note that $\delta_{w,v,t} F^k(w)$ is a continuous operator on $\mathcal{V}_h$ in case that F is a continuously differentiable function.

Theorem 3.2 (Solubility)**.** *If $a \in L^\infty(\boldsymbol{B})$, $F \in C^2(\mathbb{R})$ and $F'' \in L^\infty(\mathbb{R})$, then the numerical model (3.7) is solvable for any set of initial conditions.*

Proof. We will proceed by induction. Beforehand, notice that the initial approximation is determined by the initial data of problem (3.7), so let us suppose that the solution of (3.7) at the time $k \in \overline{I}_{K-1}$ has been calculated. Let us define the function $f : \mathcal{V}_h \to \mathcal{V}_h$ as

$$f(W)_j = \frac{W_j - U_j^k}{\tau} - \nabla_h \cdot \left(a^2_{j-\frac{1}{2}} \nabla_h \left(\frac{W_{j-1} + U^k_{j-1}}{2} \right) \right) + \delta_{W,U,t} F^k_j(W), \quad \forall W \in \mathcal{V}_h. \tag{3.11}$$

After some calculations, using the Cauchy–Schwarz inequality and the smoothness and boundedness of the functions a and F, it is possible to check that there exist non-negative constants A and L which depend only on U^k, such that

$$\begin{aligned}
\langle f(W), W \rangle &= \frac{1}{\tau} \left(\|W\|^2 - \langle U^k, W \rangle \right) - \frac{1}{2} \left(-\|a \nabla_h W\|^2 + \langle \nabla_h a^2_{j-\frac{1}{2}} \nabla_h U^k, W \rangle \right) + \langle \delta_{W,U,t} F^k(W), W \rangle \\
&\geq \frac{1}{\tau} \left(\|W\|^2 - \|U^k\| \|W\| \right) - \frac{1}{2} \| \nabla_h a^2_{j-\frac{1}{2}} \nabla_h U^k \| \|W\| - L\|W\| \\
&\geq \frac{1}{\tau} \left(\|W\|^2 - \|U^k\| \|W\| \right) - \frac{1}{2} A \|W\| - L\|W\| = \frac{1}{\tau} \|W\| \left(\|W\| - \|U^k\| - \frac{\tau}{2} A - \tau L \right) \\
&= \frac{1}{\tau} \|W\| \left(\|W\| - \lambda \right).
\end{aligned} \tag{3.12}$$

Here, $\lambda = \|u^k\| + \frac{\tau}{2} A + \tau L$. Using Brouwer's fixed-point theorem, it follows that there exists some $U^{k+1} \in \mathcal{V}_h$ which satisfies the finite-difference scheme (3.7). The conclusion of this theorem follows by mathematical induction. $\square$

Finally, we will propose a discrete version of Gibbs' free energy function for the finite-difference method (3.7), in such a way that it satisfies a discrete form of Theorem (2.2). The next standard result will be used to that end.

Lemma 3.3. *If $i \in I_d$ and $U, V \in \mathcal{V}_h$, then $\left\langle -\delta^2_{x_i} U, V \right\rangle = \langle \delta_{x_i} U, \delta_{x_i} V \rangle$.* $\square$

The next theorem establishes the dissipation of the discrete system (3.7).

Theorem 3.4 (Discrete dissipation of energy)**.** *Let $(U^k)_{k=0}^K$ be a solution of (3.7), and define*

$$E^k = \frac{1}{2} \|a \nabla_h U^k\|_2^2 + \left\langle F(U^k), 1 \right\rangle, \quad \forall k \in I_{K-1}. \tag{3.13}$$

Then $\delta_t E^k = -\|\delta_t U^k\|_2^2$, for each $k \in I_{K-1}$. Additionally, $E^k \geq 0$ for each $k \in I_{K-1}$, if F is non-negative.

Proof. For each $(j,k) \in J \times I_{K-1}$, let Θ^k_j represent the left-hand side of the difference equation in (3.7), and define the finite sequence $\Theta^k = (\Theta^k_j)_{j \in J}$. Recall that $(U^k)_{k=0}^K$ is a solution of the numerical model (3.7). After we calculate the inner product of Θ^k with $\delta_t u^k$, and doing some algebraic calculations, we obtain that

$$\begin{aligned}
0 = \langle \Theta^k, \delta_t u^k \rangle &= \left\langle \delta_t u^k - \nabla_h \left(a^2 \nabla_h \mu_t u^k \right) + \delta_{u,t} F(u^k), \delta_t u^k \right\rangle \\
&= \left\langle \delta_t u^k, \delta_t u^k \right\rangle + \left\langle a \nabla_h \mu_t u^k, a \nabla_h \delta_t u^k \right\rangle + \left\langle \delta_{u,t} F(u^k), \delta_t u^k \right\rangle \\
&= \|\delta_t u^k\|_2^2 + \frac{1}{2} \delta_t \|a \nabla_h u^k\|_2^2 + \delta_t \left\langle F(u^k), 1 \right\rangle \\
&= \|\delta_t u^k\|_2^2 + \delta_t E^k, \quad \forall k \in I_{K-1}.
\end{aligned} \tag{3.14}$$

It readily follows that $\delta_t E^k = -\|\delta_t u^k\|_2^2$, for each $k \in I_{K-1}$. The second part of the conclusion is obvious. $\square$

In light of this last result, we conclude that the method is an energy-dissipative technique. In that sense, this technique falls inside the class of structure-preserving methods for partial differential equations. Next, we will prove the consistency, the stability and the convergence of the finite-difference scheme (3.7).

4. Numerical results

Now we will provide the proofs for the main numerical properties of the method (3.7), namely, the consistency, the stability and the convergence of the scheme. Firstly, we prove that the numerical model is a second-order consistent technique. The following continuous function will help to that end:

$$\mathcal{L}u(x,t) = \frac{\partial u(x,t)}{\partial t} - \nabla \cdot \left(a^2(x) \nabla u(x,t)\right) + F'(u(x,t)), \quad \forall (x,t) \in \boldsymbol{B}_T. \tag{4.1}$$

We also define the discrete functional

$$Lu_j^k = \delta_t u_j^k - \nabla_h \cdot \left(a^2_{j-\frac{1}{2}} \nabla_h \mu_t u_{j-1}^k\right) + \delta_{u,t} F(u_j^k), \quad \forall (j,k) \in J \times I_{K-1} \tag{4.2}$$

Theorem 4.1 (Consistency)**.** *If $u \in C^{4,3}_{x,t}(\overline{\boldsymbol{B}_T})$, a is continuous and $F(u)$ is continuously differentiable and bounded, then there exists a constant $C \geq 0$ which is independent of h and τ, such that*

$$\left|Lu(x_j,t_k) - \mathcal{L}u(x,t)\right| \leq C(\tau^2 + \|h\|_2^2), \quad \forall (j,k) \in J \times I_{K-1}. \tag{4.3}$$

Proof. We proceed as typically by using Taylor's Theorem. Under the hypotheses of continuous differentiability and boundedness, there are constants $C_1, C_2, C_3 \in \mathbb{R}$ with are independent of H and τ, with the properties that

$$\left|\delta_t u_j^k - \frac{\partial}{\partial t}(x_j, t_{k+\frac{1}{2}})\right| \leq C_1 \tau^2, \quad \forall (j,k) \in J \times I_{K-1}, \tag{4.4}$$

$$\left|\nabla_h \left(a^2_{j-\frac{1}{2}} \nabla_h \mu_t u_{j-1}^k\right) - \nabla \cdot \left(a^2(x) \nabla u(x_j, t_{k+\frac{1}{2}})\right)\right| \leq C_2(\tau^2 + \|h\|_2^2), \quad \forall (j,k) \in J \times I_{K-1}, \tag{4.5}$$

$$\left|\delta_{u,t} F(u_j^k) - F'(u(x_j, t_{k+\frac{1}{2}}))\right| \leq C_3 \tau^2, \quad \forall (j,k) \in J \times I_{K-1}. \tag{4.6}$$

The desired inequality of this theorem is reached after using the triangle inequality, to obtain a constant $C \geq 0$ which depends only on C_i, for $i \in I_3$. As a consequence, C is independent of τ and h, as desired. □

The next step in our investigation is to prove the stability and convergence of the finite-difference scheme (3.7). To that end, we will require the following discrete version of Gronwall's inequality.

Lemma 4.2 (Pen-Yu [29])**.** *Let $(\omega^k)_{k=0}^K$ and $(\rho^k)_{k=0}^K$ be finite sequences of non-negative mesh functions, and suppose that there exists $C_0 \geq 0$ such that*

$$\omega^{n+1} \leq \rho^{n+1} + C_0 \tau \sum_{k=0}^{n} \omega^k, \quad \forall n \in I_{K-1}. \tag{4.7}$$

Then $\omega^k \leq \rho^k e^{C_0 k \tau}$ for each $k \in \overline{I}_K$. □

The first step for the stability Theorem is to consider two sets of solutions for the finite-difference model (3.7) corresponding to two different sets of initial data. More precisely, U will denote a solution of the discrete scheme (3.7), while $\tilde{U}$ will denote a solution of the discrete initial-boundary-value problem

$$\begin{aligned} &\delta_t \tilde{U}_j^{k+1} - \nabla_h \cdot \left(a^2_{j-\frac{1}{2}} \nabla_h \mu_t \tilde{U}_{j-1}^{k+1}\right) + \delta_{\tilde{U},t} F(\tilde{U}_j^{k+1}) = 0, \quad \forall (j,k) \in J \times I_{K-1}, \\ &\text{such that } \begin{cases} \tilde{U}_j^0 = \tilde{u}_0(x_j), & \forall j \in \overline{J}, \\ \tilde{U}_j^k = 0, & \forall (j,k) \in \partial J \times \overline{I}_K. \end{cases} \end{aligned} \tag{4.8}$$

Here, $\tilde{u}_0 : \overline{\boldsymbol{B}} \to \mathbb{R}$ is a function. We also consider the discrete operator $\tilde{F}_j^{k+1} = \delta_{u,t} F(u_j^{k+1}) - \delta_{\tilde{u},t} F(\tilde{u}_j^{k+1})$, for each $(j,k) \in \partial J \times \overline{I}_K$. The proofs of stability and convergence of the numerical model will hinge on the next lemma.

Lemma 4.3. *Let $F \in C^2(\mathbb{R})$ and $F'' \in L^\infty(\mathbb{R})$, and suppose that $(\epsilon^k)_{k=0}^K$, and $(R^k)_{k=0}^K$ are sequences in $\mathcal{V}_h$. Then the following are satisfied, for each $k \in I_{K-1}$:*

(a) $\|\tilde{F}^{k+1}\|_2^2 \leq 2(\|\epsilon^{k+1}\|_2^2 + \|\epsilon^k\|_2^2)$.
(b) $\langle \delta_t \epsilon^k, 2\mu_t \epsilon^k \rangle = \delta_t \|\epsilon^{k-1}\|_2^2$.
(c) $\langle -\nabla_h \left(a^2 \nabla_h \mu_t \epsilon^k\right), 2\mu_t \epsilon^k \rangle = 2\|a \nabla_h \mu_t \epsilon^k\|_2^2$.
(d) $\displaystyle\sum_{k=1}^{n} \left|\langle \tilde{F}^k, 2\mu_t \epsilon^k \rangle\right| \leq \frac{5}{2}\left(\|\epsilon^n\|_2^2 + \|\epsilon^0\|_2^2\right) + 5\sum_{k=1}^{n-1} \|\epsilon^k\|_2^2$.
(e) $\displaystyle\sum_{k=1}^{n-1} \left|\langle R^k, 2\mu_t \epsilon^k \rangle\right| \leq \frac{1}{2}\left(\|\epsilon^n\|_2^2 + \|\epsilon^0\|_2^2\right) + \sum_{k=1}^{n-1} \left(\|\epsilon^k\|_2^2 + \|R^k\|_2^2\right)$.

Proof. Property (a) is a direct result of the mean value theorem and the fact that the solution of the system exists. We obtain (b) and (c) from the definition of the discrete operators and after some algebraic manipulation. To prove (d) now, we firstly make use of (a) to obtain

$$\left|\langle \tilde{F}^k, 2\mu_t \epsilon^k \rangle\right| \leq \|\tilde{F}^k\|_2^2 + \|\mu_t \epsilon^k\|_2^2 \leq \frac{5}{2}\left(\|\epsilon^k\|_2^2 + \|\epsilon^{k-1}\|_2^2\right). \tag{4.9}$$

Then take the sum from k from 1 to n. In such way, we reach the inequalities

$$\sum_{k=1}^{n} \left|\langle \tilde{F}^k, 2\mu_t \epsilon^k \rangle\right| \leq \frac{5}{2}\sum_{k=1}^{n}\left(\|\epsilon^k\|_2^2 + \|\epsilon^{k-1}\|_2^2\right) \leq \frac{5}{2}\left(\|\epsilon^n\|_2^2 + \|\epsilon^0\|_2^2\right) + 5\sum_{k=1}^{n-1} \|\epsilon^k\|_2^2 \tag{4.10}$$

which is what we wanted to prove. The proof of identity (e) is similar to (d) and we omit it for that reason. □

Theorem 4.4 (Stability)**.** *Let $a \in L^\infty(\boldsymbol{B})$, $F \in C^2(\mathbb{R})$ and $F'' \in L^\infty(\mathbb{R})$, and suppose that U and $\tilde{U}$ are solutions of problems (3.7) and (4.8), respectively. Define $\epsilon^k = U^k - \tilde{U}^k$, for each $k \in \overline{I}_K$. If $\tau < \frac{1}{4}$, then the inequality $\|\epsilon^k\|_2^2 \leq \left(1 + \frac{5\tau}{2}\right)\|\epsilon^0\|_2^2 e^{5k\tau}$ holds, for each $k \in \overline{I}_K$.*

Proof. Beforehand, notice that Theorem 3.2 guarantees that the respective solutions U and $\tilde{U}$ of the discrete systems (3.7) and (4.8) exist. Calculating the difference between the respective equations and the initial data of the system, we readily check that the following discrete problem is satisfied:

$$\begin{aligned} &\delta_t \epsilon_j^{k+1} - \nabla_h \cdot \left(a^2_{j-\frac{1}{2}} \nabla_h \mu_t \epsilon_{j-1}^{k+1}\right) + \tilde{F}_j^{k+1} = 0, \qquad \forall (j,k) \in J \times I_{K-1}, \\ &\text{such that } \begin{cases} \epsilon_j^0 = u_0(x_j) - \tilde{u}_0(x_j), & \forall j \in \overline{J}, \\ \epsilon_j^k = 0, & \forall (j,k) \in \partial J \times \overline{I}_K. \end{cases} \end{aligned} \tag{4.11}$$

Next, obtain the inner product of the iterative formula in (4.11) with $2\mu_t \epsilon^k$, and use the properties established in Lemma 4.3. In this way, it is possible to obtain the discrete equations

$$\delta_t \|\epsilon^k\|_2^2 + 2\|a \nabla_h \mu_t \epsilon^k\|_2^2 + \langle \tilde{F}^k, 2\mu_t \epsilon^k \rangle = 0, \qquad \forall k \in I_{K-1}. \tag{4.12}$$

Let $n \in I_{K-1}$, and take the sum from $k = 0$ to $k = n$ on both sides of this last identity. After noticing the presence of a telescopic sum, performing some algebraic simplifications, using Young's inequality and employing one of the bounds in (4.3), we derive the following identities and inequalities:

$$\begin{aligned} \|\epsilon^n\|_2^2 &= \|\epsilon^0\|_2^2 - \tau\sum_{k=1}^{n} \|a \nabla_h \mu_t \epsilon^k\|_2^2 - \tau\sum_{k=1}^{n} \langle \tilde{F}^k, 2\mu_t \epsilon^k \rangle \leq \|\epsilon^0\|_2^2 + \tau\sum_{k=1}^{n} \left|\langle \tilde{F}^k, 2\mu_t \epsilon^k \rangle\right| \\ &\leq \|\epsilon^0\|_2^2 + \frac{5}{2}\tau\left(\|\epsilon^n\|_2^2 + \|\epsilon^0\|_2^2\right) + 5\tau\sum_{k=1}^{n-1} \|\epsilon^k\|_2^2. \end{aligned} \tag{4.13}$$

Subtract the term $\frac{5}{2}\tau\|\epsilon^n\|_2^2$ from both ends of these inequalities, rearrange terms and simplify algebraically. Notice then that the discrete version of Gronwall's inequality (4.7) is satisfied, for each $n \in I_{K-1}$. To that end, the terms in Gronwall's inequality are as follows: $\omega^n = \|\epsilon^n\|_2^2$ for each $n \in \overline{I}_K$, $C_0 = 5$ and $\rho^n = \left(1 + \frac{5}{2}\tau\right)\|\epsilon^0\|_2^2$. The conclusion of this theorem is readily obtained now from Lemma 4.2. □

Corollary 4.5 (Unique solubility)**.** *If $a \in L^\infty(\boldsymbol{B})$, $F \in C^2(\mathbb{R})$ and $F'' \in L^\infty(\mathbb{R})$, then the finite-difference scheme* (3.7) *is uniquely solvable, for any initial condition.*

Proof. Suppose that U and $\tilde{U}$ are solutions of the same initial-value problem (3.7), and define ε as in Theorem 4.4. Note that $\varepsilon^0 = 0$ holds. Also, as a consequence of Theorem 4.4, we get that

$$0 \leq \|\varepsilon^k\|_2^2 \leq \left(1 + \frac{5}{2}\tau\right)\|\varepsilon^0\|_2^2 e^{5k\tau} = 0, \qquad \forall k \in \overline{I}_K. \tag{4.14}$$

It follows that $\|\varepsilon^k\|_2^2 = 0$, for each $k \in \overline{I}_K$, whence the conclusion of the theorem follows. □

We now establish the convergence properties of our finite-difference scheme. To that end, we will assume that u_j^k represents a sufficiently smooth solution of the initial-value problem (2.1). As a consequence, $Lu_j^k = -R_j^k$, for each $(j,k) \in J \times \overline{I}_K$. Obviously, R_j^k represents here the local truncation error.

Theorem 4.6 (Convergence)**.** *Let $u \in C_{x,t}^{4,3}(\overline{\boldsymbol{B}}_T)$ be a solution of* (2.1)*. If $a \in L^\infty(\boldsymbol{B})$, $F \in C^2(\mathbb{R})$ and $F'' \in L^\infty(\mathbb{R})$, then the solution of* (3.7) *converges to the solution of* (2.1) *in the Euclidean norm, whenever τ is sufficiently small.*

Proof. As before, let U denote the solution of (3.7). For the sake of convenience, define $\eta_j^k = U(x_j, t_k) - u_j^k$, for each $k \in \overline{I}_K$. Notice that η satisfies the following discrete initial-boundary-value problem:

$$\begin{aligned}
&\delta_t \eta_j^{k+1} - \nabla_h\left(a_{j-\frac{1}{2}}^2 \nabla_h \mu_t \eta_{j-1}^{k+1}\right) + \tilde{F}_j^{k+1} + R_j^k = 0, \qquad \forall (j,n) \in J \times I_{K-1}, \\
&\text{such that } \begin{cases} \eta_j^0 = U(x_j, 0) - u_0(x_j), & \forall j \in \overline{J}, \\ \eta_j^k = 0, & \forall (j,n) \in \partial J \times \overline{I}_K, \end{cases}
\end{aligned} \tag{4.15}$$

The regularity of u and Theorem 4.1 assume that there exists a bound $C > 0$ for R_j^k which is independent of h and τ. More precisely, this constant satisfies $|R_j^k| \leq C(\tau^2 + \|h\|_2^2)$, for each $(j,k) \in J \times \overline{I}_K$. Proceeding as in the proof for the stability, take the inner product of the difference equation in (4.15) with $2\mu_t \eta^k$, and use the identities from Lemma 4.3. After rearranging some terms algebraically, we reach the equation

$$\delta_t \|\eta^k\|_2^2 + 2\|a \nabla_h \mu_t \eta^k\|_2^2 + \langle \tilde{F}^k + R_j^k, 2\mu_t \eta^k \rangle = 0, \qquad \forall n \in I_{K-1}. \tag{4.16}$$

Let $n \in \overline{I}_K$ and sum on both sides of this last identity from $k = 0$ to $k = n$. Using the formula for telescopic sums, rearranging terms, performing algebraic simplifications, using Young's inequality, and applying the bounds in Lemma 4.3 and the bound for the local truncation error, we conclude that there is a $C_1 \geq 0$ independent of τ and h, such that

$$\begin{aligned}
\left(1 - \frac{5\tau}{2}\right)\|\eta^n\|_2^2 &\leq \left(1 + \frac{5\tau}{2}\right)\|\eta^0\|_2^2 + 5\tau \sum_{k=1}^{n-1} \|\eta^k\|_2^2 + \tau \sum_{k=1}^{n} \langle R^k, 2\mu_t \eta^k \rangle \\
&\leq \left(1 + \frac{5\tau}{2}\right)\|\eta^0\|_2^2 + 5\tau \sum_{k=1}^{n-1} \|\eta^k\|_2^2 + \tau \sum_{k=1}^{n-1} \|R^k\|_2^2 + \tau \sum_{k=1}^{n-1} \|\eta^k\|_2^2 + \frac{\tau}{2}\left(\|\eta^0\|_2^2 + \|\eta^n\|_2^2\right) \\
&\leq \left(1 + \frac{5\tau}{2}\right)\|\eta^0\|_2^2 + C_1(\tau^2 + \|h\|_2^2)^2 + 6\tau \sum_{k=1}^{n-1} \|\eta^k\|_2^2 + \frac{\tau}{2}\|\eta^n\|_2^2.
\end{aligned} \tag{4.17}$$

Subtracting $\frac{\tau}{2}\|\eta^n\|_2^2$ from both ends of these inequalities, we observe that the inequality (4.7) is satisfied, for each $n \in I_{K-1}$. It is worth pointing out here that, in this case, $C_0 = 6$, $\omega^n = \|\eta^n\|_2^2$ and $\rho^n = \left(1 + \frac{5\tau}{2}\right)\|\eta^0\|_2^2 + C_1(\tau^2 + \|h\|_2^2)^2$, for each $n \in \overline{I}_K$. Lemma 4.2 guarantees now that

$$\|\eta^n\|_2^2 \leq C_2(\tau^2 + \|h\|_2^2)^2, \qquad \forall (j,n) \in J \times \overline{I}_K, \tag{4.18}$$

where $C_2 = \rho^n e^{C_0 k T}$. As a consequence, $\|\eta^n\|_2 \leq \sqrt{C_2}(\tau^2 + \|h\|_2^2)$, for each $(j,n) \in J \times \overline{I}_K$, which means that the finite-difference scheme (3.7) converges to the exact solution of (2.1) in the Euclidean norm. □

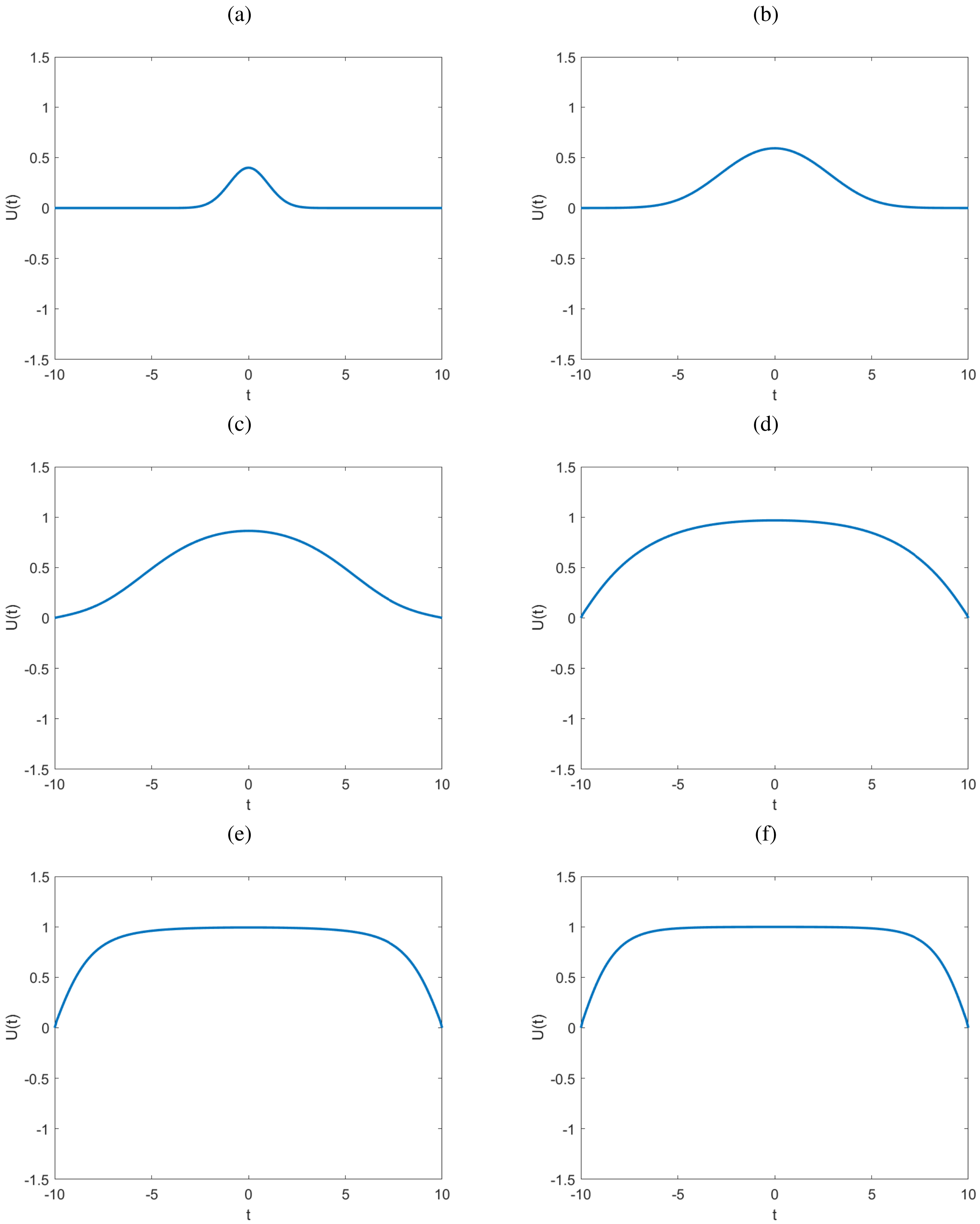

Figure 1: Graphs of the approximate solution of the one-dimensional mathematical model (2.1) obtained using the finite-difference method (3.7). The graphs represent the approximate solution u versus x at the times (a) $t = 0$, (b) $t = 2$, (c) $t = 4$, (d) $t = 6$, (e) $t = 8$ and (f) $t = 10$. Here, we used $\boldsymbol{B} = (-10, 10)$, $T = 10$, $h = 0.1$, $\tau = 0.01$ and $a \equiv 1$. The potential F was fixed as (4.19), and we used the standard normal distribution as the initial condition.

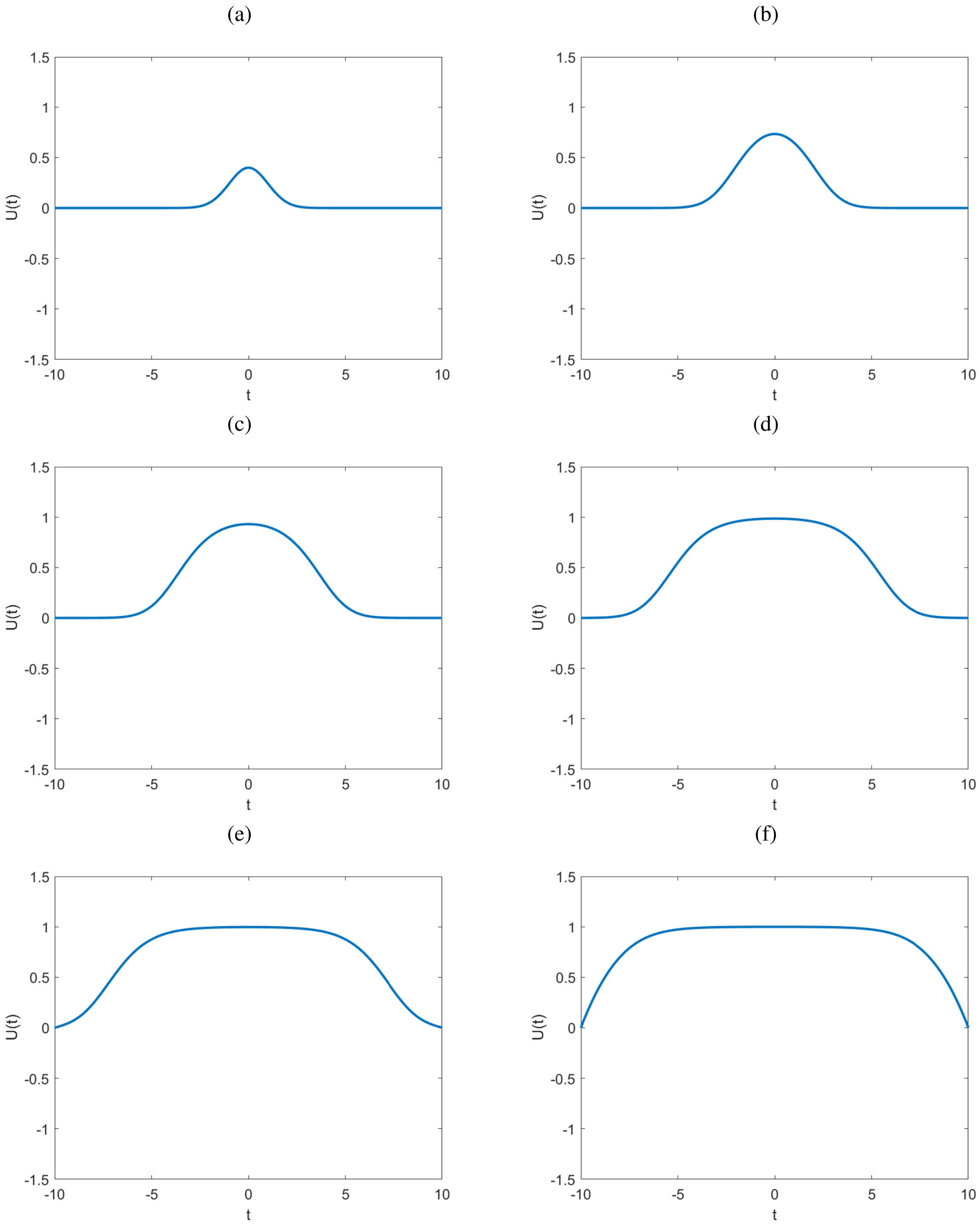

Figure 2: Graphs of the approximate solution of the one-dimensional mathematical model (2.1) obtained using the finite-difference method (3.7). The graphs represent the approximate solution u versus x at the times (a) $t = 0$, (b) $t = 2$, (c) $t = 4$, (d) $t = 6$, (e) $t = 8$ and (f) $t = 10$. Here, we used $\boldsymbol{B} = (-10, 10)$, $T = 10$, $h = 0.1$, $\tau = 0.01$ and $a \equiv 0.25$. The potential F was fixed as (4.19), and we used the standard normal distribution as the initial condition.

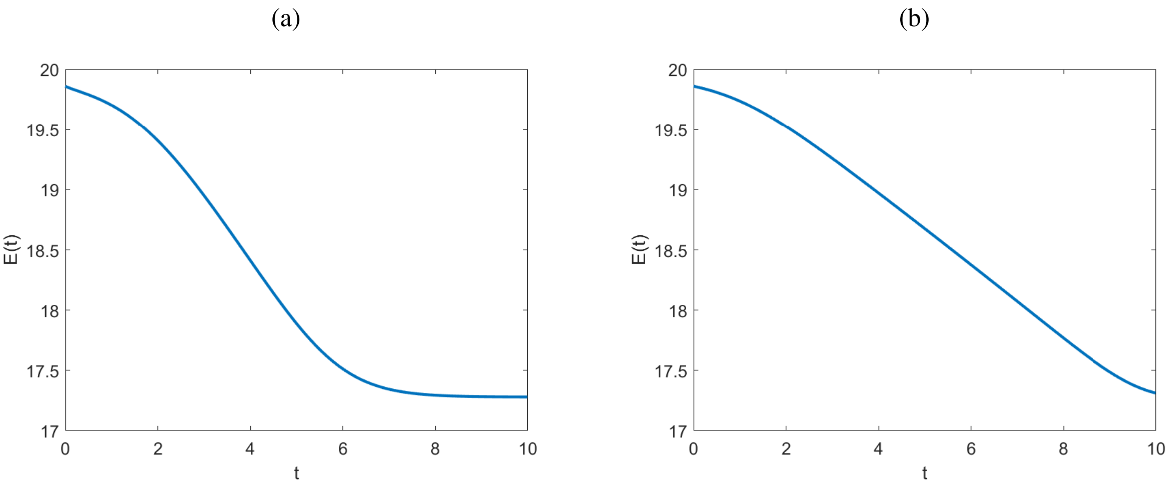

Figure 3: Graphs of the Gibbs' free energy versus time for the numerical experiments carried out in (a) Figure 1 and (b) Figure 2.

The last paragraphs of this section will be devoted to provide simulations obtained with a Matlab implementation of the finite-difference scheme (3.7), in one and two spatial dimensions. In view of the nonlinear and implicit nature of the scheme, our implementation was carried out using a fixed-point approach. This implementation is motivated by the proof on the existence of solutions which was based on Brouwer's fixed-point theorem. In our implementation, we required a tolerance of 1×10^{-6} in the Euclidean norm, and a maximum number of iterations equal to 20. It is worth to point out that, in the practice, the required number of iterations at each temporal step was much smaller than the maximum. In all of our simulations, we will let $h = h_1 = h_2 = 0.1$ and $\tau = 0.01$, and we will fix

$$F(u) = \frac{1}{3}u^3 - \frac{1}{2}u^2 + 1, \quad \forall u \in \mathbb{R}. \tag{4.19}$$

In a first example, we let $d = 1$, consider the spatial domain $\boldsymbol{B} = (-10, 10)$ and fix a time period $T = 10$. Assume that $a \equiv 1$, and consider the usual standard normal distribution as the initial condition. Under these circumstances, Figure 1 snapshots of the approximate solutions obtained using the numerical model (3.7), at the times (a) $t = 0$, (b) $t = 2$, (c) $t = 4$, (d) $t = 6$, (e) $t = 8$ and (f) $t = 10$. For illustration purposes, we will consider also the same setting, except that now we consider $a \equiv 0.25$. The results are presented in Figure 2 for the same times. In turn, the Gibbs' free energy for these two experiments are presented in Figure 3. Observe that the energy functional is decreasing in both cases. This is in obvious agreement with the theoretical results derived in this work.

Before closing this section, we would like to present a final set of simulations for the two-dimensional scenario. To that end, we will consider the continuous model (2.1) in two spatial dimensions, and let us fix the bounded spatial domain $\boldsymbol{B} = (-12, 12) \times (-12, 12)$. Set $T = 15$, and let $a \equiv 1$. The potential F will be given by (4.19), and we will use the two-dimensional standard normal distribution, which has mean equal to zero and the identity as the variance matrix. The results of our simulations are presented in Figure 4, for the times (a) $t = 0$, (b) $t = 3$, (c) $t = 6$, (d) $t = 9$, (e) $t = 12$ and (f) $t = 15$. In turn, Figure 5 provides the graph of the Gibbs' free energy versus time for this experiment. Again, the simulations confirm the fact that the free energy function is dissipated with respect to time, in agreement with our theoretical results.

5. Conclusions

In this work, we considered a multidimensional parabolic partial differential equation, together with initial and boundary conditions on a closed and bounded spatial domain. The mathematical model is a generalization of various systems appearing in the physical sciences, and considers a general nonlinear reaction term and a non-constant diffusion coefficient that depends on the spatial variable. Meanwhile, homogeneous data are considered at the boundary of the spatial domain. It is well known that there is a Gibbs' free energy functional associated to the mathematical

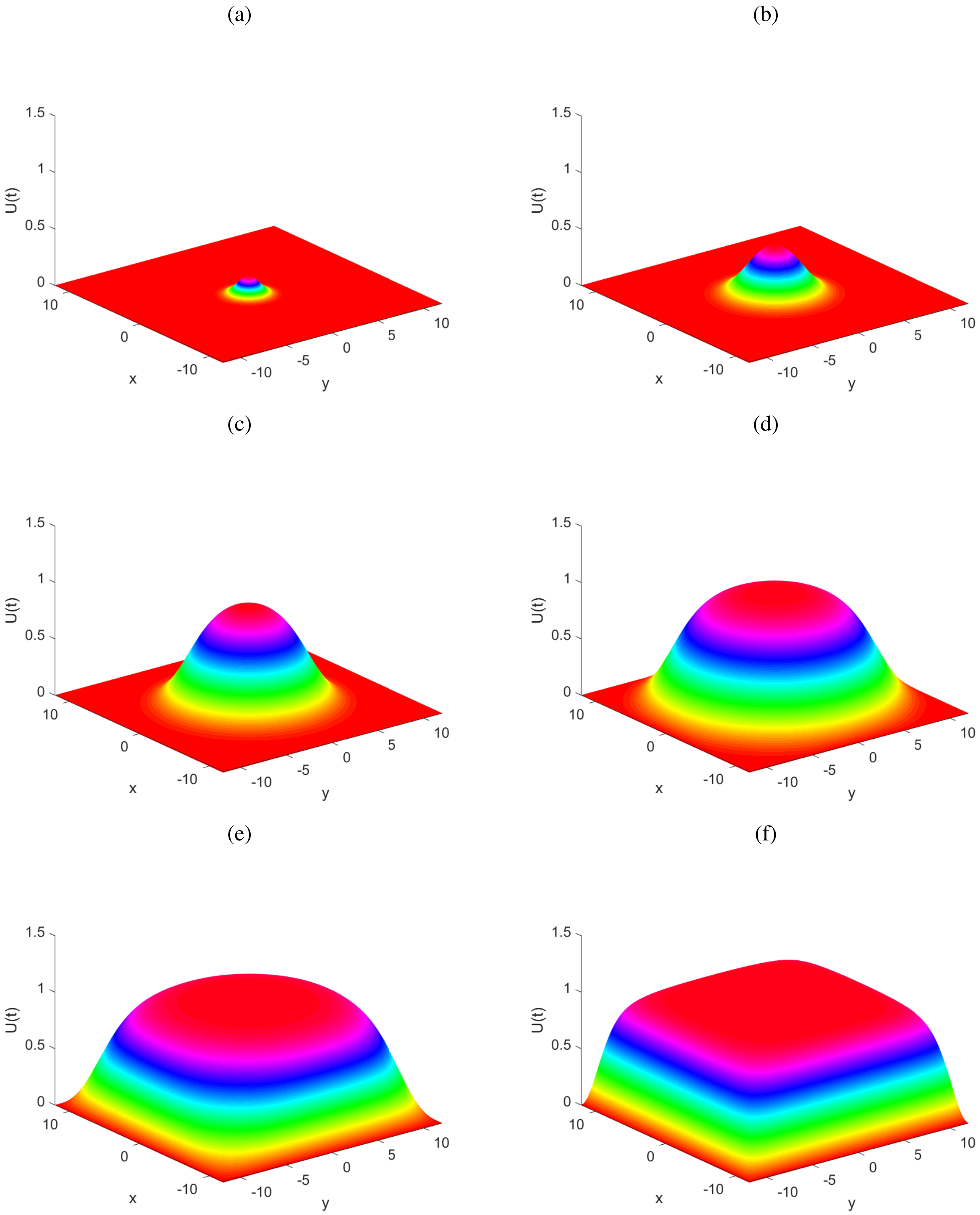

Figure 4: Graphs of the approximate solution of the two-dimensional mathematical model (2.1) obtained using the finite-difference method (3.7). The graphs represent the approximate solution u versus (x, y) at the times (a) $t = 0$, (b) $t = 3$, (c) $t = 6$, (d) $t = 9$, (e) $t = 12$ and (f) $t = 15$. Here, we used $\boldsymbol{B} = (-12, 12) \times (-12, 12)$, $T = 15$, $h = 0.1$, $\tau = 0.01$ and $a \equiv 1$. The potential F was fixed as (4.19), and we used the standard normal distribution in two dimensions as the initial condition.

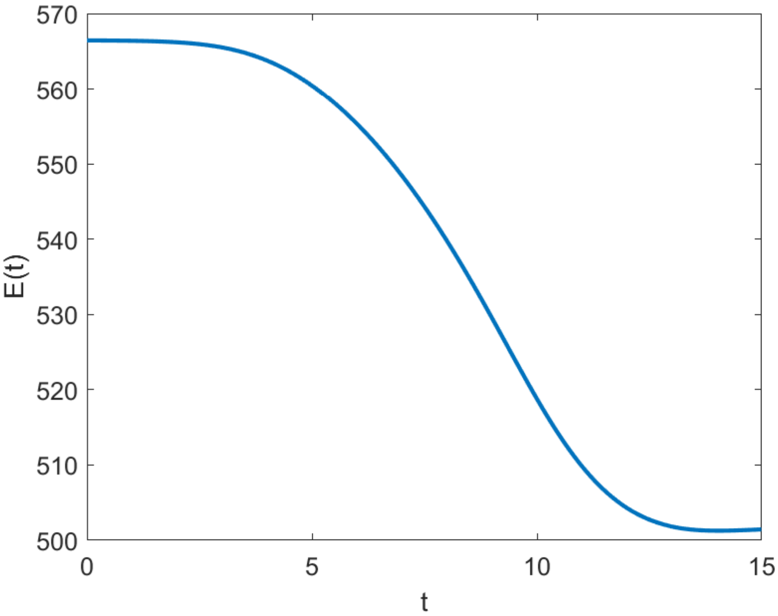

Figure 5: Graphs of the Gibbs' free energy versus time for the numerical experiment carried out in Figure 4.

problem, and we showed here that this functional is decreasing with respect to time. Moreover, under suitable conditions, the Gibbs' energy is a non-negative function. Motivated by these facts, we proposed a finite-difference method to approximate the solutions of the mathematical model. The numerical scheme is a two-step implicit technique, and we prove that it is solvable for any set of initial conditions under suitable regularity assumptions on the component functions of the model. To that end, we employ Brouwer's fixed-point theorem. Moreover, we propose a discrete form of the Gibbs' free energy, and showed that this discrete functional is dissipated with respect to the discrete time. This is in obvious agreement with the continuous model investigated in this work. Additionally, we establish the quadratic consistency of the scheme, the stability and the quadratic convergence in the Euclidean norm. As a consequence of the stability, we prove the uniqueness of the solubility of the numerical model. We provide some illustrative simulations in one and two spatial dimensions, to show that the numerical model is capable of preserving the dissipation of Gibbs' free energy, in agreement with the theoretical results derived in this manuscript.

After the completion of this work, various avenues of research still remain open. In particular, one natural direction of study is the investigation of the mathematical model (2.1) with fractional derivatives in space and time [30]. Usually, Caputo fractional operators are used in connection with partial derivatives with respect to time, while Riemann–Liouville or Riesz fractional operators are employed for partial derivatives with respect to space [31]. Naturally, one natural question is whether there is a fractional extension of the present model which for which a Gibbs' free energy functional is associated. Moreover, one may wonder whether the free energy is dissipated with respect to time. The design and theoretical analysis of a dissipation-preserving numerical model to solve that fractional problem would be an interesting avenue of research in that case. It is worth pointing out that the authors of this manuscript have devoted some efforts to design some energy-preserving techniques to solve fractional extensions of the Klein–Gordon–Zakharov equations [32, 33] and the Gross–Pitaevskii system [34]. *A priori*, the authors of the present manuscript believe that such investigation is feasible, though substantial efforts need to be carried out to that end. Obviously, this may be the topic of a future work for which the present manuscript would be a departing point.

Acknowledgments. The authors wish to thank the anonymous reviewers for their comments and criticisms. All of their comments were taken into account in the revised version of the paper, resulting in a substantial improvement with respect to the original submission.

Funding. The corresponding author (J.E.M.-D.) wishes to acknowledge the financial support from the National Council for Science and Technology of Mexico (CONACYT) through grant A1-S-45928.

Competing interests. The authors do hereby declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability statement. The data that support the findings of this study are available from the corresponding author, J.E.M.-D., upon reasonable request.

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