LINEARIZED RUNGE-KUTTA METHODS FOR THE ε-DEPENDENT CAHN-HILLIARD/ALLEN-CAHN EQUATION

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Dedicated to the memory of Professor Vassilios Dougalis

ABSTRACT. In this paper, for a small parameter $\varepsilon > 0$, we consider the Cahn-Hilliard/Allen-Cahn equation in dimensions $d = 1, 2, 3$ as introduced in [8], with weights $\delta(\varepsilon) > 0$, $\mu(\varepsilon) \geq 0$ on the Cahn-Hilliard and Allen-Cahn operators, respectively. This equation corresponds to the model B/A of critical dynamics, where ε is the order of the width of the transition layers developed during the phase separation of a binary alloy. We apply a rescaled in ε algebraically stable Runge-Kutta-SAV extrapolated time-discrete method in the sense of [1], which is adjusted properly for our problem. The discrete energy as in the continuous case is proven decaying, and optimal order error estimates are derived. The scheme is further discretized in space by piece-wise quadratic finite elements and implemented by 1D and 2D numerical simulations. These simulations are the first for the mixed problem and reveal thus, especially in the multi-dimensional case, the very interesting solution's transitional profile in the context of phase separation. The transition layers seem to change significantly depending on the selection of the weights, as rigorously proven so far only in 1D in [8].

1. Introduction

1.1. The ε-dependent Cahn-Hilliard/Allen-Cahn equation.

Letting $\varepsilon > 0$ be a small positive parameter, we consider the mixed problem for the Cahn-Hilliard and Allen-Cahn operators which is given as follows

$$
\begin{aligned}
&u_t = -\delta(\varepsilon)\,\Delta\big(\varepsilon^2\Delta u - f(u)\big) \;+\; \mu(\varepsilon)(\varepsilon^2\Delta u - f(u)),\ x \in \mathcal{D},\ \ t > 0,\\
&u(x,0) = u_0(x;\varepsilon),\ x \in \mathcal{D},\\
&\frac{\partial u}{\partial \nu} = \frac{\partial \Delta u}{\partial \nu} = 0 \ \text{ on } \ \partial\mathcal{D}.
\end{aligned}
\tag{1.1}
$$

Here, $\mathcal{D}$ is a bounded domain in $\mathbb{R}^d$, $d = 1, 2, 3$, while the nonlinearity $f(u) = F'(u)$, is the derivative of a double equal-well potential; a typical example, to be used throughout this manuscript, is $f(u) = u^3 - u$, for a potential $F(u) := \frac{1}{4}(u^2 - 1)^2$. The ε-dependent weights satisfy

$$\delta(\varepsilon) > 0,\ \ \mu(\varepsilon) \geq 0. \tag{1.2}$$

The existence and regularity properties of (1.1) in dimensions $d = 1, 2, 3$ have been analyzed in [21]. There, for the equivalent system representation for u, and v that defines the chemical potential, it has been proven that if the initial condition u_0 is in $H^1(D)$ then for any $T > 0$ there exists a unique regular solution (u, v) in $C([0,T]; H^1(D)) \times L^2([0,T]; H^1(D))$, while when $u_0 \in H^2(D)$ then u belongs to $C([0,T]; H^2(D))$ which is the critical space for the combined model. Higher regularity can be then derived as in [12] by differentiating in space the equation, for sufficiently smooth initial condition. We also refer to the stochastic version of the problem with

2020 *Mathematics Subject Classification.* 65M12, 65L06, 35B36, 35G20.

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a non-smooth multiplicative space-time noise, cf. [7]; the authors proved local existence, uniqueness, and path-regularity in dimensions $d = 1, 2, 3$, global existence when $d = 1$, and for $d = 2, 3$ existence of maximal solutions. In [6], for the same stochastic problem and $d = 1$, existence of a density has been derived through Malliavin calculus. Recently, in [8], D.C. Antonopoulou, G. Karali and K. Tzirakis studied for $d = 1$ the dynamics of the ε-dependent Cahn-Hilliard/Allen-Cahn equation of (1.1) within a neighborhood of an equilibrium of N transition layers. The spectrum of the linearized operator was estimated, and wide families of weights $\delta(\varepsilon), \mu(\varepsilon)$ were identified for which the dynamics are stable and rest exponentially small in ε.

Remark 1.1. *The initial and boundary value problem* (1.1) *is not mass-conserving when $\mu(\varepsilon) > 0$, as the mass defined by $\int_{\mathcal{D}} u(x,t)dx$ changes in time. This is not the case for the Cahn-Hilliard equation ($\mu(\varepsilon) := 0$), where due to the Neumann b.c. it holds that $\int_{\mathcal{D}} u(x,t)dx = \int_{\mathcal{D}} u(x,0)dx$ for all $t > 0$. However, in* [8] *the authors considered the problem* (1.1) *for $d = 1$ and $\mu(\varepsilon) > 0$, in the interval $\mathcal{D} := (0,1)$, and imposed mass conservation by replacing the 4th boundary condition $u_{xxx}(1,t) = 0$ by the non-local condition $\int_0^1 u(x,t)dx = \int_0^1 u(x,0)dx$, $\forall t > 0$. This problem was proven well-posed and was approximated in the mass-conserving manifold of* [9, 10] *which was initially implemented for the Cahn-Hilliard equation, and then applied with certain modifications in* [4] *for the stochastic Cahn-Hilliard equation.*

Remark 1.2. *Let $\delta(\varepsilon)$, $\mu(\varepsilon)$ satisfy* (1.2)*, and additionally the spectral condition*

$$\varepsilon^2\mu(\varepsilon) \geq \tilde{C}_1\delta(\varepsilon), \tag{1.3}$$

for some $\tilde{C}_1 > 0$ independent of ε. In [8], (1.3) *was derived by the analysis of the spectrum of the linearized operator, and $\tilde{C}_1$ was determined. Moreover, under* (1.2), (1.3)*, the authors therein constructed a stable approximation of the solution of* (1.1) *to the non mass-conserving manifold of static solutions of the Allen-Cahn equation; this manifold has been defined and analyzed in* [11]*. When $\delta(\varepsilon) = 1$, $\mu(\varepsilon) = c_0\varepsilon^{-2}$, which satisfies* (1.3)*, it has been proven in higher dimensions that the sharp interface limit as $\varepsilon \to 0^+$, a curve, or a surface for $d = 2$ or $d = 3$, respectively, is evolving by velocity proportional to its mean curvature,* [20]*. This limiting profile has essentially the same qualitative behaviour with the Allen-Cahn equation limit problem where the velocity is equal to the mean curvature.*

Let $u(x,t)$ be the solution of (1.1). A simple rescaling by setting $z = x\varepsilon^{-1}$, $r = t\mu(\varepsilon)$, and $v(z,r) := u(x,t)$, yields that $\nabla u = \varepsilon^{-1}\nabla v$, $\Delta u = \varepsilon^{-2}\Delta v$, $\Delta^2 u = \varepsilon^{-4}\Delta v$, and thus $\Delta(f(u)) = \varepsilon^{-2}\Delta(f(v))$, while $u_t = \mu(\varepsilon)v_r$. Therefore, v satisfies the combined problem

$$v_r = -\frac{\delta(\varepsilon)}{\mu(\varepsilon)\varepsilon^2}\Delta(\Delta v - f(v)) + (\Delta v - f(v)).$$

When $\frac{\delta(\varepsilon)}{\mu(\varepsilon)\varepsilon^2} = \mathcal{O}(1)$ and $u_0(z\varepsilon) = v(z,0)$ is independent of ε then v is independent of ε and so u, $\varepsilon^k\nabla^k u$, $k \in \mathbb{N}$ are upper bounded uniformly in ε. If $\frac{\delta(\varepsilon)}{\mu(\varepsilon)\varepsilon^2} \ll 1$ then the Allen-Cahn operator is dominant; such a result has been proven rigorously in [8] in dimensions one. In particular, mass-conservation classifies the dynamically stable mixed problem into two main categories. The non mass-conserving solution (i.e., the solution of (1.1) with $\mu > 0$) is close to Allen-Cahn where due to the stability condition μ dominates δ, or, when the mass is conserved, close to the Cahn-Hilliard solution where δ dominates μ. In higher dimensions the problem is open. As a first step, in this work we aim to investigate numerically this behaviour in dimensions $d = 1, 2, 3$.

Equation (1.1) is a gradient flow with respect to an ε-weighted metric for the problem's free energy functional (defined by (2.5)), [8]; for some very interesting recent results on SAV formulations for gradient flows see in [25, 26, 27]. The SAV approach was initially proposed by J. Shen, J. Xu, and J. Yang in [26], and had so far a successful application in developing energy-stable schemes for several dissipative systems, e.g., [25, 27, 24, 13]. Motivated by the extrapolated RK-SAV methods of G. Akrivis, B. Li and D. Li in [1], which stand as linearized versions with extrapolation of the RK methods of [18], we approximate the problem (1.1). We introduce a linear combination of linearized Runge-Kutta schemes with general weights $\delta(\varepsilon) > 0$, $\mu(\varepsilon) \geq 0$. Optimal order error estimates ($\mathcal{O}(\tau^{q-\frac{1}{2}})$, $q \geq 2$) are established for the RK nodes in H^2 due to the presence of the 4th order operator ($\delta > 0$). In [1] this estimate was of order $\mathcal{O}(\tau^{q-\frac{3}{2}})$ since there only the Allen-Cahn equation was analyzed where $\delta = 0$. We also carefully treat the constants of the error bounds in ε. When $\mu = 0$ the Cahn-Hilliard equation is covered by our error analysis. The scheme, and the 1D and 2D experiments presented at the last section are the first for the mixed problem. As the simulations show, the transitional profile of the two different phases seems to change, being closer to this of the Allen-Cahn or this of the Cahn-Hilliard equation, depending on the order of the weights $\delta(\varepsilon)$, $\mu(\varepsilon)$ in ε.

For various numerical schemes on Cahn-Hilliard or Allen-Cahn equations and their rigorous error analysis we refer, for example, to [1, 14, 15, 16, 17, 23, 3, 2, 5]. We stress that ε-dependent approximations for such equations are very sensitive to rounding errors when $\varepsilon \ll 1$ which is the physical problem's scale. In [16, 17, 3, 2, 5] the authors analyzed the ε-dependent problems for ε small, where the equations are stated near the sharp-interface limit, and estimated the error bounds coefficients by constants of negative polynomial order in ε.

1.2. **The physical problem.** In the study of surface processes, combinations of Cahn-Hilliard and Allen-Cahn equations arise as phase-field models of microstructural evolution at the mesoscale regime. When the parameter ε is sufficiently small they approximate sharp-interface limits of free surface problems. Such equations model two surface processes taking place simultaneously for example catalysis, chemical vapor deposition and epitaxial growth that typically involve transport and chemical reaction of precursors in a gas phase. Unconsumed reactants and radicals adsorb onto the surface of a substrate where processes like surface diffusion, reactions and desorption back to the gas phase occur. The Cahn-Hilliard operator corresponds to mass conservative phase separation and surface diffusion, while the Allen-Cahn operator relates to phase transition and stands as a diffuse interface model for antiphase boundary coarsening.

In [22], the mesoscopic models are derived from microscopic lattice models in the local mean field limit where the interaction potential range becomes infinite. At the microscopic level dynamic Ising type systems are employed which are defined on an n-dimensional lattice. At each lattice site an order parameter is allowed to take the values 0 and 1 describing vacant and occupied sites respectively. In the classical Ising model, the order parameter at a lattice point x is referred to as spin $\sigma(x)$. The energy H of the system is given by a Hamiltonian $H = \sum_{x\neq y} J(x,y)\sigma(x)\sigma(y) + h\sum\sigma(x)$, where h corresponds to an external field, and J is the interparticle potential which is assumed to be even, rapidly decaying at infinity, and nonnegative i.e., the interactions are attractive. The assumption that J is nonnegative implies that clusters of particles are energetically preferred to totally disordered structures, while it yields the mathematical condition $\delta(\varepsilon) > 0$ imposed at (1.1) on the weight of the Cahn-Hilliard operator. In this context, the microscopic mechanisms involved in the mesoscopic model are the spin-flip and the spin-exchange. A spin-flip at the site x is a spontaneous change in the order parameter, 1 is converted to 0 and vice versa. Physically this mechanism describes the desorption of a particle from the surface to the gas phase and conversely the adsorption of a particle from the gas phase to the surface. A spin-exchange between the neighboring sites x and y is a spontaneous exchange of the values of the order parameter at x and y, this mechanism describes the diffusion of a particle on a flat surface.

At large space/time scales and for long range potentials, the small scale random fluctuations of the Ising systems are suppressed and a deterministic pattern dominates. The mesoscopic local mean field equation describing the diffusion/spin-exchange mechanism combining the spin flip/exchange simultaneous mechanisms, Arrhenius adsorption/desorption dynamics, Metropolis surface diffusion, and a simple unimolecular reaction is given by, cf. [22],

$$u_t = D\nabla\cdot\big[\nabla u - \beta u(1-u)\nabla J_m * u\big] + \big[k_\alpha p(1-u) - k_d u\exp(-\beta J_d * u)\big] - k_r u, \tag{1.4}$$

where u denotes the surface coverage of the adsorbed species, J_d and J_m are the interparticle potentials for surface desorption and migration, D is the diffusion constant, β is the inverse temperature, k_r, k_d, k_α denote respectively the reaction, desorption, and adsorption constants, p is the partial pressure of the gaseous species, while the parameters k_α, k_d stem from the Hamiltonian of the system.

In [22], the authors proposed a simplification of (1.4) which preserves its fundamental structure and can be obtained after rescaling when $k_r = 0$ and $J_m = J_d = J$

$$u_t = -D\Delta(\Delta u - f(u)) + \Delta u - f(u), \tag{1.5}$$

where the Cahn-Hilliard term corresponds to surface diffusion, while the Allen-Cahn term to adsorption/desorption. The ε-dependent Cahn-Hilliard/Allen-Cahn equation of (1.1) can be derived from (1.5) after further rescaling in ε. It has been first introduced in [20] in order to describe the long-time behavior of large clusters when $\varepsilon \ll 1$, for weights $\delta = \mathcal{O}(1)$ and $\mu = \varepsilon^{-2}$.

1.3. **The Scalar Auxiliary Variable (SAV) approach.** Notice that the b.c. $\partial_\nu u = \partial_\nu \Delta u = 0$ yield that $\partial_\nu u = \partial_\nu(\varepsilon^2\Delta u - f(u)) = 0$ on $\partial\mathcal{D}$, since $f(u) = u^3 - u$. Thus, the initial and boundary value problem (1.1) is written in the equivalent form given by

$$\begin{aligned} &u_t = -\delta(\varepsilon)\,\Delta\big(\varepsilon^2\Delta u - r(u)W(u)\big) \;+\; \mu(\varepsilon)(\varepsilon^2\Delta u - r(u)W(u)),\; x \in \mathcal{D},\;\; 0 < t \le T,\\ &u(x,0) = u_0(x;\varepsilon),\; x \in \mathcal{D}, \qquad \partial_\nu u = \partial_\nu(\varepsilon^2\Delta u - f(u)) = 0 \;\text{ on }\; \partial\mathcal{D}, \end{aligned} \tag{1.6}$$

where the operators r, W are given by

$$r(u) := r(u(\cdot,t)) := \Big(\int_{\mathcal{D}} F(u(x,t))dx + E_0\Big)^{1/2}, \quad W(u) := W(u(x,t),t) := f(u)r(u)^{-1}, \tag{1.7}$$

for $E_0 > 0$ an arbitrary constant. As used in [1], it holds that

$$\partial_t r(u) = \frac{1}{2}\Big(\int_{\mathcal{D}} F(u(x,t))dx + E_0\Big)^{-1/2}\Big(\int_{\mathcal{D}} F'(u)u_t dx + 0\Big) = \frac{1}{2}(W(u), u_t). \tag{1.8}$$

The SAV approach consists of stating the gradient flow-type problem (1.1) as a system for (u, r), given by (1.6)-(1.7), and then construct energy-stable numerical schemes in order to approximate u, r.

1.4. **Main results and contributions.** In this paper, we introduce a novel class of efficient fully-discrete numerical schemes for the ε-dependent Cahn-Hilliard/Allen-Cahn problem (1.1). Section 2 is devoted to the construction of the SAV formulation for the time discretization of the equivalent to (1.1) system (1.6)-(1.7). The scheme is given by a coupled linear elliptic system for the internal stages of an algebraically stable linearized RK method with weights $\delta(\varepsilon)$, $\mu(\varepsilon)$, i.e., (2.2), (2.3), and the direct formulae (2.4) for the discrete approximations of u and $r(u)$. The energy of (1.1) defined by (2.5) is decaying, [8], we prove that the discrete energy given through the numerical solution by (2.7) is decaying as well, cf. Theorem 2.1. In Section 3, we present the error analysis of the time-discrete RK method where we state the error equations and prove Theorem 3.1. A fully-discrete space-time scheme of piece-wise quadratic finite elements coupled with (2.2), (2.3), and (2.4) is introduced at Section 4, and is implemented by a series of 1D and 2D numerical simulations.

The main contributions of the present paper are summarized as follows:

- Theorem 2.1 shows the unconditional energy-stability of the semi-discrete scheme, fact that justifies the SAV approach. Such results are proven by combining algebraically stable Runge-Kutta methods with extrapolation and using the recently developed SAV formulation.
- We present the rigorous and quite challenging error analysis of the semi-discrete scheme. By Theorem 3.1, we obtain the optimal error estimates (3.15) in L^2, and in H^2 when the RK internal stages are considered, by using the consistency error, *a priori* estimates of the discrete scheme, and by determining carefully the appearing coefficients in ε. When $\mu(\varepsilon) = 0$, this result covers the SAV formulation error analysis of the 4th order Cahn-Hilliard case which was not presented in [1]. Our estimates hold for sufficiently small step-size τ of the RK nodes, with bounds depending on ε, $\delta(\varepsilon)$, $\mu(\varepsilon)$.
- In Section 4, we present an effective implementation of the fully-discrete scheme where the Runge-Kutta internal stages $U_{n,j}$, $R_{n,j}$, and the Runge-Kutta endpoints U_{n+1}, R_{n+1} can be obtained directly; see in Section 4.1. where the fully-discrete system is written in matrix form. In contrast, in previous implementations of SAV-type numerical schemes, one needs to introduce a temporary variable and then decouple the system, cf. [26] and the papers cited therein.
- The numerical scheme, its error analysis, and the simulations are the very first numerical results in the literature of the mixed CH/AC problem. In Section 4, we confirm numerically the optimal error, and as expected the decay of the discrete energy. We also investigate the numerical solution for various weights to observe that when $\delta \gg \mu$ the solution is closer to this of the Cahn-Hilliard, while when $\delta \ll \mu$ closer to this of the Allen-Cahn equation.
- As the 2D simulations show, the transition layers seem to change significantly depending on the selection of $\delta(\varepsilon)$, $\mu(\varepsilon)$ and their order in ε. This was proven rigorously only in dimensions $d = 1$ in [8].

2. SAV-type semi-discrete formulation for the CH/AC

2.1. **The Runge-Kutta numerical scheme in time.** Let a uniform partition of the time interval $[0,T]$, $t_0 = 0 < t_1 < \cdots < t_N = T$, with stepsize $\tau = T/N$, and let $t_{n,i} := t_n + c_i\tau$, $i = 1,\dots,q$, $n = 0,\dots,N-1$ be the Runge-Kutta nodal points. Here, we consider the RK method given by the tableau

$$\begin{array}{c|c} a_{11}\cdots a_{1q} & c_1 \\ \vdots \quad\quad \vdots & \vdots \\ a_{q1}\cdots a_{qq} & c_q \\ \hline b_1\cdots b_q & \end{array}$$

where there exists $\mathbf{A}^{-1}$ for $\mathbf{A} := (a_{ij})_{i,j=1}^q$, $b_i > 0$ for $i = 1,\dots,q$, $c_i \neq c_j$ for all $i \neq j$, while the matrix

$$M = (m_{ij})_{i,j=1}^q, \quad m_{ij} := b_i a_{ij} + b_j a_{ji} - b_i b_j, \tag{2.1}$$

is positive semidefinite, and so the RK method as introduced in [1] is algebraically stable.

For given stages $u_{n-1,i}$, $i = 1,\dots,q$, let $u_{n-1}^\tau(t)$ be the Lagrange interpolation polynomial of degree at most $q-1$ at the points $(t_{n-1,i}, u_{n-1,i}) \in \mathbb{R}^2$, for $i = 1,\dots,q$. We also define, for any $i = 1,\dots,q$, $I_{n-1}^\tau u_{n,i} := u_{n-1}^\tau(t_{n,i})$, and denote by $I_{n-1}^\tau u(t)$ the Lagrange interpolation polynomial of degree at most $q-1$ at the points $(t_{n-1,i}, u(t_{n-1,i})) \in \mathbb{R}^2$, for $i = 1,\dots,q$.

Given the approximations u_n, r_n, and $u_{n-1,i}$, $i = 1,\dots,q$, we define the coupled linear elliptic system of equations for the internal stages $(u_{n,i}, w_{n,i}, r_{n,i})$, $i = 1,\dots,q$, given by the following linearized RK method

$$\begin{aligned} \dot{u}_{n,i} &= \delta(\varepsilon)\Delta w_{n,i} - \mu(\varepsilon) w_{n,i} \quad \text{in } \mathcal{D}, \\ w_{n,i} &= -\varepsilon^2 \Delta u_{n,i} + r_{n,i} W(I_{n-1}^\tau u_{n,i}) \quad \text{in } \mathcal{D}, \\ u_{n,i} &= u_n + \tau \sum_{j=1}^q a_{ij}\dot{u}_{n,j} \quad \text{in } \mathcal{D}, \\ \partial_\nu u_{n,i} &= \partial_\nu w_{n,i} = 0 \quad \text{on } \partial\mathcal{D}, \end{aligned} \tag{2.2}$$

and

$$\dot{r}_{n,i} = \frac{1}{2}(W(I_{n-1}^\tau u_{n,i}), \dot{u}_{n,i}), \qquad r_{n,i} = r_n + \tau \sum_{j=1}^q a_{ij}\dot{r}_{n,j}. \tag{2.3}$$

We shall consider sufficiently smooth initial data so that the system is solvable and $\dot{u}_{n,i}$ belongs to $H^2(\mathcal{D})$, and thus $u_{n,i} \in H^6(\mathcal{D})$.

The values u_{n+1}, r_{n+1} are then calculated by the direct formulae

$$u_{n+1} = u_n + \tau \sum_{i=1}^q b_i \dot{u}_{n,i}, \qquad r_{n+1} = r_n + \tau \sum_{i=1}^q b_i \dot{r}_{n,i}. \tag{2.4}$$

2.2. **Discrete energy decay.** The relevant to the scaling of the standard Allen-Cahn operator $\varepsilon^2\Delta u - f(u)$, free energy functional is defined as follows

$$E(u) := \int_{\mathcal{D}} \Big(\frac{\varepsilon^2 |\nabla u|^2}{2} + F(u)\Big) dx. \tag{2.5}$$

A direct calculation, see in [8], yields the free energy decreasing property for the initial and boundary value problem (1.6) (or of the equivalent (1.1)), since $\delta(\varepsilon) > 0$ and $\mu(\varepsilon) \geq 0$, i.e.,

$$\frac{\partial E(u)}{\partial t} = -\delta(\varepsilon)\|\nabla\big(\varepsilon^2\Delta u - f(u)\big)\|^2 - \mu(\varepsilon)\|\varepsilon^2\Delta u - f(u)\|^2 \leq 0. \tag{2.6}$$

Let us consider the discrete version of the energy as introduced in [1], defined for our problem by

$$E_\tau[u_n, r_n] := \frac{\varepsilon^2}{2}\|\nabla u_n\|^2 + |r_n|^2 - E_0. \tag{2.7}$$

The discrete energy decay is proven by the next Main Theorem.

Theorem 2.1. *Suppose that the Runge-Kutta method satisfies* (2.1) *and is thus algebraically stable. Then, the discrete energy given by* (2.7) *is decaying, i.e.,*

$$E_\tau[u_{n+1}, r_{n+1}] \le E_\tau[u_n, r_n], \ \ \forall\, 0 \le n \le N-1. \tag{2.8}$$

Proof. By [1] (cf. (3.2) therein), due to the positive semidefiniteness of the matrix M given by (2.1), it holds that

$$\|\nabla u_{n+1}\|^2 \le \|\nabla u_n\|^2 + 2\tau \sum_{i=1}^q b_i (\nabla \dot{u}_{n,i}, \nabla u_{n,i}). \tag{2.9}$$

By (2.2), and using that $\partial_\nu u_{n,i} = 0$ on $\partial\mathcal{D}$, we obtain

$$(w_{n,i}, \dot{u}_{n,i}) = -(\Delta\varepsilon^2 u_{n,i}, \dot{u}_{n,i}) + (r_{n,i} W(I^\tau_{n-1} u_{n,i}), \dot{u}_{n,i}) = (\varepsilon^2 \nabla u_{n,i}, \nabla \dot{u}_{n,i}) + (r_{n,i} W(I^\tau_{n-1} u_{n,i}), \dot{u}_{n,i}),$$

which gives that

$$(\varepsilon^2 \nabla u_{n,i}, \nabla \dot{u}_{n,i}) = (\dot{u}_{n,i}, w_{n,i} - r_{n,i} W(I^\tau_{n-1} u_{n,i})). \tag{2.10}$$

By using (2.10) in (2.9), we get

$$\|\nabla u_{n+1}\|^2 \le \|\nabla u_n\|^2 + 2\tau\varepsilon^{-2} \sum_{i=1}^q b_i (\dot{u}_{n,i}, w_{n,i} - r_{n,i} W(I^\tau_{n-1} u_{n,i})). \tag{2.11}$$

Obviously it holds that (cf. (3.4) of [1])

$$|r_{n+1}|^2 \le |r_n|^2 + \tau \sum_{i=1}^q b_i r_{n,i} (W(I^\tau_{n-1} u_{n,i}), \dot{u}_{n,i}). \tag{2.12}$$

Relations (2.11) and (2.12), and the first equation of (2.2), yield

$$\begin{aligned} \frac{\varepsilon^2}{2}\|\nabla u_{n+1}\|^2 + |r_{n+1}|^2 &\le \frac{\varepsilon^2}{2}\|\nabla u_n\|^2 + \tau \sum_{i=1}^q b_i (\dot{u}_{n,i}, w_{n,i} - r_{n,i} W(I^\tau_{n-1} u_{n,i})) \\ &+ |r_n|^2 + \tau \sum_{i=1}^q b_i r_{n,i} (W(I^\tau_{n-1} u_{n,i}), \dot{u}_{n,i}) = \frac{\varepsilon^2}{2}\|\nabla u_n\|^2 + |r_n|^2 - \tau\delta(\varepsilon) \sum_{i=1}^q b_i \|\nabla w_{n,i}\|^2 \\ &- \tau\mu(\varepsilon) \sum_{i=1}^q b_i \|w_{n,i}\|^2 \le \frac{\varepsilon^2}{2}\|\nabla u_n\|^2 + |r_n|^2, \end{aligned} \tag{2.13}$$

where we used the Neumann b.c. of $w_{n,i}$, that $\delta(\varepsilon) > 0$, $\mu(\varepsilon) \ge 0$, and that $\tau,\ b_i > 0$.

Inequality (2.13), by substracting E_0, gives the discrete energy decay property (2.8). ☐

3. Error analysis

3.1. **The error equations.** Let u be the solution of (1.6) and $u_{n,i}$, $r_{n,i}$ the solutions of (2.2) and (2.3). We define the error terms

$$\begin{aligned} &e_n := u(\cdot, t_n) - u_n \ \text{ for } \ n = 0, \dots, N, \ \text{ and} \\ &e_{n,i} := u(\cdot, t_n + c_i\tau) - u_{n,i}, \quad \dot{e}_{n,i} := \dot{u}^*_{n,i} - \dot{u}_{n,i} \ \text{ for } \ n = 0, \dots, N-1, \ \ i = 1, \dots, q, \end{aligned} \tag{3.1}$$

and

$$\begin{aligned} &\eta_n := r(u(\cdot, t_n)) - r_n \ \text{ for } \ n = 0, \dots, N, \ \text{ and} \\ &\eta_{n,i} := r(u(\cdot, t_n + c_i\tau)) - r_{n,i}, \quad \dot{\eta}_{n,i} := \dot{r}^*_{n,i} - \dot{r}_{n,i} \ \text{ for } \ n = 0, \dots, N-1, \ \ i = 1, \dots, q. \end{aligned} \tag{3.2}$$

In the above, $\dot{u}^*_{n,i}$ is defined by

$$\dot{u}^*_{n,i} := \delta(\varepsilon)\Delta\tilde{u}_{n,i} - \mu(\varepsilon)\tilde{u}_{n,i}, \tag{3.3}$$

for

$$\tilde{u}_{n,i} := -\,\varepsilon^2 \Delta u(\cdot, t_n + c_i\tau) + r(u(\cdot, t_n + c_i\tau)) W(I^\tau_{n-1} u(\cdot, t_n + c_i\tau)), \tag{3.4}$$

and

$$\begin{aligned} u(\cdot,t_n+c_i\tau) &= u(\cdot,t_n)+\tau\sum_{j=1}^{q}a_{ij}\dot{u}^*_{n,j}+\varepsilon_{n,i},\\ \partial_\nu u(\cdot,t_n+c_i\tau) &= \partial_\nu \Delta u(\cdot,t_n+c_i\tau)=\partial_\nu\tilde{u}_{n,i}=0 \quad \text{on } \partial\mathcal{D}, \end{aligned} \tag{3.5}$$

while, as in (4.2), (4.3) of [1], $\dot{r}^*_{n,i}$ is defined by

$$\dot{r}^*_{n,i} := \frac{1}{2}(W(I^\tau_{n-1}u(\cdot,t_n+c_i\tau)),\dot{u}^*_{n,i}), \quad r(u(\cdot,t_n+c_i\tau)) = r(u(\cdot,t_n))+\tau\sum_{j=1}^{q}a_{ij}\dot{r}^*_{n,j}+d_{n,i}, \tag{3.6}$$

for $i=1,\dots,q$, and

$$u(\cdot,t_{n+1}) = u(\cdot,t_n)+\tau\sum_{i=1}^{q}b_i\dot{u}^*_{n,i}+\varepsilon_{n+1}, \quad r(u(\cdot,t_{n+1})) = r(u(\cdot,t_n))+\tau\sum_{i=1}^{q}b_i\dot{r}^*_{n,i}+d_{n+1}, \tag{3.7}$$

where we introduced the quantities $\varepsilon_{n,i}$, ε_{n+1}, $d_{n,i}$, d_{n+1} which are the resulting consistency errors.

Therefore, by substraction the next error equations follow for any $i=1,\dots,q$

$$\dot{e}_{n,i} = \delta(\varepsilon)\Delta\tilde{e}_{n,i}-\mu(\varepsilon)\tilde{e}_{n,i}, \tag{3.8}$$

$$\tilde{e}_{n,i} := -\varepsilon^2\Delta e_{n,i}+\eta_{n,i}W(I^\tau_{n-1}u_{n,i})+r(u(\cdot,t_n+c_i\tau))\Big[W(I^\tau_{n-1}u(t_n+c_i\tau))-W(I^\tau_{n-1}u_{n,i})\Big], \tag{3.9}$$

$$e_{n,i} = e_n+\tau\sum_{j=1}^{q}a_{ij}\dot{e}_{n,j}+\varepsilon_{n,i}, \quad \partial_\nu e_{n,i}=\partial_\nu\tilde{e}_{n,i}=0 \quad \text{on } \partial\mathcal{D}. \tag{3.10}$$

Moreover, as in (4.18), (4.19) of [1], we have

$$\begin{aligned} \dot{\eta}_{n,i} &= \frac{1}{2}\Big(W(I^\tau_{n-1}u(t_n+c_i\tau))-W(I^\tau_{n-1}u_{n,i}),\dot{u}^*_{n,i}\Big)+\frac{1}{2}(W(I^\tau_{n-1}u_{n,i}),\dot{e}_{n,i}),\\ \eta_{n,i} &= \eta_n+\tau\sum_{j=1}^{q}a_{ij}\dot{\eta}_{n,j}+d_{n,i}, \end{aligned} \tag{3.11}$$

for $i=1,\dots,q$, and

$$e_{n+1} = e_n+\tau\sum_{i=1}^{q}b_i\dot{e}_{n,i}+\varepsilon_{n+1}, \quad \eta_{n+1}=\eta_n+\tau\sum_{i=1}^{q}b_i\dot{\eta}_{n,i}+d_{n+1}. \tag{3.12}$$

Then (cf. (4.21), (4.22) of [1]), it follows that

$$\|e_{n+1}\|^2 = \|e_n+\tau\sum_{i=1}^{q}b_i\dot{e}_{n,i}\|^2+2(\varepsilon_{n+1},e_n+\tau\sum_{i=1}^{q}b_i\dot{e}_{n,i})+\|\varepsilon_{n+1}\|^2. \tag{3.13}$$

3.2. **The estimates.** In this section, we prove the next Main Theorem.

Theorem 3.1. *Let the initial condition u_0 of the continuous problem* (1.1) *be smooth enough, and let*

$$\begin{aligned} &\|e_1\|^2+|\eta_1|^2+\tau\sum_{i=1}^{q}b_i\|e_{0,i}\|^2 \le c\tau^{2q},\\ &\|e_{0,i}\|_{H^2(\mathcal{D})} \le \tau, \;\; \forall\, 1\le i\le q, \end{aligned} \tag{3.14}$$

it holds that

$$\begin{aligned} &\|e_{m+1}\|+|\eta_{m+1}| \le c\tau^q, \;\; \forall\, 0\le m\le N-1,\\ &\|e_{m,i}\|_{H^2(\mathcal{D})} \le c\tau^{q-\frac{1}{2}} \le \tau, \;\; \forall\, 1\le m\le N, \; 1\le i\le q, \end{aligned} \tag{3.15}$$

when τ is small enough, for any $q\ge 2$ and c a constant independent of τ.

Proof. Due to the positive semidefiniteness of M, by (3.13) we have

$$\|e_n+\tau\sum_{i=1}^{q}b_i\dot{e}_{n,i}\|^2\leq\|e_n\|^2+2\tau\sum_{i=1}^{q}b_i(\dot{e}_{n,i},e_{n,i}-\varepsilon_{n,i}). \tag{3.16}$$

Using that $\partial_\nu\tilde{e}_{n,i}=\partial_\nu e_{n,i}=0$ on $\partial\mathcal{D}$, we obtain by (3.8), and by (3.9)

$$\begin{aligned}(\dot{e}_{n,i},&e_{n,i}-\varepsilon_{n,i})=-\delta(\varepsilon)\varepsilon^2\|\Delta e_{n,i}\|^2+\delta(\varepsilon)(\nabla\tilde{e}_{n,i},\nabla\varepsilon_{n,i})+\mu(\varepsilon)\varepsilon^2(\nabla e_{n,i},\nabla\varepsilon_{n,i})-\mu(\varepsilon)\varepsilon^2\|\nabla e_{n,i}\|^2\\
&+\delta(\varepsilon)\Big(\eta_{n,i}W(I^\tau_{n-1}u_{n,i})+r(u(\cdot,t_n+c_i\tau))\Big[W(I^\tau_{n-1}u(t_n+c_i\tau))-W(I^\tau_{n-1}u_{n,i})\Big],\Delta e_{n,i}\Big)\\
&-\mu(\varepsilon)\Big(\eta_{n,i}W(I^\tau_{n-1}u_{n,i})+r(u(\cdot,t_n+c_i\tau))\Big[W(I^\tau_{n-1}u(t_n+c_i\tau))-W(I^\tau_{n-1}u_{n,i})\Big],e_{n,i}\Big)\\
&+\mu(\varepsilon)\Big(\eta_{n,i}W(I^\tau_{n-1}u_{n,i})+r(u(\cdot,t_n+c_i\tau))\Big[W(I^\tau_{n-1}u(t_n+c_i\tau))-W(I^\tau_{n-1}u_{n,i})\Big],\varepsilon_{n,i}\Big)\\
\leq&-\frac{1}{2}\delta(\varepsilon)\varepsilon^2\|\Delta e_{n,i}\|^2-\mu(\varepsilon)\varepsilon^2\|\nabla e_{n,i}\|^2+\frac{1}{2}[\delta(\varepsilon)\varepsilon^{-2}+\mu(\varepsilon)+\mu(\varepsilon)\varepsilon^{-3}]\Big\|\eta_{n,i}W(I^\tau_{n-1}u_{n,i})\\
&+r(u(\cdot,t_n+c_i\tau))\Big[W(I^\tau_{n-1}u(t_n+c_i\tau))-W(I^\tau_{n-1}u_{n,i})\Big]\Big\|^2\\
&+\frac{1}{2}\mu(\varepsilon)\varepsilon^3\|e_{n,i}\|^2+\frac{1}{2}\mu(\varepsilon)\|\varepsilon_{n,i}\|^2+\delta(\varepsilon)(\nabla\tilde{e}_{n,i},\nabla\varepsilon_{n,i})+\mu(\varepsilon)\varepsilon^2(\nabla e_{n,i},\nabla\varepsilon_{n,i}).\end{aligned} \tag{3.17}$$

At this point we state an induction argument, analogous to the argument in [1]: let $1\leq m\leq N$, and let

$$\|e_{n-1,i}\|_{H^2(\mathcal{D})}\leq\tau,\ \text{ for all }\ i=1,\dots,q,\ \text{ and for any }\ n\leq m. \tag{3.18}$$

The above condition at $n=1$ will be imposed on the scheme. This condition, as the H^2 norm bounds L^∞ when $d=2,3$ and obviously when $d=1$, gives that

$$\|e_{n-1,i}\|_{L^\infty(\mathcal{D})}\leq c,\ \text{ for all }\ i=1,\dots,q,\ \text{ and for any }\ n\leq m. \tag{3.19}$$

The previous, and the locally Lipschitz property of W (cf. in [1] (4.23), (4.24)) yield the upper bound

$$\Big\|\eta_{n,i}W(I^\tau_{n-1}u_{n,i})+r(u(\cdot,t_n+c_i\tau))\Big[W(I^\tau_{n-1}u(t_n+c_i\tau))-W(I^\tau_{n-1}u_{n,i})\Big]\Big\|^2\leq c|\eta_{n,i}|^2+c\|e_{n-1,i}\|^2. \tag{3.20}$$

Remark 3.2. *In general the constants in* (3.20) *depend on* ε*. However, if the upper bounds of* $\|u_0\|_\infty$, $E(u_0)$ *are independent of* ε *as* $\varepsilon\to0$*, and for layered initial data so that for small times the solution* u *stays close to* u_0 *with* ε*-independent* L^∞ *bounds, then both* c *of* (3.20) *are independent from* ε*. This is true since* $r(u)$ *is bounded by a constant independent of* ε *(due to the decreasing energy 2d term), while from the induction hypothesis* $\|u_{n-1,i}\|_{L^\infty}\leq\max_t\|u\|_{L^\infty}+c\leq c$*, which yields* $\|W(I^\tau_{n-1}u_{n,i})\|\leq c$ *for* c *independent of* ε*.*

By (3.20) and (3.17), we obtain

$$\begin{aligned}(\dot{e}_{n,i},e_{n,i}-\varepsilon_{n,i})\leq&-\frac{1}{2}\delta(\varepsilon)\varepsilon^2\|\Delta e_{n,i}\|^2-\mu(\varepsilon)\varepsilon^2\|\nabla e_{n,i}\|^2+c[\delta(\varepsilon)\varepsilon^{-2}+\mu(\varepsilon)\varepsilon^{-3}]\Big[|\eta_{n,i}|^2+\|e_{n-1,i}\|^2\Big]\\
&+\frac{1}{2}\mu(\varepsilon)\varepsilon^3\|e_{n,i}\|^2+\frac{1}{2}\mu(\varepsilon)\|\varepsilon_{n,i}\|^2+\delta(\varepsilon)(\nabla\tilde{e}_{n,i},\nabla\varepsilon_{n,i})+\mu(\varepsilon)\varepsilon^2(\nabla e_{n,i},\nabla\varepsilon_{n,i})\\
\leq&-\frac{1}{2}\delta(\varepsilon)\varepsilon^2\|\Delta e_{n,i}\|^2-\frac{1}{2}\mu(\varepsilon)\varepsilon^2\|\nabla e_{n,i}\|^2+c[\delta(\varepsilon)\varepsilon^{-2}+\mu(\varepsilon)\varepsilon^{-3}]\Big[|\eta_{n,i}|^2+\|e_{n-1,i}\|^2\Big]\\
&+\frac{1}{2}\mu(\varepsilon)\varepsilon^3\|e_{n,i}\|^2+\frac{1}{2}\mu(\varepsilon)\|\varepsilon_{n,i}\|^2+\frac{1}{2}\mu(\varepsilon)\varepsilon^2\|\nabla\varepsilon_{n,i}\|^2+\delta(\varepsilon)(\nabla\tilde{e}_{n,i},\nabla\varepsilon_{n,i}).\end{aligned} \tag{3.21}$$

The consistency error $\varepsilon_{n,i}$ satisfies for any $i = 1, \dots, q$

$$\begin{aligned} u(\cdot, t_n + c_i\tau) =& u(\cdot, t_n) + \tau \sum_{j=1}^{q} a_{ij} \dot{u}^*_{n,j} + \varepsilon_{n,i} = u(\cdot, t_n) + \tau \sum_{j=1}^{q} a_{ij} u_t(\cdot, t_{n,j}) \\ & - \tau \sum_{j=1}^{q} a_{ij} \delta(\varepsilon) r(u(\cdot, t_n + c_j\tau)) \Delta[W(u(\cdot, t_n + c_j\tau)) - W(I^\tau_{n-1} u(\cdot, t_n + c_j\tau))] \\ & + \tau \sum_{j=1}^{q} a_{ij} \mu(\varepsilon) r(u(\cdot, t_n + c_j\tau))[W(u(\cdot, t_n + c_j\tau)) - W(I^\tau_{n-1} u(\cdot, t_n + c_j\tau))] + \varepsilon_{n,i}. \end{aligned}$$

Due to the Neumann b.c. of u, Δu, and using that $\nabla(W(v)) = f'(v)\nabla v c(t)$ and $\Delta(W(v)) = (6v|\nabla v|^2 + 3v^2\Delta v - \Delta v)c(t)$, and that the Lagrange polynomial preserves the Neumann b.c. of u, Δu, we have

$$\partial_\nu u_t = \partial_\nu W(u) = \partial_\nu W(I^\tau_{n-1} u) = \partial_\nu \Delta(W(u)) = \partial_\nu \Delta(W(I^\tau_{n-1} u)) = 0 \text{ on } \partial\mathcal{D}.$$

Therefore, we get

$$\partial_\nu \varepsilon_{n,i} = 0 \text{ on } \partial\mathcal{D}. \tag{3.22}$$

So, by the above and (3.9), we have

$$\begin{aligned} \delta(\varepsilon)(\nabla\tilde{e}_{n,i}, \nabla\varepsilon_{n,i}) = -\delta(\varepsilon)(\tilde{e}_{n,i}, \Delta\varepsilon_{n,i}) = -\delta(\varepsilon)\Big(-\varepsilon^2\Delta e_{n,i} + \eta_{n,i} W(I^\tau_{n-1} u_{n,i}) \\ + r(u(\cdot, t_n + c_i\tau))\Big[W(I^\tau_{n-1} u(t_n + c_i\tau)) - W(I^\tau_{n-1} u_{n,i})\Big], \Delta\varepsilon_{n,i}\Big). \end{aligned} \tag{3.23}$$

By (3.23) and (3.21), we get

$$\begin{aligned} (\dot{e}_{n,i}, e_{n,i} - \varepsilon_{n,i}) \le -\frac{1}{4}\delta(\varepsilon)\varepsilon^2\|\Delta e_{n,i}\|^2 - \frac{1}{2}\mu(\varepsilon)\varepsilon^2\|\nabla e_{n,i}\|^2 + c[\delta(\varepsilon)\varepsilon^{-2} + \mu(\varepsilon)\varepsilon^{-3}] \\ \Big[|\eta_{n,i}|^2 + \|e_{n-1,i}\|^2\Big] + \frac{1}{2}\mu(\varepsilon)\varepsilon^3\|e_{n,i}\|^2 + \frac{1}{2}\mu(\varepsilon)\|\varepsilon_{n,i}\|^2 + \frac{1}{2}\mu(\varepsilon)\varepsilon^2\|\nabla\varepsilon_{n,i}\|^2 + 2\delta(\varepsilon)\varepsilon^2\|\Delta\varepsilon_{n,i}\|^2. \end{aligned} \tag{3.24}$$

Using (3.24) in (3.16), we arrive at

$$\begin{aligned} \|e_n + \tau\sum_{i=1}^{q} b_i\dot{e}_{n,i}\|^2 \le \|e_n\|^2 + 2\tau\sum_{i=1}^{q} b_i(\dot{e}_{n,i}, e_{n,i} - \varepsilon_{n,i}) \le \|e_n\|^2 - \frac{1}{2}\delta(\varepsilon)\varepsilon^2\tau\sum_{i=1}^{q} b_i\|\Delta e_{n,i}\|^2 \\ - \mu(\varepsilon)\varepsilon^2\tau\sum_{i=1}^{q} b_i\|\nabla e_{n,i}\|^2 + c[\delta(\varepsilon)\varepsilon^{-2} + \mu(\varepsilon)\varepsilon^{-3}]\tau\sum_{i=1}^{q} b_i|\eta_{n,i}|^2 + c[\delta(\varepsilon)\varepsilon^{-2} + \mu(\varepsilon)\varepsilon^{-3}]\tau\sum_{i=1}^{q} b_i\|e_{n-1,i}\|^2 \\ + \mu(\varepsilon)\varepsilon^3\tau\sum_{i=1}^{q} b_i\|e_{n,i}\|^2 + \frac{1}{2}\tau\sum_{i=1}^{q} b_i\Big[2\mu(\varepsilon)\|\varepsilon_{n,i}\|^2 + 2\mu(\varepsilon)\varepsilon^2\|\nabla\varepsilon_{n,i}\|^2 + 8\delta(\varepsilon)\varepsilon^2\|\Delta\varepsilon_{n,i}\|^2\Big]. \end{aligned} \tag{3.25}$$

Having estimated the first term of (3.13), we proceed to estimate the rest of the right-hand side. Recall from (3.7) that $u(\cdot, t_{n+1}) = u(\cdot, t_n) + \tau\sum_{i=1}^{q} b_i\dot{u}^*_{n,i} + \varepsilon_{n+1}$. So, we have

$$\begin{aligned} u(\cdot, t_n) =& u(\cdot, t_n) + \tau\sum_{i=1}^{q} b_i\dot{u}^*_{n,i} + \varepsilon_{n+1} = u(\cdot, t_n) + \tau\sum_{i=1}^{q} b_i u_t(\cdot, t_{n,i}) \\ & - \tau\sum_{i=1}^{q} b_i\delta(\varepsilon) r(u(\cdot, t_n + c_i\tau))\Delta[W(u(\cdot, t_n + c_i\tau)) - W(I^\tau_{n-1} u(\cdot, t_n + c_i\tau))] \\ & + \tau\sum_{i=1}^{q} b_i\mu(\varepsilon) r(u(\cdot, t_n + c_i\tau))[W(u(\cdot, t_n + c_i\tau)) - W(I^\tau_{n-1} u(\cdot, t_n + c_i\tau))] + \varepsilon_{n+1}, \end{aligned}$$

which yields as in (3.22) that

$$\partial_\nu \varepsilon_{n+1} = 0 \quad \text{on} \quad \partial\mathcal{D}. \tag{3.26}$$

Moreover, recall that $\partial_\nu \tilde{e}_{n,i} = 0$ on $\partial\mathcal{D}$. Applying integration by parts and the previous b.c. together with (3.26), and by using (3.8) when replacing $\dot{e}_{n,i}$, we get

$$
\begin{aligned}
2(\varepsilon_{n+1}, e_n + \tau\sum_{i=1}^q b_i\dot{e}_{n,i}) + \|\varepsilon_{n+1}\|^2 &= 2(\varepsilon_{n+1}, e_n) + 2\delta(\varepsilon)\tau\Big(\Delta\varepsilon_{n+1}, \sum_{i=1}^q b_i\tilde{e}_{n,i}\Big) \\
&\quad - 2\mu(\varepsilon)\tau\Big(\varepsilon_{n+1}, \sum_{i=1}^q b_i\tilde{e}_{n,i}\Big) + \|\varepsilon_{n+1}\|^2 \\
&\le 2\tau\|\varepsilon_{n+1}/\tau\|\|e_n\| + 2\delta(\varepsilon)\tau\Big(\Delta\varepsilon_{n+1}, \sum_{i=1}^q b_i\tilde{e}_{n,i}\Big) - 2\mu(\varepsilon)\tau\Big(\varepsilon_{n+1}, \sum_{i=1}^q b_i\tilde{e}_{n,i}\Big) + \|\varepsilon_{n+1}\|^2.
\end{aligned}
\tag{3.27}
$$

Replacing now $\tilde{e}_{n,i}$ by (3.9), since $\partial_\nu e_{n,i} = 0$ on $\partial\mathcal{D}$, and due to (3.20), we get

$$
\begin{aligned}
&2(\varepsilon_{n+1}, e_n + \tau\sum_{i=1}^q b_i\dot{e}_{n,i}) + \|\varepsilon_{n+1}\|^2 \le 2\tau\|\varepsilon_{n+1}/\tau\|\|e_n\| \\
&+ 2\delta(\varepsilon)\tau\Big(\Delta\varepsilon_{n+1}, \sum_{i=1}^q b_i\Big[-\varepsilon^2\Delta e_{n,i} + \eta_{n,i}W(I^\tau_{n-1}, u_{n,i}) \\
&\qquad + r(u(\cdot, t_n + c_i\tau))\Big(W(I^\tau_{n-1}u(t_n + c_i\tau)) - W(I^\tau_{n-1}u_{n,i})\Big)\Big]\Big) \\
&- 2\mu(\varepsilon)\tau\Big(\varepsilon_{n+1}, \sum_{i=1}^q b_i\Big[-\varepsilon^2\Delta e_{n,i} + \eta_{n,i}W(I^\tau_{n-1}, u_{n,i}) \\
&\qquad + r(u(\cdot, t_n + c_i\tau))\Big(W(I^\tau_{n-1}u(t_n + c_i\tau)) - W(I^\tau_{n-1}u_{n,i})\Big)\Big]\Big) + \|\varepsilon_{n+1}\|^2,
\end{aligned}
$$

and so,

$$
\begin{aligned}
&2(\varepsilon_{n+1}, e_n + \tau\sum_{i=1}^q b_i\dot{e}_{n,i}) + \|\varepsilon_{n+1}\|^2 \le 2\tau\|\varepsilon_{n+1}/\tau\|\|e_n\| + \frac{1}{4}\delta(\varepsilon)\varepsilon^2\tau\sum_{i=1}^q b_i\|\Delta e_{n,i}\|^2 \\
&+ \frac{1}{2}\mu(\varepsilon)\varepsilon^2\tau\sum_{i=1}^q b_i\|\nabla e_{n,i}\|^2 + c[\delta(\varepsilon) + \mu(\varepsilon)]\tau\sum_{i=1}^q b_i|\eta_{n,i}|^2 + c[\delta(\varepsilon) + \mu(\varepsilon)]\tau\sum_{i=1}^q b_i\|e_{n-1,i}\|^2 \\
&+ c\delta(\varepsilon)\varepsilon^2\tau\|\Delta\varepsilon_{n+1}\|^2 + c\mu(\varepsilon)\varepsilon^2\tau\|\nabla\varepsilon_{n+1}\|^2 + \|\varepsilon_{n+1}\|^2.
\end{aligned}
\tag{3.28}
$$

Collecting all the terms, and by (3.13), (3.25) and (3.28), for $\varepsilon < 1$, we arrive at

$$
\begin{aligned}
\|e_{n+1}\|^2 \le &\|e_n\|^2 - \frac{1}{4}\delta(\varepsilon)\varepsilon^2\tau\sum_{i=1}^q b_i\|\Delta e_{n,i}\|^2 - \frac{1}{2}\mu(\varepsilon)\varepsilon^2\tau\sum_{i=1}^q b_i\|\nabla e_{n,i}\|^2 \\
&+ c[\delta(\varepsilon)\varepsilon^{-2} + \mu(\varepsilon)\varepsilon^{-3}]\tau\sum_{i=1}^q b_i|\eta_{n,i}|^2 + c[\delta(\varepsilon)\varepsilon^{-2} + \mu(\varepsilon)\varepsilon^{-3}]\tau\sum_{i=1}^q b_i\|e_{n-1,i}\|^2 \\
&+ \mu(\varepsilon)\varepsilon^3\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2 + \frac{1}{2}\tau\sum_{i=1}^q b_i\Big[2\mu(\varepsilon)\|\varepsilon_{n,i}\|^2 + 2\mu(\varepsilon)\varepsilon^2\|\nabla\varepsilon_{n,i}\|^2 + 8\delta(\varepsilon)\varepsilon^2\|\Delta\varepsilon_{n,i}\|^2\Big] \\
&+ 2\tau\|\varepsilon_{n+1}/\tau\|\|e_n\| + c\delta(\varepsilon)\varepsilon^2\tau\|\Delta\varepsilon_{n+1}\|^2 + c\mu(\varepsilon)\varepsilon^2\tau\|\nabla\varepsilon_{n+1}\|^2 + \|\varepsilon_{n+1}\|^2.
\end{aligned}
\tag{3.29}
$$

By the second equation of (3.12), we have

$$
|\eta_{n+1}|^2 \le (1 + c\tau)|\eta_n + \tau\sum_{i=1}^q b_i\dot{\eta}_{n,i}|^2 + (1 + c\tau^{-1})|d_{n+1}|^2.
\tag{3.30}
$$

The second equation of (3.11) and the algebraic stability of the Runge-Kutta method yield

$$|\eta_n+\tau\sum_{i=1}^{q}b_i\dot\eta_{n,i}|^2\le|\eta_n|^2+2\tau\sum_{i=1}^{q}b_i|\dot\eta_{n,i}|^2+\tau\sum_{i=1}^{q}b_i|\eta_{n,i}|^2+\tau\sum_{i=1}^{q}b_i|d_{n,i}|^2. \tag{3.31}$$

We observe now that $W(v)=f(v)c(t)$ and thus, $\nabla(W(v))=c(t)f'(v)\nabla v$, which gives, for $v:=I^\tau_{n-1}u(\cdot,t_{n,i})$, $\nabla(W(I^\tau_{n-1}u(\cdot,t_{n,i}))=c(t)f'(I^\tau_{n-1}u(\cdot,t_{n,i}))\nabla(I^\tau_{n-1}u(\cdot,t_{n,i}))$. By the definition of $I^\tau_{n-1}u(\cdot,t_{n,i})$ which is implemented by extrapolation in t by using the values $u_{n-1,i}$ for $i=1,\dots,q$, and due to the Neumann b.c. of $u(\cdot,t_{n,i})$ on $\partial\mathcal{D}$ for all n, i, it follows that the Neumann b.c. is satisfied as well by $I^\tau_{n-1}u(\cdot,t_{n,i})$, and therefore

$$\partial_\nu(W(I^\tau_{n-1}u(\cdot,t_{n,i})))=0 \quad\text{on}\quad \partial\mathcal{D}. \tag{3.32}$$

The same argument follows for $\partial_\nu\Delta(W(I^\tau_{n-1}u(\cdot,t_{n,i})))$ due to the Neumann condition of Δu, i.e.,

$$\partial_\nu\Delta(W(I^\tau_{n-1}u(\cdot,t_{n,i})))=0 \quad\text{on}\quad \partial\mathcal{D}. \tag{3.33}$$

We use the first equation of (3.11), we apply integration by parts and use the b.c. (3.32), (3.33), and the Neumann b.c. of $\tilde e_{n,i}$, $\Delta\tilde e_{n,i}$ to arrive at

$$\begin{aligned}&|\dot\eta_{n,i}|^2\le c\Big\|W(I^\tau_{n-1}u(t_n+c_i\tau))-W(I^\tau_{n-1}u_{n,i})\Big\|^2+c(W(I^\tau_{n-1}u_{n,i}),\dot e_{n,i})^2\le c\|e_{n-1,i}\|^2\\&\quad+c(W(I^\tau_{n-1}u_{n,i}),\dot e_{n,i})^2=c\|e_{n-1,i}\|^2+\mathcal{H}+c(W(I^\tau_{n-1}u(\cdot,t_{n,i})),\dot e_{n,i})^2=c\|e_{n-1,i}\|^2+\mathcal{H}\\&\quad+c[(\Delta(W(I^\tau_{n-1}u(\cdot,t_{n,i}))),\delta(\varepsilon)\tilde e_{n,i})-(W(I^\tau_{n-1}u(\cdot,t_{n,i})),\mu(\varepsilon)\tilde e_{n,i})]^2\\&\le c\|e_{n-1,i}\|^2+\mathcal{H}+c[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\|e_{n,i}\|^2+c[\delta(\varepsilon)^2+\mu(\varepsilon)^2]|\eta_{n,i}|^2+c[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\|e_{n-1,i}\|^2,\end{aligned} \tag{3.34}$$

for $\mathcal{H}:=c(W(I^\tau_{n-1}u_{n,i})-W(I^\tau_{n-1}u(\cdot,t_{n,i})),\dot e_{n,i})^2$. In the above, we integrated two times by parts the term $\varepsilon^2\Delta e_{n,i}$ stemming from $(\Delta(W(I^\tau_{n-1}u(\cdot,t_{n,i}))),\delta(\varepsilon)\tilde e_{n,i})$, and from $(W(I^\tau_{n-1}u(\cdot,t_{n,i})),\mu(\varepsilon)\tilde e_{n,i})$ after we replaced $\tilde e_{n,i}$ by (3.9), and then used (3.20). Here we need initial data smooth enough in space (in $H^6(\mathcal{D})$) so that $\|\Delta^2(W(I^\tau_{n-1}u(\cdot,t_{n,i})))\|^2$, $\|\Delta(W(I^\tau_{n-1}u(\cdot,t_{n,i})))\|^2$ are bounded by $c=c(\varepsilon)$ in general. In this way we reduced the norms at the right and only the L^2 norm of $e_{n,i}$ appears, which will be bounded summed by $\|e_n\|$ and higher order terms in τ including $\Delta e_{n,i}$, see (3.45) and the preceding inequality there.

We use now (3.34) in (3.31), and obtain

$$\begin{aligned}|\eta_n+\tau\sum_{i=1}^{q}b_i\dot\eta_{n,i}|^2&\le|\eta_n|^2+c\tau\sum_{i=1}^{q}b_i\Big[[1+\delta(\varepsilon)^2+\mu(\varepsilon)^2]\|e_{n-1,i}\|^2\\&+\mathcal{H}+[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\|e_{n,i}\|^2+[\delta(\varepsilon)^2+\mu(\varepsilon)^2]|\eta_{n,i}|^2\Big]+\tau\sum_{i=1}^{q}b_i|\eta_{n,i}|^2+\tau\sum_{i=1}^{q}b_i|d_{n,i}|^2.\end{aligned} \tag{3.35}$$

So, (3.35) and (3.30) yield for $\tau<1$

$$\begin{aligned}|\eta_{n+1}|^2\le&(1+c\tau)|\eta_n|^2+c\tau\sum_{i=1}^{q}b_i\Big[[1+\delta(\varepsilon)^2+\mu(\varepsilon)^2]\|e_{n-1,i}\|^2+\mathcal{H}+[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\|e_{n,i}\|^2\\&+[\delta(\varepsilon)^2+\mu(\varepsilon)^2]|\eta_{n,i}|^2\Big]+c\tau\sum_{i=1}^{q}b_i|\eta_{n,i}|^2+c\tau\sum_{i=1}^{q}b_i|d_{n,i}|^2+(1+c\tau^{-1})|d_{n+1}|^2.\end{aligned} \tag{3.36}$$

Adding (3.36) and (3.29), we get

$$
\begin{aligned}
&\|e_{n+1}\|^2+|\eta_{n+1}|^2+\frac{1}{4}\delta(\varepsilon)\varepsilon^2\tau\sum_{i=1}^q b_i\|\Delta e_{n,i}\|^2+\frac{1}{2}\mu(\varepsilon)\varepsilon^2\tau\sum_{i=1}^q b_i\|\nabla e_{n,i}\|^2\leq\\
&\|e_n\|^2+(1+c\tau)|\eta_n|^2+c[\delta(\varepsilon)\varepsilon^{-2}+\mu(\varepsilon)\varepsilon^{-3}]\tau\sum_{i=1}^q b_i|\eta_{n,i}|^2+c[\delta(\varepsilon)\varepsilon^{-2}+\mu(\varepsilon)\varepsilon^{-3}]\tau\sum_{i=1}^q b_i\|e_{n-1,i}\|^2\\
&+\mu(\varepsilon)\varepsilon^3\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2+\frac{1}{2}\tau\sum_{i=1}^q b_i\Big[2\mu(\varepsilon)\|\varepsilon_{n,i}\|^2+2\mu(\varepsilon)\varepsilon^2\|\nabla\varepsilon_{n,i}\|^2+8\delta(\varepsilon)\varepsilon^2\|\Delta\varepsilon_{n,i}\|^2\Big]\\
&+2\tau\|\varepsilon_{n+1}/\tau\|\|e_n\|+c\delta(\varepsilon)\varepsilon^2\tau\|\Delta\varepsilon_{n+1}\|^2+c\mu(\varepsilon)\varepsilon^2\tau\|\nabla\varepsilon_{n+1}\|^2+\|\varepsilon_{n+1}\|^2\\
&+c\tau\sum_{i=1}^q b_i\Big[[1+\delta(\varepsilon)^2+\mu(\varepsilon)^2]\|e_{n-1,i}\|^2+[\delta(\varepsilon)^2+\mu(\varepsilon)^2]|\eta_{n,i}|^2\Big]+c\tau\sum_{i=1}^q b_i|\eta_{n,i}|^2\\
&+c\tau\sum_{i=1}^q b_i|d_{n,i}|^2+(1+c\tau^{-1})|d_{n+1}|^2+c\tau\sum_{i=1}^q b_i\mathcal{H}+c[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2=:\mathcal{A},
\end{aligned}
\tag{3.37}
$$

$$
\begin{aligned}
\mathcal{A}\leq&(1+c\tau)\|e_n\|^2+(1+c\tau)|\eta_n|^2+c[1+\delta(\varepsilon)\varepsilon^{-2}+\mu(\varepsilon)\varepsilon^{-3}+\delta(\varepsilon)^2+\mu(\varepsilon)^2]\tau\sum_{i=1}^q b_i|\eta_{n,i}|^2\\
&+c[1+\delta(\varepsilon)\varepsilon^{-2}+\mu(\varepsilon)\varepsilon^{-3}+\delta(\varepsilon)^2+\mu(\varepsilon)^2]\tau\sum_{i=1}^q b_i\|e_{n-1,i}\|^2+\mu(\varepsilon)\varepsilon^3\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2\\
&+\frac{1}{2}\tau\sum_{i=1}^q b_i\Big[2\mu(\varepsilon)\|\varepsilon_{n,i}\|^2+2\mu(\varepsilon)\varepsilon^2\|\nabla\varepsilon_{n,i}\|^2+8\delta(\varepsilon)\varepsilon^2\|\Delta\varepsilon_{n,i}\|^2\Big]\\
&+c\tau\|\varepsilon_{n+1}/\tau\|^2+c\delta(\varepsilon)\varepsilon^2\tau\|\Delta\varepsilon_{n+1}\|^2+c\mu(\varepsilon)\varepsilon^2\tau\|\nabla\varepsilon_{n+1}\|^2+\|\varepsilon_{n+1}\|^2\\
&+c\tau\sum_{i=1}^q b_i|d_{n,i}|^2+(1+c\tau^{-1})|d_{n+1}|^2+c\tau\sum_{i=1}^q b_i\mathcal{H}+c[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2.
\end{aligned}
\tag{3.38}
$$

Remark 3.3. *The next consistency error estimate holds true*

$$
\|\varepsilon_{n+1}\|_{H^2(\mathcal{D})}+|d_{n+1}|+\tau\sum_{i=1}^q(\|\varepsilon_{n,i}\|_{H^2(\mathcal{D})}+|d_{n,i}|)\leq c\tau^{q+1}.
\tag{3.39}
$$

The proof of the above is analogous to this of Lemma 4.1 of [1] *proven for the Allen-Cahn equation. However, due to the 4-th order CH/AC equation we considered, $H^2(\mathcal{D})$ consistency estimates are needed for the error analysis. These follow if we assume smooth enough initial data, resulting in a regular solution. More specifically, the expansions in Lemma 4.1 of* [1] *involve time derivatives of the continuous problem solution. By using there $H^2(\mathcal{D})$ norms in place of $H^1(\mathcal{D})$ yields the result.*

By (3.39), we obtain

$$
\begin{aligned}
&\frac{1}{2}\tau\sum_{i=1}^q b_i\Big[2\mu(\varepsilon)\|\varepsilon_{n,i}\|^2+2\mu(\varepsilon)\varepsilon^2\|\nabla\varepsilon_{n,i}\|^2+8\delta(\varepsilon)\varepsilon^2\|\Delta\varepsilon_{n,i}\|^2\Big]+c\tau\|\varepsilon_{n+1}/\tau\|^2+c\delta(\varepsilon)\varepsilon^2\tau\|\Delta\varepsilon_{n+1}\|^2\\
&+c\mu(\varepsilon)\varepsilon^2\tau\|\nabla\varepsilon_{n+1}\|^2+\|\varepsilon_{n+1}\|^2+c\tau\sum_{i=1}^q b_i|d_{n,i}|^2+(1+c\tau^{-1})|d_{n+1}|^2\leq c\tau^{2q+1}.
\end{aligned}
\tag{3.40}
$$

Due to the bound (3.40), (3.38), and (3.37), for $\mathcal{J} := 1+\delta(\varepsilon)\varepsilon^{-2}+\mu(\varepsilon)\varepsilon^{-3}+\delta(\varepsilon)^2+\mu(\varepsilon)^2$, we arrive at

$$\begin{aligned}&\|e_{n+1}\|^2+|\eta_{n+1}|^2+\frac{1}{4}\delta(\varepsilon)\varepsilon^2\tau\sum_{i=1}^q b_i\|\Delta e_{n,i}\|^2+\frac{1}{2}\mu(\varepsilon)\varepsilon^2\tau\sum_{i=1}^q b_i\|\nabla e_{n,i}\|^2\le\mathcal{A}\le(1+c\tau)\|e_n\|^2\\&+(1+c\tau)|\eta_n|^2+c\mathcal{J}\tau\sum_{i=1}^q b_i|\eta_{n,i}|^2+c\mathcal{J}\tau\sum_{i=1}^q b_i\|e_{n-1,i}\|^2+\mu(\varepsilon)\varepsilon^3\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2+c\tau^{2q+1}+c\tau\sum_{i=1}^q b_i\mathcal{H}\\&+c[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2.\end{aligned}\tag{3.41}$$

We use now the second equation of (3.11), i.e., $\eta_{n,i}=\eta_n+\tau\sum_{j=1}^q a_{ij}\dot{\eta}_{n,j}+d_{n,i}$, which yields that

$$|\eta_{n,i}|^2\le c|\eta_n|^2+c\tau^2\Big(\sum_{j=1}^q a_{ij}\dot{\eta}_{n,j}\Big)^2+c|d_{n,i}|^2\le c|\eta_n|^2+c\tau^2\sum_{j=1}^q|\dot{\eta}_{n,j}|^2+c|d_{n,i}|^2.$$

So, by (3.34) and the above, we get

$$\begin{aligned}|\eta_{n,i}|^2\le& c|\eta_n|^2+c\tau^2\sum_{j=1}^q|\dot{\eta}_{n,j}|^2+c|d_{n,i}|^2\le c|\eta_n|^2+c\tau^2\sum_{i=1}^q b_i\mathcal{H}+c\tau^2[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\sum_{j=1}^q\|e_{n,j}\|^2\\&+c\tau^2[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\sum_{j=1}^q|\eta_{n,j}|^2+c\tau^2[1+\delta(\varepsilon)^2+\mu(\varepsilon)^2]\sum_{j=1}^q\|e_{n-1,j}\|^2+c|d_{n,i}|^2.\end{aligned}\tag{3.42}$$

Therefore, by the estimate (3.39) it follows that

$$\begin{aligned}&\tau\sum_{i=1}^q b_i|\eta_{n,i}|^2\le c\tau|\eta_n|^2+c\tau^3\sum_{i=1}^q b_i\mathcal{H}+c\tau^3[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\sum_{i=1}^q\|e_{n,i}\|^2+c\tau^3[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\sum_{i=1}^q|\eta_{n,i}|^2\\&+c\tau^3[1+\delta(\varepsilon)^2+\mu(\varepsilon)^2]\sum_{i=1}^q\|e_{n-1,i}\|^2+c\tau\sum_{i=1}^q b_i|d_{n,i}|^2\le c\tau|\eta_n|^2+c\tau^3[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\sum_{i=1}^q\|e_{n,i}\|^2\\&+c\tau^3[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\sum_{i=1}^q|\eta_{n,i}|^2+c\tau^3[1+\delta(\varepsilon)^2+\mu(\varepsilon)^2]\sum_{i=1}^q\|e_{n-1,i}\|^2+c\tau^3\sum_{i=1}^q b_i\mathcal{H}+c\tau^{2q+1}.\end{aligned}\tag{3.43}$$

So, for $\tau<G(\delta(\varepsilon),\mu(\varepsilon),\varepsilon)$ small enough, (3.43) and (3.41) give

$$\begin{aligned}&\|e_{n+1}\|^2+|\eta_{n+1}|^2+\frac{1}{8}\delta(\varepsilon)\varepsilon^2\tau\sum_{i=1}^q b_i\|\Delta e_{n,i}\|^2+\frac{1}{2}\mu(\varepsilon)\varepsilon^2\tau\sum_{i=1}^q b_i\|\nabla e_{n,i}\|^2\\&\le(1+c\tau)\|e_n\|^2+(1+c\tau)|\eta_n|^2+c[1+\delta(\varepsilon)\varepsilon^{-2}+\mu(\varepsilon)\varepsilon^{-3}+\delta(\varepsilon)^2+\mu(\varepsilon)^2]\tau\sum_{i=1}^q b_i\|e_{n-1,i}\|^2\\&+\mu(\varepsilon)\varepsilon^3\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2+c\tau\sum_{i=1}^q b_i\mathcal{H}+c[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2+c\tau^{2q+1}\\&\le(1+c\tau)\|e_n\|^2+(1+c\tau)|\eta_n|^2+c[1+\delta(\varepsilon)\varepsilon^{-2}+\mu(\varepsilon)\varepsilon^{-3}+\delta(\varepsilon)^2+\mu(\varepsilon)^2]\tau\sum_{i=1}^q b_i\|e_{n-1,i}\|^2\\&+\mu(\varepsilon)\varepsilon^3\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2+c\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2+c\tau\|e_n\|^2+c[\delta(\varepsilon)^2+\mu(\varepsilon)^2]\varepsilon^4\tau\sum_{i=1}^q b_i\|e_{n,i}\|^2+c\tau^{2q+1},\end{aligned}\tag{3.44}$$

where we used that $\dot{e}_{n,i} \leq c\tau^{-1}\sum_{j=1}^{q}(\|e_{n,j}-e_n\|+\|\varepsilon_{n,j}\|)$ ([1]), which yielded by the induction hypothesis that $c\tau\sum_{i=1}^{q} b_i\mathcal{H} \leq c\tau\sum_{i=1}^{q} b_i\|e_{n,i}\|^2 + c\tau\|e_n\|^2 + c\tau^{2q+1}$. By (3.10) (as in [1] after (4.30)), we have

$$\sum_{i=1}^{q}\|e_{n,i}\|^2 \leq c\|e_n\|^2 + c\tau\sum_{i,j=1}^{q} a_{ij}(\dot{e}_{n,j}, e_{n,i}) + c\sum_{i=1}^{q}\|\varepsilon_{n,i}\|^2 = c\|e_n\|^2 + c\tau\sum_{i,j=1}^{q} a_{ij}\Big(\delta(\varepsilon)\Delta\Big[-\varepsilon^2\Delta e_{n,j}$$
$$+\eta_{n,j}W(I_{n-1}^{\tau}u_{n,j}) + r(u(\cdot,t_n+c_j\tau))\Big[W(I_{n-1}^{\tau}u(t_n+c_j\tau)) - W(I_{n-1}^{\tau}u_{n,j})\Big]\Big], e_{n,i}\Big) - c\tau\sum_{i,j=1}^{q} a_{ij}\Big(\mu(\varepsilon)$$
$$\Big[-\varepsilon^2\Delta e_{n,j} + \eta_{n,j}W(I_{n-1}^{\tau}u_{n,j}) + r(u(\cdot,t_n+c_j\tau))\Big[W(I_{n-1}^{\tau}u(t_n+c_j\tau)) - W(I_{n-1}^{\tau}u_{n,j})\Big]\Big], e_{n,i}\Big) + c\sum_{i=1}^{q}\|\varepsilon_{n,i}\|^2$$

where we used (3.8) and (3.9). Integration by parts and using that $r(u)$, $\eta_{n,j}$ are independent of x, and since $\partial_\nu\Delta e_{n,i} = \partial_\nu e_{n,i} = \partial_\nu(W(I_{n-1}^{\tau}u(t_n+c_j\tau))) = \partial_\nu(W(I_{n-1}^{\tau}u_{n,j})) = 0$ on $\partial\mathcal{D}$ then yields

$$\sum_{i=1}^{q}\|e_{n,i}\|^2 \leq c\|e_n\|^2 + c\tau\sum_{i,j=1}^{q} a_{ij}\Big(\delta(\varepsilon)\Big[-\varepsilon^2\Delta e_{n,j} + \eta_{n,j}W(I_{n-1}^{\tau}u_{n,j}) + r(u(\cdot,t_n+c_j\tau))\Big[W(I_{n-1}^{\tau}u(t_n+c_j\tau))$$
$$- W(I_{n-1}^{\tau}u_{n,j})\Big]\Big], \Delta e_{n,i}\Big) - c\tau\sum_{i,j=1}^{q} a_{ij}\Big(\mu(\varepsilon)\Big[-\varepsilon^2\Delta e_{n,j} + \eta_{n,j}W(I_{n-1}^{\tau}u_{n,j}) + r(u(\cdot,t_n+c_j\tau))$$
$$\Big[W(I_{n-1}^{\tau}u(t_n+c_j\tau)) - W(I_{n-1}^{\tau}u_{n,j})\Big]\Big], e_{n,i}\Big) + c\sum_{i=1}^{q}\|\varepsilon_{n,i}\|^2 \leq c\|e_n\|^2 + c\tau\sum_{i=1}^{q}[\delta(\varepsilon)\varepsilon^2 + \delta(\varepsilon)^2 + \varepsilon^4]\|\Delta e_{n,i}\|^2$$
$$+ c\tau\sum_{i=1}^{q}(|\eta_{n,i}|^2 + \|e_{n-1,i}\|^2) + c\tau\sum_{i=1}^{q}\mu(\varepsilon)^2\|e_{n,i}\|^2 + c\sum_{i=1}^{q}\|\varepsilon_{n,i}\|^2$$

where we used (3.20). Therefore, we get for $\mathcal{G} := \mu(\varepsilon)\varepsilon^3 + 1 + [\delta(\varepsilon)^2 + \mu(\varepsilon)^2]\varepsilon^4$

$$\begin{aligned}\mathcal{G}\tau\sum_{i=1}^{q} b_i\|e_{n,i}\|^2 \leq c\mathcal{G}\Big[\tau\|e_n\|^2 + \tau^2\sum_{i=1}^{q}[\delta(\varepsilon)\varepsilon^2 + \delta(\varepsilon)^2 + \varepsilon^4]\|\Delta e_{n,i}\|^2 \\ + \tau^2\sum_{i=1}^{q}(|\eta_{n,i}|^2 + \|e_{n-1,i}\|^2) + \tau^2\sum_{i=1}^{q}\mu(\varepsilon)^2\|e_{n,i}\|^2 + c\tau^{2q+1}\Big],\end{aligned} \tag{3.45}$$

where we used (3.40) and that $b_i > 0$. By (3.45), and by (3.43) as $b_i > 0$, and for $\tau < M(\delta(\varepsilon), \mu(\varepsilon), \varepsilon)$ small enough, we bound

$$(\mu(\varepsilon)\varepsilon^3 + 1 + [\delta(\varepsilon)^2 + \mu(\varepsilon)^2]\varepsilon^4)\tau\sum_{i=1}^{q} b_i\|e_{n,i}\|^2$$

by the existing terms in (3.44) apart from $1\|e_n\|^2$. This gives for some $c_1(\varepsilon) > 0$ (never vanishing for any $\delta > 0$, $\mu \geq 0$)

$$\begin{aligned}\|e_{n+1}\|^2 + |\eta_{n+1}|^2 + \frac{1}{16}\delta(\varepsilon)\varepsilon^2\tau\sum_{i=1}^{q} b_i\|\Delta e_{n,i}\|^2 + \frac{1}{2}\mu(\varepsilon)\varepsilon^2\tau\sum_{i=1}^{q} b_i\|\nabla e_{n,i}\|^2 + c_1(\varepsilon)\tau\sum_{i=1}^{q} b_i\|e_{n,i}\|^2 \\ \leq (1+c\tau)\|e_n\|^2 + (1+c\tau)|\eta_n|^2 + c_1(\varepsilon)\tau\sum_{i=1}^{q} b_i\|e_{n-1,i}\|^2 + c\tau^{2q+1}.\end{aligned} \tag{3.46}$$

By taking maximum for $1 \leq n \leq m$ and using (3.14), then (3.15) is derived. This completes the induction for $q \geq 2$ for $\tau < \min\{c(\varepsilon)^{-2}, 1\}$ for $c = c(\varepsilon)$ this of the estimate (3.15). The smallness of $c(\varepsilon)$ is independent of m, [1]. ∎

Remark 3.4. *As in (4.34) of* [1], $\|\dot{e}_{n,i}\| \leq c\tau^{q-\frac{3}{2}}$, *while by* (3.8), (3.9) *and since* δ, μ *are non-negative we get* $\|\nabla\tilde{e}_{n,i}\|^2 \leq c\|\dot{e}_{n,i}\|^2$. *Using then* (3.42), *we obtain* $\|\tilde{e}_{n,i}\|_{H^2(\mathcal{D})} \leq c\tau^{q-\frac{3}{2}}$, $\forall\, 1 \leq n \leq N$, $1 \leq i \leq q$.

Remark 3.5. *Since $\partial_\nu e_{n,i} = \partial_\nu \Delta e_{n,i} = 0$ on $\partial\mathcal{D}$, we have $\|e_{n,i}\|_{H^2(\mathcal{D})} \sim \|e_{n,i}\| + \|\Delta e_{n,i}\|$, and thus for $\mu(\varepsilon) = 0$ (Cahn-Hilliard case)* (3.15) *is valid. When $\delta(\varepsilon) = 0$ (Allen-Cahn case) the Laplacian term is missing at* (3.46)*; we refer to* [1] *for the derivation of an $\mathcal{O}(\tau^{q-3/2})$ H^2-estimate there.*

Remark 3.6. *A rescaling $u(x,t) \to v(z,r)$ as presented at the introduction, and for $\frac{\delta(\varepsilon)}{\mu(\varepsilon)\varepsilon^2} = \mathcal{O}(1)$, would have led to optimal order numerical approximations for $v(z,r)$, $z \in \mathcal{D}$, $r \in (0,T)$, with $\tau(r) = \mathcal{O}(1)$ (ε-independent), and subsequently of $u(x,t)$, but there only for any x such that $|x| \le c\varepsilon$, and any $t \le c\mu(\varepsilon)^{-1}$. In case of the Allen-Cahn dominance ($\frac{\delta(\varepsilon)}{\mu(\varepsilon)\varepsilon^2} \ll 1$) the order of convergence in ε of the 2d of* (3.15) *would approximate the Allen-Cahn reduced order.*

4. Numerical experiments

In this section, we construct a fully-discrete space-time scheme, and then present the results of a series of numerical experiments for the ε-dependent Cahn-Hilliard/Allen-Cahn problem (1.1) for various choices of the weights $\delta(\varepsilon)$, $\mu(\varepsilon)$.

4.1. **The fully-discrete scheme.** As in [1], the linearized RK method defined by (2.2), (2.3), (2.4) will be applied on a spatially semi-discrete scheme of conforming piece-wise quadratic finite elements, which is given as follows: Let $S_h = \text{span}\{\varphi_1, \dots, \varphi_J\}$, $h < 1$, be the finite element space on $\mathcal{D}$, we seek $u_h(x,t), w_h(x,t) \in S_h$, and $R(t) \in \mathbb{R}$ such that

$$\begin{aligned}
&\big(u_{h,t}, v_h\big) = \delta(\varepsilon)\big(\nabla w_h, \nabla v_h\big) + \mu(\varepsilon)\big(w_h, v_h\big),\ \forall v_h \in S_h,\\
&\big(w_h, v_h\big) = -\varepsilon^2\big(\nabla u_h, \nabla v_h\big) - R\big(W_h(u_h), v_h\big),\ \forall v_h \in S_h, \quad R_t = \frac{1}{2}\big(W_h(u_h), u_{h,t}\big),
\end{aligned}$$

where $(\cdot,\cdot)$ denotes the $L^2(\mathcal{D})$ inner product, and $W_h\big(u_h\big) := f(u_h)\big(\int_{\mathcal{D}} F(u_h)dx + E_0\big)^{-1/2}$.

Let

$$u_h = \sum_{i=1}^{J} u_i(t)\varphi_i, \quad w_h = \sum_{i=1}^{J} w_i(t)\varphi_i, \quad U := [u_1(t), \dots, u_J(t)]^T, \quad V := [w_1(t), \dots, w_J(t)]^T.$$

Then, the above equations can be rewritten as

$$AU_t = \delta(\varepsilon)BV + \mu(\varepsilon)AV, \quad AV = -\varepsilon^2 BU - R\mathcal{F}(U), \quad R_t = \frac{1}{2}\mathcal{F}(U)^T U_t,$$

for

$$A := \big[\big(\varphi_j, \varphi_i\big)\big]_{J\times J}, \quad B := \big[\big(\nabla\varphi_j, \nabla\varphi_i\big)\big]_{J\times J}, \quad \mathcal{F}(U) = \big[\big(W_h(u_h), \varphi_1\big), \dots, \big(W_h(u_h), \varphi_J\big)\big]^T.$$

By substituting V in the first equation of the above, we obtain

$$\begin{aligned}
&U_t = -\varepsilon^2\big(\delta(\varepsilon)A^{-1}BA^{-1}B + \mu(\varepsilon)A^{-1}B\big)U - R\big(\delta(\varepsilon)A^{-1}BA^{-1} + \mu(\varepsilon)A^{-1}\big)\mathcal{F}(U) := M_1U + M_2\mathcal{F}(U)R\\
&R_t = \frac{1}{2}\mathcal{F}(U)^T U_t = \frac{1}{2}\mathcal{F}(U)^T M_1 U + R\frac{1}{2}\mathcal{F}(U)^T M_2\mathcal{F}(U),
\end{aligned} \tag{4.1}$$

where $M_1 := -\varepsilon^2\big(\delta(\varepsilon)A^{-1}BA^{-1}B + \mu(\varepsilon)A^{-1}B\big)$ and $M_2 := \big(\delta(\varepsilon)A^{-1}BA^{-1} + \mu(\varepsilon)A^{-1}\big)$.

We shall use q-stage ($q = 2,3,4$) Gauss methods to construct the corresponding linearized Runge-Kutta methods, which we name as q-stage linearized Gauss methods. Then, we use the derived linearized Gauss scheme in order to solve numerically (4.1).

Let $0 = t_0 < t_1 < \cdots < t_N = T$ be a uniform partition of the interval $[0,T]$ with step size $\tau = T/N$. Let also

$$U_n \approx U(t_n), \quad R_n \approx R(t_n), \quad U_{n,i} \approx U(t_n + c_i\tau), \quad R_{n,i} \approx R(t_n + c_i\tau), \quad i = 1, \dots, q.$$

The fully discrete scheme is defined, for any $1 \leq n \leq N$, by

$$
\begin{aligned}
U_{n,i} &= U_n + \tau \sum_{j=1}^{q} a_{ij}\Big(M_1 U_{n,j} + M_2 \mathcal{F}(I_{n-1}^{\tau} U_{n,j}) R_{n,j}\Big), i = 1, \dots, q,\\
R_{n,i} &= R_n + \tau \sum_{j=1}^{q} a_{ij}\big(\frac{1}{2}\mathcal{F}(I_{n-1}^{\tau} U_{n,j})^T M_1 U_{n,j} + R_{n,j}\frac{1}{2}\mathcal{F}(I_{n-1}^{\tau} U_{n,j})^T M_2 \mathcal{F}(I_{n-1}^{\tau} U_{n,j})\big),\ i = 1, \dots, q,\\
U_{n+1} &= U_n + \tau \sum_{i=1}^{q} b_i\Big(M_1 U_{n,i} + M_2 \mathcal{F}(I_{n-1}^{\tau} U_{n,i}) R_{n,i}\Big),\\
R_{n+1} &= R_n + \tau \sum_{i=1}^{q} b_i\big(\frac{1}{2}\mathcal{F}(I_{n-1}^{\tau} U_{n,i})^T M_1 U_{n,i} + R_{n,i}\frac{1}{2}\mathcal{F}(I_{n-1}^{\tau} U_{n,i})^T M_2 \mathcal{F}(I_{n-1}^{\tau} U_{n,i})\big),
\end{aligned}
\tag{4.2}
$$

where a_{ij}, b_i, c_i for $i, j = 1, \dots, q$ are the coefficients of the Gauss methods given in [19], and for $n = 0$, $U_{0,i}$, $R_{0,i}$ $i = 1, \dots, q$, U_1, R_1, are computed by the standard Gauss methods.

Remark 4.1. *Note that $\mathcal{F}(I_{n-1}^{\tau} U_{n,j})$ in the above equation is known at the time t_n, while the first two formulae in (4.2) are linear with respect to $U_{n,i}, R_{n,i}, i = 1, \dots, q$. Therefore, $U_{n,i}, R_{n,i}, i = 1, \dots, q$ can be obtained directly. Then, we substitute $U_{n,i}, R_{n,i}, i = 1, \dots, q$ into the last two formulae in (4.2), and compute U_{n+1}, R_{n+1}.*

4.2. **Simulations.** Let us select the ε-weights by

I. $\delta(\varepsilon) = 1,\ \mu(\varepsilon) = 8\varepsilon^{-2}$, II. $\delta(\varepsilon) = \varepsilon^2,\ \mu(\varepsilon) = \varepsilon^{-1}$, III. $\delta(\varepsilon) = \varepsilon^{-1},\ \mu(\varepsilon) = \varepsilon^2$, IV. $\delta(\varepsilon) = 1,\ \mu(\varepsilon) = 1$.

We also define the discrete energy by

$$E(u_{h,n}, r_{h,n}) = \int_{\mathcal{D}} \frac{\varepsilon^2}{2} |\nabla u_{h,n}|^2 dx + r_{h,n}^2 - E_0,$$

for $u_{h,n}$, $r_{h,n}$ the fully discrete approximations of u, r.

4.2.1. *1D Runs.* We consider first the one dimensional ε-dependent Cahn-Hilliard/Allen-Cahn problem (1.1), posed in $\mathcal{D} := (-3, 3)$, and layered initial condition

$$u(x, 0) := \tanh\Big(\frac{x}{\sqrt{2\varepsilon}}\Big),\ x \in \mathcal{D},$$

for a mesh size $h := 0.05$.

We first examine the accuracy of the proposed methods. The $2, 3, 4$-stage linearized Gauss methods are used for the Case II, with $\varepsilon = 0.1$. Here, the numerical solution u_h^*, with sufficiently small time step $\tau = 10^{-4}$, is chosen as the solution of reference. We then compute the L^2-norm errors $\|u_{h,n} - u_h^*\|_{L^2}$ at $T = 1$. The numerical results are shown in 4.2.1, from which we can clearly see that the q-stage linearized Gauss methods have q-th order accuracy. These are consistent with the theoretical results of the paper.

Table 1. L^2-norm errors and convergence rates of the q-stage linearized Gauss methods.

τ	$q = 2$		$q = 3$		$q = 4$	
	$\|u_{h,n} - u_h^*\|_{L^2}$	*rate*	$\|u_{h,n} - u_h^*\|_{L^2}$	*rate*	$\|u_{h,n} - u_h^*\|_{L^2}$	*rate*
1/200	2.9928e-06	-	4.5974e-08	-	6.0506e-10	-
1/400	7.5863e-07	1.98	6.1901e-09	2.89	3.7672e-11	4.01
1/800	1.9005e-07	2.00	8.0325e-10	2.95	2.3515e-12	4.00
1/1600	4.6746e-08	2.02	1.0198e-10	2.98	1.6339e-13	3.85

We apply the 2-stage linearized Gauss method. Figure 4.1 presents the evolution of $E(u_{h,n}, r_{h,n})$ which decays, as well as the numerical solutions, for weights defined by Case IV, with $\varepsilon = 0.1$,0.01 ,0.001, which clearly illustrates that the proposed methods are energy-stable. For all other Cases I-III the results were similar, and the numerical solutions seemed to converge to the step function ± 1, as in Case IV.

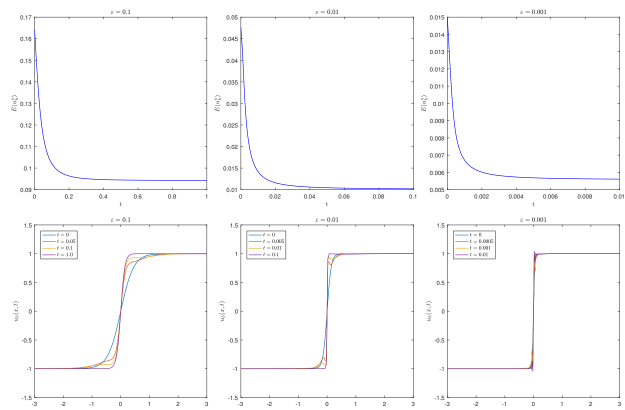

FIGURE 4.1. *Evolutions of the energy (top) and the solutions (bottom) in Case* IV *with* $\varepsilon = 0.1$, $\varepsilon = 0.01$, $\varepsilon = 0.001$ *(from the right to the left) using* 2*-stage linearized Gauss methods with stepsize* $\tau = 10^{-4}, 10^{-5}, 10^{-6}$*, respectively.*

4.2.2. *2D Runs.* We consider the two dimensional problem (1.1), posed in $\mathcal{D} := (0,1) \times (0,1)$, and initial condition

$$u(x,y,0) = \cos(\pi x)\cos(\pi y),\ (x,y) \in \mathcal{D},$$

for the mesh sizes $h_x,\ h_y := 0.1$.

We investigate first the accuracy of the proposed scheme. The $2,3,4$-stage linearized Gauss methods are used to approximate the problem with weights defined in Case II with $\varepsilon = 0.01$. Here, we use the numerical solution u_h^* with small step size $\tau = 10^{-5}$ as the solution of reference and we compute the L^2-norm error at $T = 0.1$. These numerical results are listed in 4.2.2. From the table, one can see that the q-stage linearized Gauss methods have convergence orders q.

TABLE 2. L^2-norm errors and convergence orders of q-stage linearized Gauss methods

τ	$q=2$		$q=3$		$q=4$	
	$\Vert u_{h,n} - u_h^*\Vert_2$	*rate*	$\Vert u_{h,n} - u_h^*\Vert_2$	*rate*	$\Vert u_{h,n} - u_h^*\Vert_2$	*rate*
1/1000	5.8366e-04	-	2.1095e-05	-	5.5372e-07	-
1/2000	1.5272e-04	1.93	2.6069e-06	3.02	3.2353e-08	4.10
1/4000	3.8991e-05	1.97	3.2353e-07	3.01	1.9542e-09	4.05
1/8000	9.8070e-06	1.99	4.0266e-08	3.01	1.2006e-10	4.02
1/16000	2.4172e-06	2.02	5.0051e-09	3.01	7.4468e-12	4.01

The evolution of the discrete energy $E(u_{h,n}, r_{h,n})$, and the numerical solutions for weights defined by all the four Cases I-IV, with $\varepsilon = 0.1, 0.01, 0.001$, by using the 2-stage extrapolated Gauss methods, are presented in Figures 4.2, 4.3 respectively. The discrete energy is decaying for all cases. As we can observe the evolution of the numerical solutions for Case I, and Case II is similar to this of Allen-Cahn equation. For Case III, and Case IV, the evolution is closer to this of Cahn-Hilliard equation; see Figure 4.4 for a comparison, where the numerical solutions of Cahn-Hiliard and Allen-Cahn equations are presented.

When $\varepsilon = 10^{-1}$, which is a rather large value, in Cases I, II, one of the phases rapidly vanishes, while for the Cases III, IV, the problem seems static. In Cases I where $\frac{\delta(\varepsilon)}{\mu(\varepsilon)\varepsilon^2} = \mathcal{O}(1)$, and II where $\delta(\varepsilon) \ll \mu(\varepsilon)\varepsilon^2$ as $\varepsilon \to 0$, for smaller values of ε the evolution slows down. Layer generation and annihilation is observed for $\varepsilon = 10^{-2}, 10^{-3}$ in the cases III, IV where $\delta(\varepsilon) \gg \mu(\varepsilon)\varepsilon^2$ as $\varepsilon \to 0$.

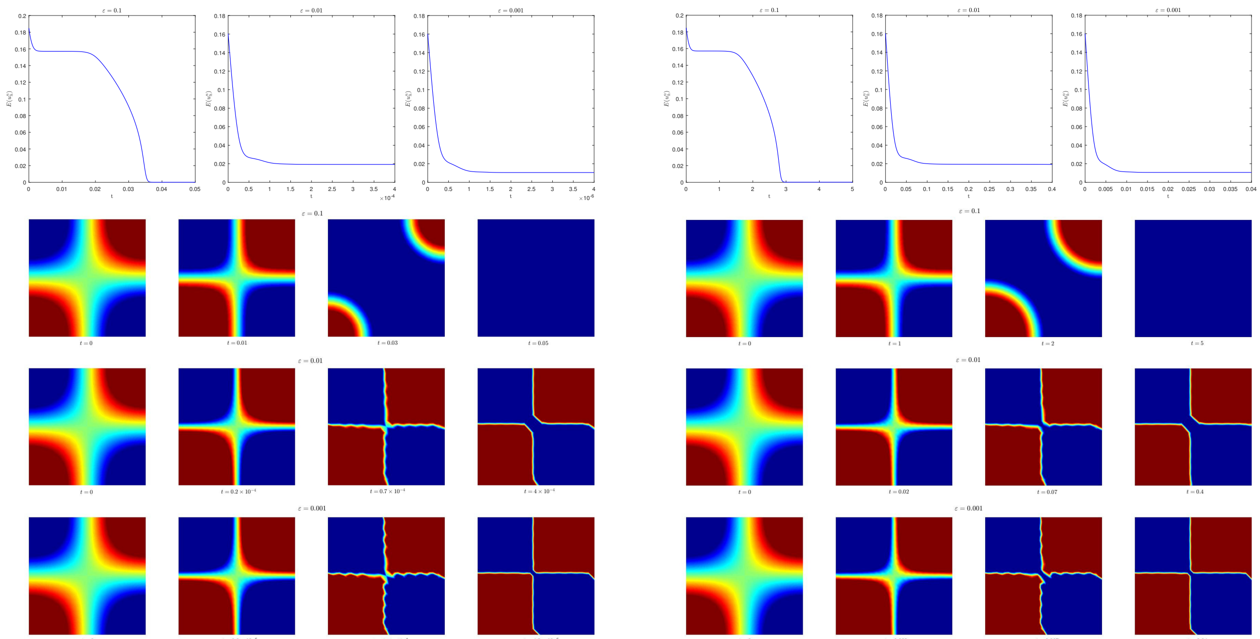

FIGURE 4.2. *Left: Evolutions of the energy and snapshots of the solutions. Left: Case* I *with* $\varepsilon = 0.1$, $\varepsilon = 0.01$, $\varepsilon = 0.001$, *with stepsize* $\tau = 10^{-4}, 10^{-6}, 10^{-8}$, *respectively. Right: Case* II *with* $\varepsilon = 0.1$, $\varepsilon = 0.01$, $\varepsilon = 0.001$, *with stepsize* $\tau = 10^{-2}, 10^{-3}, 10^{-4}$, *respectively.*

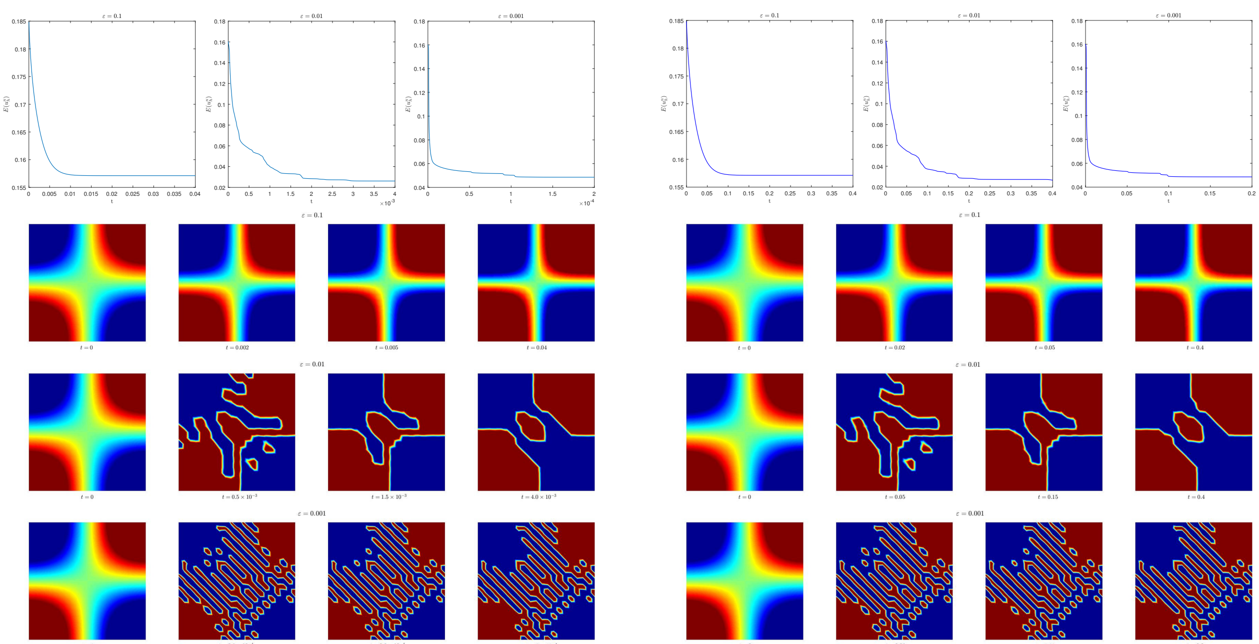

FIGURE 4.3. *Evolutions of the energy and snapshots of the solutions. Left: Case* III *with* $\varepsilon = 0.1$, $\varepsilon = 0.01$, $\varepsilon = 0.001$, *with stepsize* $\tau = 10^{-4}, 10^{-7}, 10^{-8}$, *respectively. Right: Case* IV *with* $\varepsilon = 0.1$, $\varepsilon = 0.01$, $\varepsilon = 0.001$, *with stepsize* $\tau = 10^{-3}, 10^{-5}, 10^{-7}$, *respectively.*

For our final set of runs, we considered (1.1), posed in $\mathcal{D} := (-1,1) \times (-1,1)$, with a layered initial condition near ± 1

$$u(x,y,0) = \tanh\Big(\frac{1}{\sqrt{2\varepsilon}} \min\{\sqrt{(x+0.3)^2+y^2} - 0.3, \sqrt{(x-0.3)^2+y^2} - 0.25\}\Big), \ (x,y) \in \mathcal{D},$$

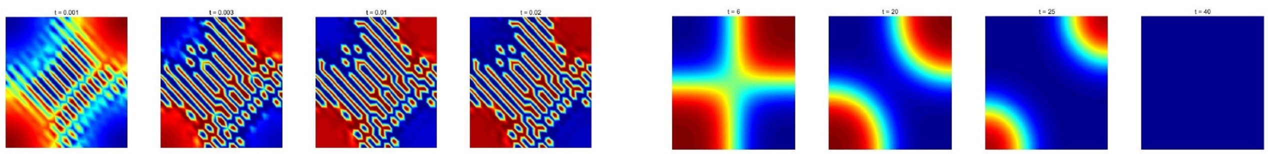

FIGURE 4.4. *Left: Cahn-Hilliard case with* $\sigma(\varepsilon) = 1$, $\mu(\varepsilon) = 0$, *for* $\varepsilon = 0.0001$, *and* $\tau = 10^{-5}$. *Right: Allen-Cahn case with* $\sigma(\varepsilon) = 0$, $\mu(\varepsilon) = 1$, *for* $\varepsilon = 0.1$, *and* $\tau = 10^{-1}$.

and $h_x,\ h_y := 0.1$. Such ε-dependent layered initial data are selected when evolution is observed after the so-called time of layer generation where the different layers of ε-dependent width have been formed around the two phases of the binary alloy with concentrations $u = \pm 1$.

The numerical solutions with 2-stage extrapolated Gauss methods for Cases I, II, III, IV are presented in the next Figures 4.5, 4.6. There, the evolution seems to be influenced by the selection of weights and the smallness of ε, τ, with Case IV presenting the slowest transitional change for $\varepsilon = 10^{-3}$ and $\tau = 10^{-7}$. Moreover, when $\varepsilon = 10^{-1}$, in all cases and in very short times one phase survives (red) while the second phase (blue) evolves rapidly towards concentration values near the first (light blue).

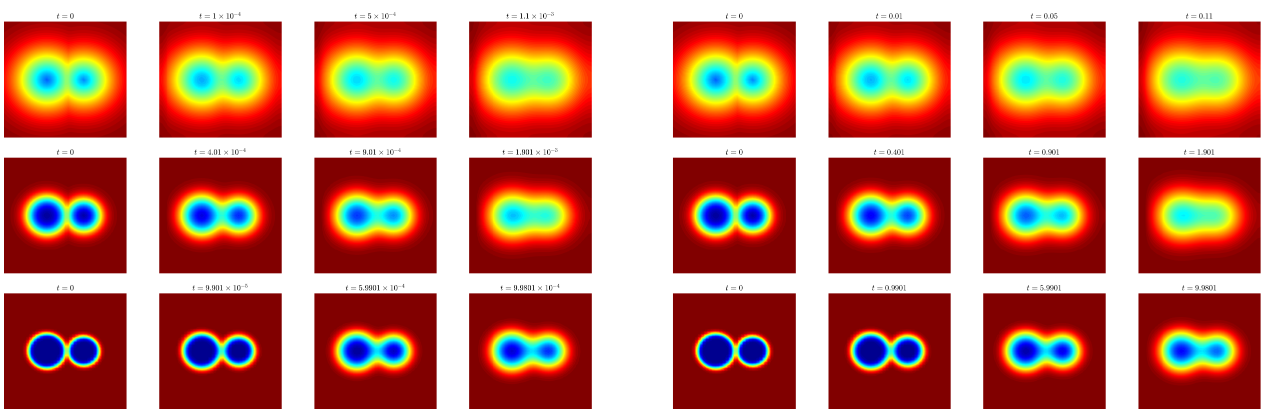

FIGURE 4.5. *Numerical solutions. Left: Case I with* $\varepsilon = 0.1$, $\varepsilon = 0.01$, $\varepsilon = 0.001$, *and* $\tau = 10^{-4}, 10^{-6}, 10^{-8}$ *(from top to bottom), respectively. Right: Case II with* $\varepsilon = 0.1$, $\varepsilon = 0.01$, $\varepsilon = 0.001$, *and* $\tau = 10^{-2}, 10^{-3}, 10^{-4}$ *(from top to bottom), respectively.*

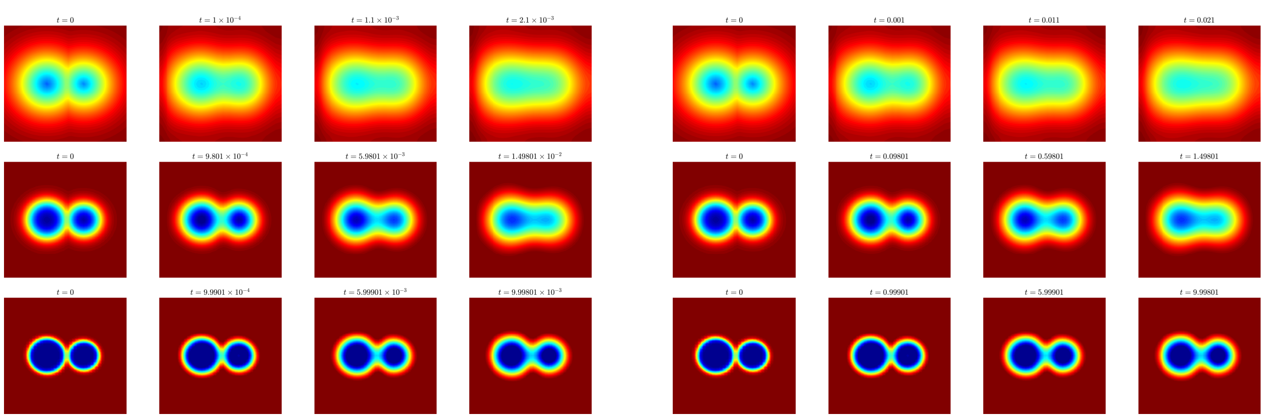

FIGURE 4.6. *Numerical solutions. Left: Case III with* $\varepsilon = 0.1$, $\varepsilon = 0.01$, $\varepsilon = 0.001$, *and* $\tau = 10^{-4}, 10^{-7}, 10^{-8}$ *(from top to bottom), respectively. Right: Case IV with* $\varepsilon = 0.1$, $\varepsilon = 0.01$, $\varepsilon = 0.001$, *and* $\tau = 10^{-3}, 10^{-5}, 10^{-7}$ *(from top to bottom), respectively.*

Acknowledgment

The authors would like to thank Prof. G. Akrivis for stimulating discussions. The research work was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the First Call for H.F.R.I. Research Projects to support Faculty members and Researchers and the procurement of high-cost research equipment grant (Project Number: HFRI-FM17-45). The research work was also supported by the National Nature Science Foundation of China, Project numbers 11771162, 12231003.

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