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Error analysis for a second order approximation of a viscoelastic phase separation model

Aaron Brunk[1] · **Herbert Egger**[2,3] · **Oliver Habrich**[3] · **Maria Lukáčová-Medviďová**[1]

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Abstract
We consider a systematic numerical approximation of a viscoelastic phase separation model that describes the demixing of a polymer-solvent mixture. An unconditionally stable discretisation method is proposed based on a finite element approximation in space and a variational time discretization strategy. The proposed method preserves the energy-dissipation structure of the underlying system exactly and allows us to establish a fully discrete nonlinear stability estimate in natural norms based on the concept of relative energy. These estimates are used to derive order optimal error estimates for the method under minimal smoothness assumptions on the problem data, despite the presence of various strong nonlinearities in the equations. The theoretical results and main properties of the method are illustrated by numerical simulations, which also demonstrate the capability to reproduce the relevant physical effects observed in experiments.

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Herbert Egger, Oliver Habrich, and Maria Lukáčová-Medvid'ová have contributed equally to this work.

✉ Aaron Brunk
abrunk@uni-mainz.de

Herbert Egger
herbert.egger@jku.at

Oliver Habrich
oliver.habrich@jku.at

Maria Lukáčová-Medvid'ová
lukacova@uni-mainz.de

1 Institute of Mathematics, Johannes Gutenberg-University, Mainz, Germany

2 Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria

3 Institute for Numerical Mathematics, Johannes Kepler University, Linz, Austria

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1 Introduction

The separation of polymer-solvent mixtures after a deep quench is strongly influenced by dynamic asymmetry, i.e., by different length and time scales of two components [44, 49]. This leads to meta-stable states and the formation of transient network-like structures of a slow polymer phase and its volume shrinking. Such intermediate states are not observed in the classical demixing of binary fluids. Examples of viscoelastic phase separation include polymeric porous media used as advanced materials in lithium-ion batteries biofilters. An overview of applications of viscoelastic phase separation is presented, e.g., in [48, 50]. In [47], Tanaka made a first attempt to model such viscoelastic phase separation phenomena by introducing an internal relaxation variable, the elastic stress tensor and the bulk stress. The latter originates from (microscopic) intermolecular attractive interactions and can be seen as additional viscoelastic pressure q. We refer a reader to our work [16] for a detailed, physically motivated discussion. Tanaka's model provided good qualitative agreement with experimental observations. To guarantee thermodynamic consistency, i.e. non-increasing total energy, the model was further improved by Zhou et al. [55]. The resulting system of partial differential equations is of parabolic-hyperbolic type and combines the Cahn-Hilliard equation for the volume fraction, a relaxation equation for the bulk stress, the Navier-Stokes equations for the fluid flow, and the Oldroyd-B model for the elastic stress tensor. Well-posedness of the viscoelastic phase separation model and suitable modifications were thoroughly analyzed in [15, 19]. The viscoelastic phase separation model studied in [19] includes a stress diffusion term in the time evolution equation for the elastic stress tensor, which is governed by the Peterlin model, a nonlinear version of the classical Olroyd-B equations. Following Barrett and Süli [9], we note that the diffusive term appearing in the evolution equation for the elastic stress tensor is not a mathematical regularization but rather an outcome of detailed physical modelling allowing a heterogeneous fluid velocity around microscopic dumbbells. Indeed, as discussed in Málek et al. [42] the stress diffusion term can be interpreted either as a consequence of a non-local energy storage mechanism or as a consequence of a non-local entropy production mechanism, see also [24, 43] for related studies.

2 Basic model under consideration.

In [55], a simplified model for viscoelastic phase separation was studied, where the effects of fluid flow and of the so-called elastic shear stress were neglected. In the absence of initial flow, the system gave qualitatively similar results to the full system. Being inspired by [55] we will consider here the following simplified system for viscoelastic phase separation

$$\partial_t \phi = \operatorname{div}\big(b(\phi)\nabla\mu + c(\phi)\nabla(A(\phi)q)\big), \tag{0.1}$$

$$\mu = -\gamma\Delta\phi + f'(\phi), \tag{0.2}$$

$$\partial_t q = -\kappa(\phi)\, q - A(\phi)\,\mathrm{div}\,\big(c(\phi)\nabla\mu - d(\phi)\nabla(A(\phi)q)\big) + \varepsilon\Delta q. \tag{0.3}$$

Here ϕ is the volume fraction of the polymer component, i.e. $\phi = 1$ represents pure polymer phase and $\phi = 0$ pure solvent phase, μ is the chemical potential, and q denotes a pressure-like quantity called the bulk stress in the mixture that models viscoelastic effects. Further, $\gamma > 0$ is the interface parameter, $f(\cdot)$ is the derivative of internal energy of the mixture, $b(\cdot)$, $c(\cdot)$, $d(\cdot)$ are phase dependent mobility parameters, $\kappa(\cdot)$ is an inverse relaxation time, $A(\cdot)$ a bulk modulus, and $\varepsilon > 0$ is the center-of-mass diffusion coefficient. The value of ε lies between 10^{-9} to 10^{-7} and depends on the fraction of small and large characteristic length-scales and on the Weissenberg number characterizing the elastic relaxation property of the fluid [8, 9]. For $\varepsilon = 0, b(\phi) = M(\phi)\phi^2(1-\phi)^2, c(\phi) = M(\phi)\phi(1-\phi)$, and $d(\phi) = M(\phi) = \mathrm{const}$ the above system amounts to the problem studied in [55, Section III], where the constant mobility equals to the inverse of the friction coefficient between polymer and solvent. The first simulation results for this simplified model of viscoelastic phase separation were obtained in [55] by explicit time-stepping methods. A good qualitative agreement was observed with the experimental data from [47]. In [41, 46], linear-implicit energy-stable approximations were developed for the above system guaranteeing energy dissipation on the discrete level. Extensive numerical tests were performed for the simplified model (0.1)–(0.3) above as well as for the full model coupled to viscoelastic fluid flow. A rigorous error analysis for corresponding discretization methods seems to be missing up to date.

2.1 Related work

The problem under consideration shares similarities with cross-diffusion systems; see [34] for an introduction and references. Discretization schemes preserving the underlying entropy-dissipation structure have been proposed and investigated in [12, 35, 37, 37]. Typically, finite-volume schemes are used in this context since they accommodate a discrete version of the chain rule, which is important to deal with the nonlinearities of the model. Various discretisation methods have been devised for the Cahn-Hilliard equation and similar gradient systems, see, e.g. [26, 27]. Recent developments, like the *scalar auxiliary variable* (SAV) approach [45] or the *energy quadratisation* (EQ) approach [32] aim at improving computational efficiency. This is achieved by relaxing the nonlinear relation between energy and chemical potential to some extent by introducing auxiliary variables. Similar ideas are also used in [3, 20, 38] and in [21, 52, 54]. We refer to [22] and [51] for rigorous error analysis of second order schemes for the Cahn-Hilliard equation using SAV or EQ. Applying such methods to the system under consideration seems interesting and is left for future work. In our previous work [18], we proposed a structure-preserving discretization scheme for the Cahn-Hilliard equation and provided a full stability and error analysis based on the relative energy estimates. In the present work, we concentrate for simplicity on a variable but strictly positive mobility. We note that the degenerate mobility $b(\phi) = \phi^2(1-\phi)^2$ as employed in [55] can be considered applying the techniques from [5, 33]. If full elastic stress tensor is considered, one has to include a time evolution equation for the elastic stress, see, e.g., the Oldroyd-B, FENE-P or Giesekus models. Numerical approximations of viscoelastic fluid flows, without phase separation effects, can be found, e.g., in [6, 10] for the Oldroyd-B system and [7] for the FENE-P model.

From a mechanical point of view, the equation for the elastic stress tensor is very similar to the equation of the left Cauchy-Green tensor in elasticity. In this context, viscoelastic models with phase-field are used in the context of tumour growth and are given in [28, 30, 30], where the authors considered the existence of generalized solutions and their approximation. A model with a phase-dependent elastic energy is considered in [40].

The interpretation as left Cauchy-Green tensor enables one to develop also (visco)-elastic systems based on the deformation gradient. We refer to [1] and [2] for modelling and existence of two variants of the Cahn-Hilliard equation with the viscoelastic effects based on the deformation gradient. We emphasize that [2] also contains two numerical methods based on convex-concave splitting and SAV.

2.2 Scope and main contributions.

In this paper, we propose a fully discrete approximation scheme for the system (0.1)–(0.3) based on a finite element approximation in space and a variational time discretization strategy. The resulting method is unconditionally energy stable, preserves the underlying energy-dissipation structure of the problem, and yields order optimal error estimates under minimal smoothness assumptions on the problem data and on the continuous solution. The main ingredient of our analysis are *relative energy estimates*, which allow us to establish discrete stability estimates in appropriate norms. Together with the variational structure of the approximation scheme, this allows us to bound the discretization errors by the corresponding projection and interpolation errors, leading to the optimal quantitative a-priori error bounds. The discrete stability estimates further allow us to prove the uniqueness of the discrete solution under a mild restriction on the spatial and temporal mesh size. A key difficulty in the analysis of the problem lies in the various nonlinear terms of the model, which are, however, important to obtain good qualitative agreement with experimental data [47, 55]. This is resolved here by the nonlinear discrete stability analysis mentioned above. The technicalities, therefore, are shifted to the estimation of certain residual terms, which can be analysed independently.

2.3 Outline.

The remainder of the manuscript is organized as follows: In Section 3.1, we introduce our notation and basic assumptions. We also collect some results about the analysis of the problem (0.1)–(0.3). In Section 4.1, we then present our discretization scheme and state the main results of the paper. The essential parts of the proofs are elaborated in Sections 5.1–8.1, and further technical details are provided in the appendices. For an illustration of our theoretical findings, we present some numerical tests in Section 9.1 and then close with a brief discussion.

3 Notation, assumptions, and preliminaries

We consider for simplicity a periodic setting and assume that $\Omega \subset \mathbb{R}^d$ is a hypercube in dimension $d = 2, 3$ which is identified with the d-dimensional torus. Functions on Ω are assumed periodically extendable to $\mathbb{R}^d$ under preservation of class. We denote by $L^p(\Omega)$, $W^{k,p}(\Omega)$ the corresponding Lebesgue and Sobolev spaces and write $\|\cdot\|_{0,p}$, $\|\cdot\|_{k,p}$ for the respective norms. If the meaning is clear from the context, we will sometimes omit the symbol Ω and write L^p for $L^p(\Omega)$. Analogous notation holds for other spaces. We further abbreviate $H^k(\Omega) = W^{k,2}(\Omega)$ and $\|\cdot\|_k = \|\cdot\|_{k,2}$. The corresponding dual spaces are denoted by $H^{-s}(\Omega) = H^s(\Omega)'$. Note that for $s = 0$, we have $H^s(\Omega) = H^{-s}(\Omega) = L^2(\Omega)$, where we tacitly identified $L^2(\Omega)$ with its dual space. The norm of the dual spaces is given by

$$\|r\|_{-s} = \sup_{v \in H^s(\Omega)} \frac{\langle r, v\rangle}{\|v\|_s}, \tag{1.1}$$

where $\langle\cdot,\cdot\rangle$ denotes for the duality product on $H^{-s}(\Omega) \times H^s(\Omega)$ for $s \geq 0$. The same symbol will be used for the scalar product of $L^2(\Omega)$. For functions $u, v \in H^0(\Omega) = L^2(\Omega)$, we use the same symbol $\langle u, v\rangle = \int_\Omega uv\, dx$ to denote the scalar product on $L^2(\Omega)$. We further denote by $L^p(a, b; X)$, $W^{k,p}(a, b; X)$, and $H^k(a, b; X)$ the Bochner spaces of integrable or differentiable functions on the time interval (a, b) with values in some Banach space X. If $(a, b) = (0, T)$, we will omit reference to the time interval and briefly write $L^p(X)$, for instance.

The following assumptions on the problem data will be used throughout the manuscript.

Assumption 1 (A0) $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ is a hypercube and identified with the d-dimensional torus. Functions on Ω are assumed periodically extendable to $\mathbb{R}^d$; $T > 0$ given.

(A1) $b \in C^2(\mathbb{R})$ with $0 < b_1 \leq b(s) \leq b_2$ for all $s \in \mathbb{R}$ and $\|b'\|_{0,\infty} + \|b''\|_{0,\infty} \leq b_3$; $c \in C^2(\mathbb{R})$ with $0 \leq c_1 \leq c(s) \leq c_2$ for all $s \in \mathbb{R}$ and $\|c'\|_{0,\infty} + \|c''\|_{0,\infty} \leq c_3$; $d(s) = d_0 > 0$ and $b(s) \geq c(s)^2/d_0 + \varepsilon$.

(A2) $f \in C^4(\mathbb{R})$ with $f(s), f''(s) \geq -f_1$, $|f^{(k)}(s)| \leq f_2^{(k)} + f_3^{(k)}|s|^{4-k}$, $f_1, f_i^{(k)} \geq 0$.

(A3) $A \in C^2(\mathbb{R})$ with $0 \leq A_1 \leq A(s) \leq A_2$ and $\|A'\|_{0,\infty} + \|A''\|_{0,\infty} \leq A_3$.

(A4) $\kappa \in C^2(\mathbb{R})$ with $0 < \kappa_1 \leq \kappa(s) \leq \kappa_2$ and $\|\kappa'\|_{0,\infty} + \|\kappa''\|_{0,\infty} \leq \kappa_3$.

(A5) $\gamma, \varepsilon > 0$ constant.

The above assumptions allow us to prove the existence of weak solutions to (0.1)–(0.3) for appropriate initial values. We emphasize that the dependence on ε in the lower bound of $b(s) \geq c(s)^2/d_0 + \varepsilon$ is due to simplified notations. One can prove the existence of a weak solution of the viscoelastic phase separation system (0.1)-(0.3) also in the case that $b(s) = c(s)^2/d_0, d_0 = 1$ and $\varepsilon > 0$ holds. Corresponding results for a more complex model have been obtained in [15, 19] and imply the following existence result for the simplified model considered here.

Theorem 2 *For given initial data $(\phi_0, q_0) \in [H^1(\Omega) \times L^2(\Omega)]$ and time $T > 0$ there exists a global-in-time weak solution of (0.1)–(0.3) in the sense that*

$$\begin{aligned}
&\phi \in L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega)) \cap H^1(0,T;H^{-1}(\Omega)),\\
&q \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)) \cap W^{1,4/3}(0,T;H^{-1}(\Omega)),\\
&A(\phi)q, \mu \in L^{5/3}(0,T,W^{1,5/3}(\Omega)),\\
&c(\phi)\nabla\mu - \nabla\big(A(\phi)q\big) \in L^2(0,T;L^2(\Omega)),
\end{aligned}$$

and

$$\begin{aligned}
&\langle \partial_t\phi, \psi\rangle + \langle c(\phi)\big[c(\phi)\nabla\mu - \nabla(A(\phi)q)\big]m\nabla\psi\rangle = 0,\\
&\quad\langle \mu, \xi\rangle - \gamma\langle\nabla\phi, \nabla\xi\rangle - \langle f'(\phi), \xi\rangle = 0,\\
&\langle \partial_t q, \zeta\rangle + \langle\kappa(\phi)q, \zeta\rangle + \varepsilon\langle\nabla q, \nabla\zeta\rangle - \langle\big[c(\phi)\nabla\mu - \nabla(A(\phi)q)\big], \nabla(A(\phi)\zeta)\rangle = 0,
\end{aligned}$$

for any test function $\psi, \zeta, \xi \in H^1(\Omega)$ and almost every $t \in (0, T)$. Furthermore for a.a. $t \in (0, T)$ the energy following energy inequality holds

$$\begin{aligned}
&\int_\Omega \frac{\gamma}{2}|\nabla\phi(t)|^2 + F(\phi(t)) + \frac{1}{2}|q(t)|^2 \,\mathrm{d}x\\
&\quad + \int_0^t\int_\Omega \big|c(\phi)\nabla\mu - \nabla\big(A(\phi)q\big)\big|^2 + \kappa(\phi)|q|^2 + \varepsilon|\nabla q|^2 \,\mathrm{d}x\,\mathrm{d}s\\
&\le \int_\Omega \frac{\gamma}{2}|\nabla\phi(0)|^2 + F(\phi(0)) + \frac{1}{2}|q(0)|^2 \,\mathrm{d}x.
\end{aligned}$$

The error analysis can also be performed with the assumption $b(s) \ge c(s)^2/d_0$ as well as with $d(s)$ variable but sufficiently regular and suitably bounded. However, this would involve additional technical details since the estimates are obtained only in weak spaces, e.g. $\mu \in L^{5/3}(0,T;W^{1,5/3}(\Omega))$.

3.1 Variational characterization

As a starting point for designing a suitable discretization scheme, we note that sufficiently regular periodic solutions of (0.1)–(0.3) satisfy

$$\langle \partial_t\phi, \psi\rangle + \langle b(\phi)\nabla\mu - c(\phi)\nabla(A(\phi)q), \nabla\psi\rangle = 0, \tag{1.2}$$

$$\langle \mu, \xi\rangle - \gamma\langle\nabla\phi, \nabla\xi\rangle - \langle f'(\phi), \xi\rangle = 0, \tag{1.3}$$

$$\begin{aligned}
&\langle \partial_t q, \zeta\rangle + \langle\kappa(\phi)q, \zeta\rangle + \langle d_0\nabla(A(\phi)q) - c(\phi)\nabla\mu, \nabla(A(\phi)\zeta)\rangle\\
&\quad - \langle + \varepsilon\langle\nabla q, \nabla\zeta\rangle = 0,
\end{aligned} \tag{1.4}$$

for all smooth test functions ψ, ξ, ζ and all $t \in [0, T]$. Note that the solution components here depend on time, while the test functions do not. The above identities follow immediately by testing the equations appropriately and using integration-by-parts for some of the terms.

3.2 Basic properties

The variational identities (1.2)–(1.4) immediately imply the following properties of sufficiently smooth solutions: By testing with $\psi = 1$, $\xi = 0$ and $\zeta = 0$, we get

$$\frac{d}{dt} \int_\Omega \phi(t) \, \mathrm{d}x = 0, \tag{1.5}$$

which encodes the conservation of mass. Testing with $\psi = \mu(t)$, $\xi = \partial_t \phi(t)$ and $\zeta = q(t)$ on the other hand, leads to the energy dissipation identity

$$\frac{d}{dt} \mathcal{E}(\phi(t), q(t)) = -\mathcal{D}_{\phi(t)}(\mu(t), q(t)). \tag{1.6}$$

Here $\mathcal{E}(\phi, q) = \int_\Omega \frac{\gamma}{2} |\nabla \phi|^2 + f(\phi) + \frac{1}{2}|q|^2$ denotes the free energy associated to the system and we denote the corresponding dissipation functional by

$$\mathcal{D}_\phi(\mu, q) = \int_\Omega \tfrac{1}{d_0} |c(\phi)\nabla \mu - d_0 \nabla (A(\phi) q)|^2 + \tfrac{b(\phi) - c(\phi)^2}{d_0} |\nabla \mu|^2 + \varepsilon |\nabla q|^2 + \kappa(\phi)|q|^2 \, \mathrm{d}x.$$

The two properties (1.5)–(1.6) are important for proving the existence of weak solutions. Note that they are a direct consequence of the variational characterization (1.2)–(1.4) of solutions and can be preserved by appropriate discretization schemes.

4 Proposed method and main results

We start by introducing additional notation, assumptions and the approximation method for our model problem. Afterwards, we state our main results and briefly comment on the main arguments of the proofs, which are detailed in the following sections.

4.1 Notation and assumptions.

For the space discretization, we assume that

(A6) $\mathcal{T}_h$ is a geometrically conforming and quasi-uniform partition of Ω into simplices that can be extended periodically to periodic extensions of Ω.

This means that there exists a constant $\sigma > 0$ such that $\sigma h \leq \rho_K \leq h_K \leq h$ for all elements $K \in \mathcal{T}_h$, where ρ_K and h_K are the inner-circle radius and diameter of the element, and $h = \max_{K \in \mathcal{T}_h} h_K$ is the global mesh size [13]. We then denote by

$$\mathcal{V}_h := \{v \in H^1(\Omega) : v|_K \in P_2(K) \quad \forall K \in \mathcal{T}_h\},$$

the space of continuous periodic piecewise quadratic polynomials on $\mathcal{T}_h$, which yields a second order finite element approximation. By $\pi_h^0 : L^2(\Omega) \to \mathcal{V}_h$ and $\pi_h^1 : H^1(\Omega) \to \mathcal{V}_h$, we denote the L^2- and H^1-orthogonal projection operators, defined by

$$\langle \pi_h^0 u - u, v_h \rangle = 0 \qquad \forall v_h \in \mathcal{V}_h, \tag{2.1}$$

$$\langle \pi_h^1 u - u, v_h \rangle + \langle \nabla(\pi_h^1 u - u), \nabla v_h \rangle = 0 \qquad \forall v_h \in \mathcal{V}_h. \tag{2.2}$$

Some basic properties of these operators are again summarized in Appendix 11.1.. We will frequently make use of the discrete dual norm given by

$$\|r\|_{-1,h} := \sup_{v_h \in \mathcal{V}_h} \frac{\langle r, v_h \rangle}{\|v_h\|_1} \tag{2.3}$$

which is the discrete version of the dual norm. For the approximation in time, we also use piecewise polynomial functions defined on the grid

(A7) $\quad \mathcal{I}_\tau := \{0 = t^0, t^1, \ldots, t^N = T\}$ with time steps $t^n = n\tau$ and $\tau = T/N$.

We note that non-uniform time steps could be considered with minor modifications of the arguments presented in the following. We write $I_n := (t^{n-1}, t^n)$ for the *n*-th time interval and use $\langle a, b \rangle^n = \int_{I^n} \langle a, b \rangle \, \mathrm{d}s$ to abbreviate the integral over I^n. We further introduce the spaces

$$P_k(\mathcal{I}_\tau; X) \qquad \text{and} \qquad P_k^c(\mathcal{I}_\tau; X) = P_k(\mathcal{I}_\tau; X) \cap C(0, T; X), \tag{2.4}$$

consisting of all discontinuous, respectively, continuous piecewise polynomial functions of degree less or equal then *k* on the time grid $\mathcal{I}_\tau$, with values in some vector space *X*. We write $I_\tau^1 : H^1(0, T; X) \to P_1^c(\mathcal{I}_\tau; X)$ and $\bar{\pi}_\tau^0 : L^2(0, T; X) \to P_0(\mathcal{I}_\tau; X)$ for the piecewise linear interpolation, respectively, the piecewise constant projection of functions in time. Some important properties of these operators are again summarized in Appendix 11.1.. Throughout the presentation, the bar symbol $\bar{u}$ is used to indicate functions in $P_0(\mathcal{I}_\tau; X)$ which are piecewise constant in time. For ease of presentation, we use the same symbol $\bar{u} = \bar{\pi}_\tau^0 u$ also to abbreviate the piecewise constant projection in time of a function $u \in L^2(0, T; X)$.

4.2 Discretization method

As an approximation of the initial value problem for (0.1)–(0.3), we consider the following scheme, which is motivated by the variational characterization of solutions.

Problem 3 Let (A0)–(A7) hold and $\phi_{h,0}, q_{h,0} \in \mathcal{V}_h$ be given. Find $\phi_{h,\tau}, q_{h,\tau} \in P_1^c(\mathcal{I}_\tau; \mathcal{V}_h)$ and $\bar\mu_{h,\tau} \in P_0(\mathcal{I}_\tau; \mathcal{V}_h)$ such that $\phi_{h,\tau}(0) = \phi_{h,0}$ and $q_{h,\tau}(0) = q_{h,0}$, and such that

$$\langle \partial_t \phi_{h,\tau}, \bar\psi_{h,\tau}\rangle^n = -\langle b(\bar\phi_{h,\tau})\nabla\bar\mu_{h,\tau} - c(\bar\phi_{h,\tau})\nabla(A(\bar\phi_{h,\tau})\bar q_{h,\tau}), \nabla\bar\psi_{h,\tau}\rangle^n, \tag{2.5}$$

$$\langle \bar\mu_{h,\tau}, \bar\xi_{h,\tau}\rangle^n = \gamma\langle\nabla\bar\phi_{h,\tau}, \nabla\bar\xi_{h,\tau}\rangle^n + \langle f'(\phi_{h,\tau}), \bar\xi_{h,\tau}\rangle^n, \tag{2.6}$$

$$\begin{aligned}\langle \partial_t q_{h,\tau}, \bar\zeta_{h,\tau}\rangle^n = &-\langle d_0\nabla(A(\bar\phi_{h,\tau})\bar q_{h,\tau}) - c(\bar\phi_{h,\tau})\nabla\bar\mu_{h,\tau}, \nabla(A(\bar\phi_{h,\tau})\bar\zeta_{h,\tau})\rangle^n \\ &- \langle\kappa(\bar\phi_{h,\tau})\bar q_{h,\tau}, \bar\zeta_{h,\tau}\rangle^n - \varepsilon\langle\nabla\bar q_{h,\tau}\nabla\bar\zeta_{h,\tau}\rangle^n,\end{aligned} \tag{2.7}$$

for all test functions $\bar\psi_{h,\tau}, \bar\xi_{h,\tau}, \bar\zeta_{h,\tau} \in P_0(I_n; \mathcal{V}_h)$ and all time steps $1 \le n \le N$. Let us recall that $\langle a, b\rangle^n = \int_{t^{n-1}}^{t^n} \langle a, b\rangle\, ds = \int_{t^{n-1}}^{t^n}\int_\Omega a \cdot b \,\mathrm{d}x\,\mathrm{d}s$ is used for the abbreviation of space-time integrals.

In the *n*-th time step of the method, the values $\phi_{h,\tau}(t^{n-1})$, $q_{h,\tau}(t^{n-1})$ are known, and one has to find $\phi_{h,\tau}(t^n)$, $q_{h,\tau}(t^n)$ and $\bar\mu_{h,\tau}(t^n)$. The above scheme thus amounts to a fully implicit time-stepping scheme, cf. Problem 15. Solvability will be discussed below.

4.3 Main results.

As a first step of our analysis, let us comment on the well-posedness of the discrete problem and its preservation of the basic properties of the underlying system.

Theorem 4 *Let (A0)–(A7) hold. Then for any $\phi_{h,0}, q_{h,0} \in \mathcal{V}_h$, Problem 3 has at least one solution. Moreover, any such solution conserves mass and dissipates energy, i.e., $\langle\phi_{h,\tau}(t^n), 1\rangle = \langle\phi_{h,\tau}(t^m), 1\rangle$ and*

$$\mathcal{E}(\phi_{h,\tau}, q_{h,\tau})\big|_{t^m}^{t^n} = -\int_{t^m}^{t^n} \mathcal{D}_{\bar\phi_{h,\tau}}(\bar\mu_{h,\tau}, \bar q_{h,\tau})\,\mathrm{d}s \tag{2.8}$$

for all $0 \le m \le n \le N$. The energy and dissipation functionals $\mathcal{E}(\phi, q)$, $\mathcal{D}_\phi(\mu, q)$ are the same as defined after (1.6). Furthermore, any solution is uniformly bounded by

$$\|\phi_{h,\tau}\|^2_{L^\infty(H^1)} + \|q_{h,\tau}\|^2_{L^\infty(L^2)} + \|\bar q_{h,\tau}\|^2_{L^2(H^1)} + \|\bar\mu_{h,\tau}\|^2_{L^2(H^1)} \le C'. \tag{2.9}$$

The constant $C' = C'(\|\phi_{h,0}\|_{H^1}, \|q_{h,0}\|_{L^2})$ depends only on the bounds of the coefficients appearing in the assumptions and the norm of the initial data.

The two identities (2.8) follow immediately from the variational characterization of discrete solutions and the use of appropriate test functions; compare with the proof of these properties on a continuous level. They provide a-priori bounds and allow us to show the existence of a discrete solution via fixed-point arguments. The proof will be presented in Section 5.1. We continue by stating the main result on the error estimates.

Theorem 5 *Let (A0)–(A7) hold and let (ϕ, μ, q) be a smooth solution of the variational identities (1.2)–(1.4) satisfying*

$$\phi \in H^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^3(\Omega)), \tag{2.10}$$

$$\mu \in H^2(0,T;H^1(\Omega)) \cap L^\infty(0,T;W^{1,3}(\Omega)) \cap L^2(0,T;H^3(\Omega)), \tag{2.11}$$

$$q \in H^2(0,T;H^1(\Omega)) \cap L^\infty(0,T;W^{1,3}(\Omega)) \cap L^2(0,T;H^3(\Omega)). \tag{2.12}$$

Furthermore, let $(\phi_{h,\tau}, \bar{\mu}_{h,\tau}, q_{h,\tau})$ be a solution of Problem 3 for some $h, \tau > 0$ and with initial values given by $\phi_{h,0} = \pi_h^1 \phi(0)$ and $q_{h,0} = \pi_h^0 q(0)$. Then

$$\|\phi_{h,\tau} - \phi\|^2_{L^\infty(H^1)} + \|q_{h,\tau} - q\|^2_{L^\infty(L^2)} + \|\bar{\mu}_{h,\tau} - \bar{\mu}\|^2_{L^2(H^1)} + \|\bar{q}_{h,\tau} - \bar{q}\|^2_{L^2(H^1)} \leq C''(h^4 + \tau^4).$$

The constant C'' is independent of h and τ. Moreover, for the choice $h = c'\tau$ with $c' > 0$ independent of h and τ, the discrete solution is unique.

We emphasize that in contrast to the existence of discrete solutions established in Theorem 4, we need to assume the existence of a sufficiently regular continuous solution to obtain the uniqueness result for the discrete problem. The detailed proof is given in Sections 6.1–8.1. For a better orientation, we point out the main steps already here: Following standard practice, we decompose the error into a projection error and a discrete evolution error. The first can be treated by standard arguments, which also reveal that the regularity assumptions of the theorem are rather sharp. In Section 6.1, we establish a nonlinear stability estimate for the discrete problem which allows us to bound the discrete evolution error by certain residuals which arise when replacing the discrete solution in Problem 3 by projections of the continuous solution. The residuals are identified, and corresponding bounds are stated in Section 7.1, which allows us to conclude the global error estimates. The uniqueness of the discrete solution is proven in Section 8.1 using similar arguments.

- Remark 6 The theoretical results can, in principle, be extended to other boundary conditions, for instance

$$\nabla\phi \cdot \mathrm{n}|_{\partial\Omega} = \nabla\mu \cdot \mathrm{n}|_{\partial\Omega} = \nabla q \cdot \mathrm{n}|_{\partial\Omega} = 0.$$

- It remains unproved if the regularity assumptions (2.10)–(2.12) can be verified. Given the results for the Cahn-Hilliard equation [4, 11] one expects that such statements can be verified in two space dimensions. In three space dimensions, even the uniqueness of the Cahn-Hilliard equation with variable mobility is unknown. However, one might expect either a short-time existence of a regular solution or the existence of a global-in-time regular solution under stronger as-

sumptions on the initial data or mobility functions, cf. [11, 31]. This means that we obtain optimal rates under a regularity assumption which might not be fulfilled or only holds for small times.
- The result in Theorem 4 remains valid even for non-uniform meshes in space and time and can be further generalized to such adaptive settings.
- The proof of uniqueness can also be adapted to provide continuous dependence on the initial data.

5 Proof of Theorem 4

5.1 Basic properties of discrete solutions.

We start with establishing the two important identities (2.8) stated in the theorem. It suffices to consider a single time step, e.g., the case $m = n-1$, $1 \le n \le N$. Let $\phi_{h,\tau}$, $q_{h,\tau} \in P_1(I_n;\mathcal{V}_h)$ and $\bar\mu_{h,\tau} \in P_0(I_n;\mathcal{V}_h)$ solve (2.5)–(2.7). By choosing $\bar\psi_{h,\tau} = 1$, $\bar\psi_{h,\tau} = 0$, and $\bar\zeta_{h,\tau} = 0$ as test functions in the discrete variational identities, we obtain

$$\langle \phi_{h,\tau}, 1\rangle\big|_{t^{n-1}}^{t^n} = \langle \partial_t\phi_{h,\tau}, 1\rangle^n = -\langle b(\bar\phi_{h,\tau})\nabla\bar\mu_{h,\tau} - c(\bar\phi_{h,\tau})\nabla(A(\bar\phi_{h,\tau})\bar q_{h,\tau}), \nabla 1\rangle^n = 0.$$

In the first step, we used the fundamental theorem of calculus and the notation $\langle a,b\rangle^n = \int_{t^{n-1}}^{t^n}\langle a,b\rangle\, \mathrm{d}s$. This already yields conservation of mass for a single time interval. The general case follows by induction over *n* and using the continuity of $\phi_{h,\tau}$ in time. In a similar manner, we obtain

$$\mathcal{E}(\phi_{h,\tau}, q_{h,\tau})\big|_{t^{n-1}}^{t^n} = \gamma\langle\nabla\bar\phi_{h,\tau}, \nabla\partial_t\phi_{h,\tau}\rangle^n + \langle f'(\phi_{h,\tau}), \partial_t\phi_{h,\tau}\rangle^n + \langle\partial_t q_{h,\tau}, \bar q_{h,\tau}\rangle^n.$$

For the first and last term, we used that $\partial_t\nabla\phi_{h,\tau}, \partial_t q_{h,\tau}$ are constant in time on the interval I^n and hence $\langle\partial_t q_{h,\tau}, q_{h,\tau}\rangle^n = \langle\partial_t q_{h,\tau}, \bar q_{h,\tau}\rangle^n$ and similar for the first term, where $\bar q_{h,\tau} = \bar\pi_\tau^0 q_{h,\tau}$ is the piecewise constant projection in time. Using (2.6) with $\bar\xi_{h,\tau} = \partial_t\phi_{h,\tau}$ and (2.7) with $\bar\zeta_{h,\tau} = \bar q_{h,\tau}$, we obtain

$$\begin{aligned}\mathcal{E}(\phi_{h,\tau}, q_{h,\tau})\big|_{t^{n-1}}^{t^n} &= \langle\bar\mu_{h,\tau}, \partial_t\phi_{h,\tau}\rangle^n - \langle\kappa(\bar\phi_{h,\tau})\bar q_{h,\tau}, \bar q_{h,\tau}\rangle^n - \varepsilon\langle\nabla\bar q_{h,\tau}, \nabla\bar q_{h,\tau}\rangle^n\\ &\quad - \langle d_0\nabla(A(\bar\phi_{h,\tau})\bar q_{h,\tau}) - c(\bar\phi_{h,\tau})\nabla\bar\mu_{h,\tau}, \nabla(A(\bar\phi_{h,\tau})\bar q_{h,\tau})\rangle^n.\end{aligned}$$

Using (2.5) with $\bar\psi_{h,\tau} = \bar\mu_{h,\tau}$, the first term on the right-hand side can be replaced by $\langle\bar\mu_{h,\tau}, \partial_t\phi_{h,\tau}\rangle^n = \langle b(\bar\phi_{h,\tau})\nabla\bar\mu_{h,\tau} - c(\bar\phi_{h,\tau})\nabla(A(\bar\phi_{h,\tau})\bar q_{h,\tau}), \nabla\bar\mu_{h,\tau}\rangle^n$. We thus obtain

$$\begin{aligned}\mathcal{E}(\phi_{h,\tau}, q_{h,\tau})\big|_{t^{n-1}}^{t^n} &= -\langle b(\bar\phi_{h,\tau})\nabla\bar\mu_{h,\tau}, \nabla\bar\mu_{h,\tau}\rangle^n + 2\langle c(\bar\phi_{h,\tau})\nabla(A(\bar\phi_{h,\tau})\bar q_{h,\tau}), \nabla\bar\mu_{h,\tau}\rangle^n\\ &\quad - \langle d_0\nabla(A(\bar\phi_{h,\tau})\bar q_{h,\tau}), \nabla(A(\bar\phi_{h,\tau})\bar q_{h,\tau})\rangle^n - \langle\kappa(\bar\phi_{h,\tau})\bar q_{h,\tau}, \bar q_{h,\tau}\rangle^n - \varepsilon\langle\nabla\bar q_{h,\tau}, \nabla\bar q_{h,\tau}\rangle^n.\end{aligned}$$

A careful inspection of the individual terms reveals that the right-hand side of this identity exactly amounts to the dissipation term $\int_{t^{n-1}}^{t^n} \mathcal{D}_{\bar\phi_{h,\tau}}(\bar\mu_{h,\tau}, \bar q_{h,\tau})\, \mathrm{d}s$ in (2.8). We have thus established the discrete energy-dissipation identity for a single time step. The general case then follows by induction.

5.2 A-priori bounds

Using assumptions (A0)–(A5), one can immediately see that

$$\|\nabla\phi\|_{L^2}^2 + \|q\|_{L^2}^2 \le C_1\mathcal{E}(\phi, q) + C_2 f_1 \qquad \text{for all } \phi, q \in H^1(\Omega), \tag{3.1}$$

where f_1 is the lower bound for f from (A2). Furthermore, $\|\phi\|_{H^1}^2 \le C_3\|\nabla\phi\|_{L^2}^2 + C_4|\int_\Omega \phi \,\mathrm{d}x|^2$ by the Poincaré inequality. From the discrete mass conservation and energy-dissipation property, and using the positivity of the dissipation functional, we thus already obtain

$$\|\phi\|_{L^\infty(H^1)}^2 + \|q\|_{L^\infty(L^2)}^2 \le C_1',$$

with C_1' depending only on the bounds of the coefficients in (A1)–(A7) and the energy and mass of the initial data. From the energy-dissipation identity and the bounds of the coefficients, we further get

$$\|\nabla\bar\mu_{h,\tau}\|_{L^2(L^2)}^2 + \|\bar q_{h,\tau}\|_{L^2(H^1)}^2 + \|c(\bar\phi_{h,\tau})\nabla\bar\mu_{h,\tau} - d_0\nabla(A(\bar\phi_{h,\tau})\bar q_{h,\tau})\|_{L^2(L^2)}^2 \le C_2'.$$

Here C_2' again only depends on the bounds of the coefficients and the initial data. By testing the identity (2.6) with $\bar\xi_{h,\tau} = 1$, by using (A2) we further see that

$$\langle\bar\mu_{h,\tau}, 1\rangle^n = \langle f'(\phi_{h,\tau}), 1\rangle^n \le C'\tau\left(f_2^1 + f_3^1\|\phi_{h,\tau}\|_{L^\infty(L^3)}^3\right).$$

Summation over n, the continuous embedding of $H^1(\Omega)$ in $L^3(\Omega)$, the uniform bounds for $\|\phi_{h,\tau}\|_{L^\infty(H^1)}$ and $\|\nabla\bar\mu_{h,\tau}\|_{L^2(L^2)})$, and the Poincaré inequality then lead to

$$\|\bar\mu_{h,\tau}\|_{L^2(L^2)}^2 \le C_1''\|\nabla\bar\mu_{h,\tau}\|_{L^2(L^2)}^2 + C_2''\sum\nolimits_n \langle\bar\mu_{h,\tau}, 1\rangle^n \le C_3'$$

with C_3' again only depending on the bounds of the coefficients and the initial data. This completes the proof of a-priori bounds stated in the theorem.

5.3 Existence of discrete solutions

The aim of this section is to prove the existence of a discrete solution. This can be obtained by a fixed point theorem and from the a-priori estimates implied by the discrete energy-dissipation identity (2.8). In the *n*th time step of Problem 3, we have to determine the values $\phi_h^n = \phi_{h,\tau}(t^n)$, $q_h^n = q_{h,\tau}(t^n)$, and $\mu_h^n = \bar{\mu}_{h,\tau}(t^{n-1/2})$ in $\mathcal{V}_h$ such that (2.5)–(2.7) hold. Now, the functions $\phi_h^{n-1} = \phi_{h,\tau}(t^{n-1})$ and $q_h^{n-1} = q_{h,\tau}(t^{n-1})$ are already known. The system (2.5)–(2.7) can be written compactly as

$$\langle F_h(x_h), y_h\rangle^n = 0 \qquad \forall y_h \in X_h \tag{3.2}$$

with continuous operator $F_h : X_h \to X_h$, $X_h = (\mathcal{V}_h)^3$ and $x_h = (\mu_h^n, d_\tau\phi_h^n, q_h^n)$. Here we have used that $\phi_h^n = \phi_h^{n-1} + \tau d_\tau \phi_h^n$ with $d_\tau\phi_h^n = \frac{1}{\tau}(\phi_h^n - \phi_h^{n-1})$ denoting the backward difference quotient. Since $\phi_{h,\tau}$ is piecewise linear, $d_\tau\phi_h^n = \partial_t\phi_{h,\tau}$ on the interval (t^{n-1}, t^n). From our previous considerations, we know that

$$\langle F_h(x_h), x_h\rangle^n = \mathcal{E}_h^n - \mathcal{E}_h^{n-1} + \tau\mathcal{D}_h^n, \tag{3.3}$$

where $\mathcal{E}_h^n = \mathcal{E}(\phi_h^n, q_h^n)$, $\mathcal{E}_h^{n-1} = \mathcal{E}(\phi_h^{n-1}, q_h^{n-1})$, and $\mathcal{D}_h^n = \mathcal{D}_{\phi_h^{n-1/2}}(\mu_h^n, q_h^{n-1/2})$ denote the relevant values of the energy and dissipation functionals appearing in (2.8). The values at the midpoints of the time interval $[t^{n-1}, t^n]$ are given by $\phi_h^{n-1/2} = \frac{1}{2}(\phi_h^n + \phi_h^{n-1})$ and $q_h^{n-1/2} = \frac{1}{2}(q_h^n + q_h^{n-1})$. System (3.3) is equivalent to the fixed point problem

$$x_h = x_h - F_h(x_h) =: T_h(x_h) \qquad \text{in } X_h. \tag{3.4}$$

To show the existence of a fixed point, we apply the Leray-Schauder theorem; see [53, Theorem 6.A]. Assume that $x_h \in X_h$ is a solution of the parametrized equation $x_h = \lambda T_h(x_h)$ for some $0 \le \lambda < 1$. Then by (3.2) and (3.3), we have

$$\begin{aligned}\|x_h\|_h^2 := \langle x_h, x_h\rangle^n &= \lambda\langle x_h, x_h\rangle^n - \lambda\langle F_h(x_h), x_h\rangle^n \\ &= \lambda\|x_h\|_h^2 + \lambda\left(\mathcal{E}_h^n - \mathcal{E}_h^{n-1} + \tau\mathcal{D}_h^n\right).\end{aligned}$$

A slight rearrangement of the terms leads to the identity

$$(1-\lambda)\|x_h\|_h^2 + \lambda(\mathcal{E}_h^n + \tau D_h^n) = \lambda\mathcal{E}_h^{n-1}. \tag{3.5}$$

From the properties of the energy- and dissipation functionals, one can see that solutions of $x_h = \lambda T_h(x_h)$ are uniformly bounded for all values $0 \le \lambda \le 1$ by the energy $\mathcal{E}_h^{n-1}$. This allows us to apply [53, Theorem 6.A] and to conclude the existence of a fixed point of (3.4), and hence of a solution to (2.5)–(2.7) for a single time step. By induction over *n*, we obtain the existence of a solution to Problem 3.

6 A discrete relative energy estimate

In this section, we prove discrete relative energy for the difference between the solutions of the discrete problem and a suitably perturbed discrete system, which is one of the key ingredients for the proof of Theorem 5. This perturbed solution will, later on, be either another numerical solution itself, in order to show the uniqueness, or suitable projections of the exact regular solution, in order to show the error estimates. To this end, we first propose a suitable perturbed system, whose variables will be named $\hat{\phi}_{h,\tau}, \bar{\hat{\mu}}_{h,\tau}, \hat{q}_{h,\tau}$. Based on a convexified version of the energy, we propose the relative energy between a discrete solution and a solution of the perturbed system and afterwards compute the discrete time evolution of the relative energy. Finally, applying the discrete Gronwall lemma implies that the *distance* between the discrete solutions and the perturbed solutions is controlled only by the initial *distance* and the residuals of the perturbed system.

Let $(\phi_{h,\tau}, q_{h,\tau}, \bar{\mu}_{h,\tau})$ be a solution of Problem 3, and further let $\hat{\phi}_{h,\tau}$, $\hat{q}_{h,\tau} \in P_1^c(\mathcal{I}_\tau;\mathcal{V}_h)$, and $\bar{\hat{\mu}}_{h,\tau} \in P_0(\mathcal{I}_\tau;\mathcal{V}_h)$ be some given functions in the corresponding spaces. By inserting these functions into (2.5)–(2.7), we obtain

$$\langle \partial_t \hat{\phi}_{h,\tau}, \bar{\psi}_{h,\tau}\rangle^n + \langle b(\bar{\hat{\phi}}_{h,\tau})\nabla\bar{\hat{\mu}}_{h,\tau} - c(\bar{\hat{\phi}}_{h,\tau})\nabla(A(\bar{\hat{\phi}}_{h,\tau})\bar{\hat{q}}_{h,\tau}), \nabla\bar{\psi}_{h,\tau}\rangle^n =: \langle \bar{r}_{1,h,\tau}, \bar{\psi}_{h,\tau}\rangle^n, \tag{4.1}$$

$$\langle \bar{\hat{\mu}}_{h,\tau}, \bar{\xi}_{h,\tau}\rangle^n - \gamma\langle \nabla\bar{\hat{\phi}}_{h,\tau}, \nabla\bar{\xi}_{h,\tau}\rangle^n - \langle f'(\hat{\phi}_{h,\tau}), \bar{\xi}_{h,\tau}\rangle^n =: \langle \bar{r}_{2,h,\tau}, \bar{\xi}_{h,\tau}\rangle^n, \tag{4.2}$$

$$\begin{aligned} \langle \partial_t \hat{q}_{h,\tau}, \bar{\zeta}_{h,\tau}\rangle^n &+ \langle d_0\nabla(A(\bar{\hat{\phi}}_{h,\tau})\bar{\hat{q}}_{h,\tau}) - c(\bar{\hat{\phi}}_{h,\tau})\nabla\bar{\hat{\mu}}_{h,\tau}, \nabla(A(\bar{\hat{\phi}}_{h,\tau})\bar{\zeta}_{h,\tau})\rangle^n \\ &+ \langle \kappa(\bar{\hat{\phi}}_{h,\tau})\bar{\hat{q}}_{h,\tau}, \bar{\zeta}_{h,\tau}\rangle^n + \varepsilon\langle \nabla\bar{\hat{q}}_{h,\tau}, \nabla\bar{\zeta}_{h,\tau}\rangle^n =: \langle \bar{r}_{3,h,\tau}, \bar{\zeta}_{h,\tau}\rangle^n \end{aligned} \tag{4.3}$$

for all test function $\bar{\psi}_{h,\tau}$, $\bar{\xi}_{h,\tau}$, $\bar{\zeta}_{h,\tau} \in P_0(I_n;\mathcal{V}_h)$, time steps $1 \le n \le N$, and with appropriate residuals $\bar{r}_{i,h,\tau} \in P_0(\mathcal{I}_\tau;\mathcal{V}_h)$, $i = 1, 2, 3$, which are actually defined through these equations.

6.1 Relative energy

In order to estimate the distance between solutions of the discrete problem (2.5)–(2.7) and the perturbed problem (4.1)–(4.3) in terms of the residuals $\bar{r}_{i,h,\tau}$ we will measure to *distance* using the relative energy method, cf. [23]. The relative energy functional we employ is defined by

$$\begin{aligned} \mathcal{E}_\alpha(\phi, q|\hat{\phi}, \hat{q}) :=& \frac{\gamma}{2}\|\nabla\phi - \nabla\hat{\phi}\|_0^2 + \langle f(\phi) - f(\hat{\phi}) - f'(\hat{\phi})(\phi - \hat{\phi}), 1\rangle \\ &+ \frac{\alpha}{2}\|\phi - \hat{\phi}\|_0^2 + \frac{1}{2}\|q - \hat{q}\|_0^2 \end{aligned} \tag{4.4}$$

with parameter $\alpha = \max\{-f_1, 0\} + 1$. This choice guarantees that the functional is non-negative. We further observe that the relative energy functional splits naturally into contributions $\mathcal{E}_\alpha^\phi(\phi_{h,\tau}|\hat{\phi}_{h,\tau}) := \mathcal{E}_\alpha(\phi_{h,\tau}, 0|\hat{\phi}_{h,\tau}, 0)$ and

$\mathcal{E}^q_\alpha(q_{h,\tau}|\hat{q}_{h,\tau}) := \mathcal{E}_\alpha(0, q_{h,\tau}|0, \hat{q}_{h,\tau})$ for the individual variables. The following important estimates immediately follow from the Taylor expansions.

Lemma 7 *Let (A0)–(A5) hold. Then*

$$\|\phi_{h,\tau} - \hat{\phi}_{h,\tau}\|_1^2 \le C\,\mathcal{E}^\phi_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau}), \qquad \|q_{h,\tau} - \hat{q}_{h,\tau}\|_0^2 \le C\,\mathcal{E}^q_\alpha(q_{h,\tau}|\hat{q}_{h,\tau}), \textit{and} \tag{4.5}$$

$$\|\nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau})\|_0^2 + \|\nabla(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau})\|_0^2 \le C\,\mathcal{D}_{\bar{\phi}_{h,\tau}}(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}, \bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}). \tag{4.6}$$

The constant C depends only on the bounds of the parameters.

6.2 Discrete stability estimate

We can now state and prove the main result of this section.

Lemma 8 *Let (A0)–(A7) hold and $(\phi_{h,\tau}, q_{h,\tau}, \bar{\mu}_{h,\tau})$ be a solution of Problem 3. Furthermore, let $(\hat{\phi}_{h,\tau}, \hat{q}_{h,\tau}, \bar{\hat{\mu}}_{h,\tau})$ be given and $\bar{r}_{i,h,\tau}$, $i = 1, 2, 3$, be the residuals defined by (4.1)–(4.3). Then*

$$\begin{aligned} &\mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau}|\hat{\phi}_{h,\tau}, \hat{q}_{h,\tau})\big|_{t=t^n} + c\int_0^{t^n} \|\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}\|_1^2 + \|\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\|_1^2 \,\mathrm{d}s \\ &\le C_1\mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau}|\hat{\phi}_{h,\tau}, \hat{q}_{h,\tau})\big|_{t=0} + C_2\int_0^{t^n} \|\bar{r}_{1,h,\tau}\|_{-1,h}^2 + \|\bar{r}_{2,h,\tau}\|_1^2 + \|\bar{r}_{3,h,\tau}\|_{-1,h}^2 \,\mathrm{d}s \end{aligned} \tag{4.7}$$

for all $0 \le n \le N$ with constants c, C_1, C_2 that are independent of the discretization parameters.

Proof The remainder of this section, i.e. Section 4.3-4.5 is devoted to the proof of this assertion. We start with splitting $\mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau}|\hat{\phi}_{h,\tau}, \hat{q}_{h,\tau}) = \mathcal{E}^\phi_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau}) + \mathcal{E}^q_\alpha(q_{h,\tau}|\hat{q}_{h,\tau})$ and then estimate the change in the two parts of the relative energy over a single time interval separately. We note that the numbering of the constants, i.e. $C_1', C_2', \ldots$, will be reused for every component. □

6.3 Bulk stress component

By the fundamental theorem of calculus, we obtain

$$\begin{aligned} \mathcal{E}^q_\alpha(q_{h,\tau}|\hat{q}_{h,\tau})\big|_{t^{n-1}}^{t^n} &= \langle \partial_t q_{h,\tau} - \partial_t\hat{q}_{h,\tau}, q_{h,\tau} - \hat{q}_{h,\tau}\rangle^n \\ &= \langle \partial_t q_{h,\tau} - \partial_t\hat{q}_{h,\tau}, \bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\rangle^n = (*). \end{aligned}$$

In the second step, we have used the definition of the orthogonal projection $\bar{q} = \bar{\pi}^0_\tau q$. Using the test function $\bar{\zeta}_{h,\tau} = \bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}$ in (2.7) and (4.3), we further obtain

$$
\begin{aligned}
(*) = &- \langle \kappa(\bar{\phi}_{h,\tau})(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}), \bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\rangle^n \\
&- \varepsilon \|\nabla(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau})\|_0^2 + \langle \bar{r}_{3,h,\tau}, \bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\rangle^n \\
&- \langle d_0 \nabla(A(\bar{\phi}_{h,\tau})(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau})) - c(\bar{\phi}_{h,\tau})\nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}), \nabla(A(\bar{\phi}_{h,\tau})(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}))\rangle^n.
\end{aligned}
\tag{4.8}
$$

The first two terms have already appeared in the dissipation functional. The last one will be used later, and we abbreviate it by

$$
\begin{aligned}
\mathcal{R}_q^n := -\langle d_0 \nabla(A(\bar{\phi}_{h,\tau})(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau})) - c(\bar{\phi}_{h,\tau})\nabla(\bar{\mu}_{h,\tau} \\
- \bar{\hat{\mu}}_{h,\tau}), \nabla(A(\bar{\phi}_{h,\tau})(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}))\rangle^n.
\end{aligned}
$$

The third term can be estimated by

$$
\langle \bar{r}_{3,h,\tau}, \bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\rangle^n \le \delta \int_{I^n} \|\nabla(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau})\|_1^2 + C(\delta)\|\bar{r}_{3,h,\tau}\|_{-1,h}^2 \, \mathrm{d}s.
$$

The parameter $\delta > 0$ stems from the application of Young's inequality and will be chosen sufficiently small, but independent of the discretization parameters, to absorb the corresponding terms on the left-hand side. As a consequence, $C(\delta) \approx \delta^{-1}$ will only depend on the bounds in our assumptions. In summary, we thus obtain

$$
\mathcal{E}_\alpha^q(q_{h,\tau}|\hat{q}_{h,\tau})\big|_{t^{n-1}}^{t^n} \le -c_1' \int_{I^n} \|\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\|_1^2 \, \mathrm{d}s + \mathcal{R}_q^n + C_1' \int_{I_n} \|\bar{r}_{3,h,\tau}\|_{-1,h}^2 \, \mathrm{d}s \tag{4.9}
$$

with positive constants c_1', C_1' independent of the discretization parameters. The first term on the right-hand side has a negative sign and allows to compensate similar terms arising later on.

6.4 Cahn-Hilliard component

By the fundamental theorem of calculus, repeated application of the chain rule, the definition of the relative energy (4.4), and elementary computations, we obtain

$$
\begin{aligned}
\mathcal{E}_\alpha^\phi(\phi_{h,\tau}|\hat{\phi}_{h,\tau})\big|_{t^{n-1}}^{t^n} = &\ \gamma\langle \nabla(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}), \nabla\partial_t(\phi_{h,\tau} - \hat{\phi}_{h,\tau})\rangle^n \\
&+ \langle f'(\phi_{h,\tau}) - f'(\hat{\phi}_{h,\tau}), \partial_t(\phi_{h,\tau} - \hat{\phi}_{h,\tau})\rangle^n + \alpha\langle \bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}, \partial_t(\phi_{h,\tau} - \hat{\phi}_{h,\tau})\rangle^n \\
&+ \langle f'(\phi_{h,\tau}) - f'(\hat{\phi}_{h,\tau}) - f''(\hat{\phi}_{h,\tau}), \partial_t\hat{\phi}_{h,\tau}\rangle^n = I_1 + I_2 + I_3 + I_4.
\end{aligned}
\tag{4.10}
$$

6.4.1 Step 1.

By testing (2.6) and (4.2) with $\bar{\xi}_{h,\tau} = \partial_t(\phi_{h,\tau} - \hat{\phi}_{h,\tau})$, we obtain

$$
I_1 + I_2 = \langle \bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau} + \bar{r}_{2,h,\tau}, \partial_t(\phi_{h,\tau} - \hat{\phi}_{h,\tau})\rangle^n = (*).
$$

Next we use $\bar{\psi}_{h,\tau} = \bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau} + \bar{r}_{2,h,\tau}$ as test function in (2.5) and (4.1) to deduce

$$
\begin{aligned}
(*) &= \langle \bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau} + \bar{r}_{2,h,\tau}, \partial_t(\phi_{h,\tau} - \hat{\phi}_{h,\tau})\rangle^n \\
&= -\langle b(\bar{\phi}_{h,\tau})\nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}) - c(\bar{\phi}_{h,\tau})\nabla(A(\bar{\phi}_{h,\tau})(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau})), \nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau} + \bar{r}_{2,h,\tau})\rangle^n \\
&\quad + \langle \bar{r}_{1,h,\tau}, \bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau} + \bar{r}_{2,h,\tau}\rangle^n = (i) + (ii).
\end{aligned}
$$

The first term can be combined with the remainder $\mathcal{R}_q^n$ in (4.9). By decomposition of the dissipative terms, similar as in the proof of the discrete energy-dissipation identity, c.f. Subsection 5.2, estimating coefficient from below using (A1), and application of Young's inequality, we get

$$
\begin{aligned}
\mathcal{R}_q^n + (i) \le \int_{I_n} & C' \|\bar{r}_{2,h,\tau}\|_1^2 - c_2' \|\nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau})\|_0^2 \\
& - c_3' \|c(\bar{\phi}_{h,\tau})\nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}) - d_0 \nabla(A(\bar{\phi}_{h,\tau})(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}))\|_0^2 \,\mathrm{d}s.
\end{aligned} \tag{4.11}
$$

The last two terms have a negative sign and will be used to compensate for terms of this form in the other estimates. Using the definition of the discrete dual norm (1.1), Poincaré's inequality, and the bounds for the coefficients (A1), the second term can be further estimated by

$$
\begin{aligned}
(ii) &\le \int_{I_n} \|\bar{r}_{1,h,\tau}\|_{-1,h} \left(\|\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}\|_1 + \|\bar{r}_{2,h,\tau}\|_1 \right) \,\mathrm{d}s \\
&\le \int_{I_n} C_1' \|\bar{r}_{1,h,\tau}\|_{-1,h}^2 + C_2' |\langle \bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}, 1\rangle|^2 + \delta \, \|\nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau})\|_0^2 + C_3' \|\bar{r}_{2,h,\tau}\|_1^2 \,\mathrm{d}s.
\end{aligned}
$$

The parameter $\delta > 0$ is the same as before and will be chosen sufficiently small, but independent of the discretization parameters. By testing the variational identities (2.6) and (4.2) with $\bar{\xi}_{h,\tau} = 1$, we see using (A2) that

$$
\begin{aligned}
\int_{I_n} |\langle \bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}, 1\rangle|^2 \,\mathrm{d}s &= \int_{I_n} |\langle f'(\phi_{h,\tau}) - f'(\hat{\phi}_{h,\tau}) + \bar{r}_{2,h,\tau}, 1\rangle|^2 \,\mathrm{d}s \\
&\le \int_{I_n} C_4' \|\bar{r}_{2,h,\tau}\|_{0,1}^2 + C_5' \|\phi_{h,\tau} - \hat{\phi}_{h,\tau}\|_1^2 \,\mathrm{d}s.
\end{aligned} \tag{4.12}
$$

The constants C_4', C_5' depend on the bounds in the assumptions, i.e. (A2) and the uniform a-priori bounds for the discrete solution established in Theorem 4. In summary, we can thus estimate

$$
(ii) \le \int_{I_n} \delta \, \|\nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau})\|_0^2 + C_6' \|\bar{r}_{1,h,\tau}\|_{-1,h}^2 + C_7' \|\bar{r}_{2,h,\tau}\|_1^2 + C_8' \mathcal{E}_\alpha^\phi(\phi_{h,\tau}|\hat{\phi}_{h,\tau}) \,\mathrm{d}s. \tag{4.13}
$$

The first term can later be absorbed by dissipation terms and choosing δ appropriately.

6.4.2 Step 2.

By testing the variational identities (2.5) and (4.1) with $\bar{\psi}_{h,\tau} = \alpha(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})$, we get

$$I_3 = \alpha\langle \bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}, \partial_t(\phi_{h,\tau} - \hat{\phi}_{h,\tau})\rangle^n = \alpha\langle \bar{r}_{1,h,\tau}, \bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\rangle^n$$
$$- \alpha\langle b(\bar{\phi}_{h,\tau})\nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}) - c(\bar{\phi}_{h,\tau})\nabla(A(\bar{\phi}_{h,\tau})(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau})), \nabla(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})\rangle^n.$$

With similar arguments as before, we then obtain

$$\begin{aligned} I_3 \le \int_{I_n} & C_1'\|\bar{r}_{1,h,\tau}\|_{-1,h}^2 + C_2'\|\phi_{h,\tau} - \hat{\phi}_{h,\tau}\|_1^2 + C_3'\delta\|\nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau})\|_0^2 \\ & + C_4'\delta\|c(\bar{\phi}_{h,\tau})\nabla(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}) - d_0\nabla(A(\bar{\phi}_{h,\tau})(\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}))\|_0^2 \,\mathrm{d}s. \end{aligned} \tag{4.14}$$

For δ sufficiently small, the corresponding term can again be absorbed by dissipation terms.

6.4.3 Step 3.

From the bounds in assumption (A2), we can deduce that

$$|f'(\phi_{h,\tau}) - f'(\hat{\phi}_{h,\tau}) - f''(\hat{\phi}_{h,\tau})(\phi_{h,\tau} - \hat{\phi}_{h,\tau})| \le \left(f_2^{(3)} + f_3^{(3)}(|\phi_{h,\tau}| + |\hat{\phi}_{h,\tau}|)\right)|\phi_{h,\tau} - \hat{\phi}_{h,\tau}|^2.$$

Using the Hölder inequality, embedding estimates, and the uniform bounds for $\phi_{h,\tau}$ (2.9), we can further bound I_4 from above as follows

$$\begin{aligned} I_4 &\le \int_{I_n} \|\partial_t\hat{\phi}_{h,\tau}\|_0\|f'(\phi_{h,\tau}) - f'(\hat{\phi}_{h,\tau}) - f''(\hat{\phi}_{h,\tau})(\phi_{h,\tau} - \hat{\phi}_{h,\tau})\|_0 \,\mathrm{d}s \\ &\le C\int_{I_n} \|\partial_t\hat{\phi}_{h,\tau}\|_0(f_3^{(3)}\|\phi_{h,\tau} - \hat{\phi}_{h,\tau}\|_{0,4}^2 + f_2^{(3)}(\|\phi_{h,\tau}\|_{0,6} + \|\hat{\phi}_{h,\tau}\|_{0,6})\|\phi_{h,\tau} - \hat{\phi}_{h,\tau}\|_{0,6}^2) \,\mathrm{d}s \\ &\le C_1'\int_{I^n} \|\phi_{h,\tau} - \hat{\phi}_{h,\tau}\|_{0,6}^2 \,\mathrm{d}s \le C_2'\int_{I^n} \mathcal{E}_\alpha^\phi(\phi_{h,\tau}|\hat{\phi}_{h,\tau}) \,\mathrm{d}s. \end{aligned} \tag{4.15}$$

The constants C_1', C_2' only depend on the bounds of the coefficients (A2) and available uniform bounds for the discrete and exact solutions.

6.5 Stability estimate.

Combining all bounds derived so far, i.e. (4.9), (4.11), (4.13), (4.14), (4.15), and using (4.12) once again in order to bound $\|\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}\|_0^2$, we find the following inequality

$$\begin{aligned} &\mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau}|\hat{\phi}_{h,\tau}, \hat{q}_{h,\tau})\big|_{t^{n-1}}^{t^n} + c'\int_{I_n} \|\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}\|_1^2 + \|\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\|_1^2 \,\mathrm{d}s \\ &\le C_1'\int_{I_n} \mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau}|\hat{\phi}_{h,\tau}, \hat{q}_{h,\tau}) \,\mathrm{d}s + C_2'\int_{I_n} \|\bar{r}_{1,h,\tau}\|_{-1,h}^2 + \|\bar{r}_{2,h,\tau}\|_1^2 + \|\bar{r}_{3,h,\tau}\|_{-1,h} \,\mathrm{d}s. \end{aligned} \tag{4.16}$$

The constants c', C_1', C_2' only depend on available bounds for the discrete and continuous solution and the parameters. The bound of Lemma 8 then follows by a recursive application of this inequality and a discrete Gronwall estimate; see Lemma 19. □

7 Error estimates

In order to prove the global error estimates of Theorem 5, we define

$$\hat{\phi}_{h,\tau} = I_\tau^1 \pi_h^1 \phi \quad \text{and} \quad \bar{\hat{\mu}}_{h,\tau} = \bar{\pi}_\tau^0 \pi_h^0 \mu \quad \text{and} \quad \hat{q}_{h,\tau} = I_\tau^1 \pi_h^0 q \tag{5.1}$$

as approximations for the continuous solution. We can then split the error into a projection error and a discrete evolution error, using standard error estimates for the first one, and the discrete stability results of the previous section to bound the second error component.

7.1 Projection errors.

By standard estimates of polynomial interpolation and projection errors, we obtain the following estimates; see [13] and the appendix.

Lemma 9 *Let (A6)–(A7) hold and* $(\hat{\phi}_{h,\tau}, \bar{\hat{\mu}}_{h,\tau}, \hat{q}_{h,\tau})$ *be given as above. Let* (ϕ, μ, q) *be a smooth solution of (0.1)–(0.3) such that (2.10)–(2.12) holds. Then*

$$\begin{aligned}
&\|\hat{\phi}_{h,\tau} - \phi\|^2_{L^\infty(H^1)} \le C(h^4 + \tau^4), && \|\bar{\hat{\mu}}_{h,\tau} - \bar{\mu}\|^2_{L^2(H^1)} \le Ch^4, \\
&\|\hat{q}_{h,\tau} - q\|^2_{L^\infty(L^2)} \le C(h^4 + \tau^4), && \|\bar{\hat{q}}_{h,\tau} - \bar{q}\|^2_{L^2(H^1)} \le Ch^4, \\
&\|\partial_t \hat{\phi}_{h,\tau} - \bar{\pi}_\tau^0(\partial_t \phi)\|^2_{L^2(H^{-1})} \le Ch^4, && \|\partial_t \hat{q}_{h,\tau} - \bar{\pi}_\tau^0(\partial_t q)\|^2_{L^2(H^{-1})} \le Ch^4.
\end{aligned}$$

The constant C in these estimates depends only on a-priori bounds for the solution components in appropriate norms and constants in the assumptions.

7.2 Residuals

In the next step, we identify and then estimate the residuals arising from the above choice of approximate functions and (4.1)–(4.3).

Lemma 10 *Let the assumptions of Theorem 5 hold and* $(\hat{\phi}_{h,\tau}, \bar{\hat{\mu}}_{h,\tau}, \hat{q}_{h,\tau})$ *be defined as projections of the smooth solution* (ϕ, μ, q) *via (5.1). Then (2.5)–(2.7) holds with the residuals* $\bar{r}_{i,h,\tau}$ *defined by*

$$\begin{aligned}
\langle \bar{r}_{1,h,\tau}, \bar{\psi}_{h,\tau} \rangle^n &= \langle \partial_t (\pi_h^1 \phi - \phi), \bar{\psi}_{h,\tau} \rangle + \langle b(\bar{\phi}_{h,\tau}) \nabla \bar{\hat{\mu}}_{h,\tau} - c(\bar{\phi}_{h,\tau}) \nabla (A(\bar{\phi}_{h,\tau}) \bar{\hat{q}}_{h,\tau}), \nabla \bar{\psi}_{h,\tau} \rangle^n \\
&\quad - \langle b(\phi) \nabla \mu - c(\phi) \nabla (A(\phi) q)), \nabla \bar{\psi}_{h,\tau} \rangle^n, \\
\langle \bar{r}_{2,h,\tau}, \bar{\xi}_{h,\tau} \rangle^n &= \langle \bar{\hat{\mu}}_{h,\tau} - I_\tau^1 \mu, \bar{\xi}_{h,\tau} \rangle^n + \gamma \langle \nabla (\bar{\hat{\phi}}_{h,\tau} - I_\tau^1 \phi), \nabla \bar{\xi}_{h,\tau} \rangle^n \\
&\quad + \langle f'(\hat{\phi}_{h,\tau}) - I_\tau^1 f'(\phi), \bar{\xi}_{h,\tau} \rangle^n, \\
\langle \bar{r}_{3,h,\tau}, \bar{\zeta}_{h,\tau} \rangle^n &= \langle \kappa(\bar{\phi}_{h,\tau}) \bar{\hat{q}}_{h,\tau} - \kappa(\phi) \nabla q, \bar{\zeta}_{h,\tau} \rangle^n + \varepsilon \langle \nabla \bar{\hat{q}}_{h,\tau} - \nabla q, \nabla \bar{\zeta}_{h,\tau} \rangle^n \\
&\quad + \langle d_0 \nabla (A(\bar{\phi}_{h,\tau}) \bar{\hat{q}}_{h,\tau}) - c(\bar{\phi}_{h,\tau}) \nabla \bar{\hat{\mu}}_{h,\tau}, \nabla (A(\bar{\phi}_{h,\tau}) \bar{\zeta}_{h,\tau}) \rangle^n \\
&\quad - \langle d_0 \nabla (A(\phi) q) - c(\phi) \nabla \mu, \nabla (A(\phi) \bar{\zeta}_{h,\tau}) \rangle^n.
\end{aligned}$$

Proof The identities follow directly from the variational principles characterizing the exact smooth solution and its discrete projection, and some elementary manipulations. □

Using interpolation and projection error estimates, one can derive the following bounds for the residuals after some tedious calculations.

Lemma 11 *Under the assumptions of the previous lemma, we have*

$$\int_{I_n} \|\bar{r}_{1,h,\tau}\|_{-1,h}^2 + \|\bar{r}_{2,h,\tau}\|_1^2 + \|\bar{r}_{3,h,\tau}\|_{-1,h}^2 \,\mathrm{d}s \le C_1'(h^4+\tau^4) + C_2' \int_{I_n} \mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau} | \hat{\phi}_{h,\tau}, \hat{q}_{h,\tau}) \,\mathrm{d}s.$$

The constants C_1', C_2' are independent of the discretization parameters.

A detailed proof of this assertion is given in the appendix.

7.3 Discrete error

Combining Lemma 9 and Lemma 11, we can now prove the following bounds for the discrete evolution error.

Lemma 12 *Let the assumptions of Theorem 5 hold. Then*

$$\|\phi_{h,\tau} - \hat{\phi}_{h,\tau}\|_{L^\infty(H^1)}^2 + \|q_{h,\tau} - \hat{q}_{h,\tau}\|_{L^\infty(L^2)}^2 + \|\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}\|_{L^2(H^1)}^2 + \|\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\|_{L^2(H^1)}^2 \le C(h^4+\tau^4)$$

with a constant C that is independent of the discretization parameters h and τ.

Proof By using Lemma 8, the bounds of Lemma 11, and applying the discrete Gronwall lemma, cf. Lemma 19, similar to the proof of Lemma 8, we obtain

$$\mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau} | \hat{\phi}_{h,\tau}, \hat{q}_{h,\tau})\big|_{t=t^n} + c' \int_0^{t^n} \|\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}\|_1^2 + \|\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\|_1^2 \,\mathrm{d}s \le C_1 \mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau} | \hat{\phi}_{h,\tau}, \hat{q}_{h,\tau})\big|_{t=0} + C(h^4+\tau^4) \qquad \text{for all } 0 \le n \le N.$$

Due to the particular choice of the initial values $\phi_{h,0}$, $q_{h,0}$, the first term on the right-hand side drops out. Using (4.5), the first term on the left-hand side can further be estimated from below by the corresponding norms, which already yields the result. □

7.4 Conclusion

Combining the estimates for the projection errors with the discrete evolution error, we can finally obtain the global error estimates of Theorem 5.

8 Uniqueness of discrete solutions

We will now use the discrete stability results of Lemma 8 to show that, under a mild restriction on the time step τ, we can also prove the uniqueness of the discrete solution.

Lemma 13 *Let $(\phi_{h,\tau}, \bar{\mu}_{h,\tau}, q_{h,\tau})$ and $(\hat{\phi}_{h,\tau}, \bar{\hat{\mu}}_{h,\tau}, \hat{q}_{h,\tau})$ be two solutions of Problem 3 with the same initial data. Then $(\hat{\phi}_{h,\tau}, \bar{\hat{\mu}}_{h,\tau}, \hat{q}_{h,\tau})$ satisfies (4.1)–(4.3) with $\bar{r}_{2,h,\tau} = 0$ and the remaining residuals defined by*

$$
\begin{aligned}
\langle \bar{r}_{1,h,\tau}, \bar{\psi}_{h,\tau} \rangle^n &= \langle b(\bar{\phi}_{h,\tau}) \nabla \bar{\mu}_{h,\tau} - c(\bar{\phi}_{h,\tau}) \nabla (A(\bar{\phi}_{h,\tau}) \bar{q}_{h,\tau}), \nabla \bar{\psi}_{h,\tau} \rangle^n \\
&\quad - \langle b(\bar{\hat{\phi}}_{h,\tau}) \nabla \bar{\hat{\mu}}_{h,\tau} - c(\bar{\hat{\phi}}_{h,\tau}) \nabla (A(\bar{\hat{\phi}}_{h,\tau}) \bar{\hat{q}}_{h,\tau}), \nabla \bar{\psi}_{h,\tau} \rangle^n \\
\langle \bar{r}_{3,h,\tau}, \bar{\psi}_{h,\tau} \rangle^n &= \langle d_0 \nabla (A(\bar{\phi}_{h,\tau}) \bar{q}_{h,\tau}) - c(\bar{\phi}_{h,\tau}) \nabla \bar{\mu}_{h,\tau}, \nabla (A(\bar{\phi}_{h,\tau}) \bar{\zeta}_{h,\tau}) \rangle^n \\
&\quad - \langle d_0 \nabla (A(\bar{\hat{\phi}}_{h,\tau}) \bar{\hat{q}}_{h,\tau}) - c(\bar{\hat{\phi}}_{h,\tau}) \nabla \bar{\hat{\mu}}_{h,\tau}, \nabla (A(\bar{\hat{\phi}}_{h,\tau}) \bar{\zeta}_{h,\tau}) \rangle^n \\
&\quad + \langle \kappa(\bar{\phi}_{h,\tau}) \bar{q}_{h,\tau}, \bar{\zeta}_{h,\tau} \rangle^n - \langle \kappa(\bar{\hat{\phi}}_{h,\tau}) \bar{\hat{q}}_{h,\tau}, \bar{\zeta}_{h,\tau} \rangle^n.
\end{aligned}
$$

The assertions again follow directly from the definition of the discrete solutions and some elementary computations. Similar to the above, we next state appropriate bounds for the residuals in the norms relevant to our analysis.

Lemma 14 *Let (A0)–(A7) hold and $(\phi_{h,\tau}, \mu_{h,\tau}, q_{h,\tau})$ resp. $(\hat{\phi}_{h,\tau}, \bar{\hat{\mu}}_{h,\tau}, \hat{q}_{h,\tau})$ denote two solutions of Problem 3. Then the residuals of Lemma 13 can be estimated by*

$$
\int_{I_n} \|\bar{r}_{1,h,\tau}\|_{-1,h}^2 + \|\bar{r}_{3,h,\tau}\|_{-1,h}^2 \, \mathrm{d}s \leq C'' \int_{I_n} \mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau} | \hat{\phi}_{h,\tau}, \hat{q}_{h,\tau}) \, \mathrm{d}s.
$$

The constant C'' only depends on bounds of the model parameters, the initial data, and on bounds for $\|\bar{\hat{\mu}}_{h,\tau}\|_{L^\infty(W^{1,3})}$, $\|\bar{\hat{q}}_{h,\tau}\|_{L^\infty(W^{1,3})}$, $\|\bar{\hat{q}}_{h,\tau}\|_{L^\infty(L^\infty)}$, and $\|\bar{\hat{\phi}}_{h,\tau}\|_{L^\infty(W^{1,3})}$.

The detailed proof of these estimates is provided in the appendix.

8.1 Uniqueness

In order to proceed, we need to estimate the norms of the discrete solution mentioned at the end of Lemma 14 uniformly in the discretization parameters. To this end, we use the following arguments: Let $\bar{g}_{h,\tau}$ stand for $\bar{\hat{\mu}}_{h,\tau}$ or $\bar{\hat{q}}_{h,\tau}$. Then

$$
\|\bar{g}_{h,\tau}\|_{L^\infty(W^{1,3})} \leq \|\bar{g}_{h,\tau} - \pi_h^0 \bar{g}\|_{L^\infty(W^{1,3})} + \|\pi_h^0 \bar{g} - \bar{g}\|_{L^\infty(W^{1,3})} + \|\bar{g}\|_{L^\infty(W^{1,3})},
$$

where π_h^0 is the L^2-projection on the space $\mathcal{V}_h$. The second and third terms can be uniformly bounded by projection error estimates assuming sufficient spatial regularity of the function $\bar{g}$; see Lemma 9. To bound the first term, we use the inverse inequality (A.4) with $p = 3, q = 2, d \leq 3$ in space and with $p = \infty, q = 2, d = 1$ in time, and the estimates of Lemma 12. This leads to

$$\|\bar{g}_{h,\tau} - \pi_h^0 \bar{g}\|_{L^\infty(W^{1,3})} \leq Ch^{-1/2}\tau^{-1/2}(h^2 + \tau^2).$$

Similar estimates can be done for the $L^\infty(L^\infty)$ norm of $\bar{\hat{q}}_{h,\tau}$ via

$$\|\bar{g}_{h,\tau}\|_{L^\infty(L^\infty)} \leq \|\bar{g}_{h,\tau} - \pi_h^0 \bar{g}\|_{L^\infty(L^\infty)} + \|\pi_h^0 \bar{g}_{h,\tau} - \bar{g}\|_{L^\infty(L^\infty)} + \|\bar{g}\|_{L^\infty(L^\infty)}.$$

Again, the last two terms are bounded due to projection errors. For the first term we use the inverse inequality (A.4) with $p = \infty, q = 2, d \leq 3$ in space and with $p = \infty, q = 2, d = 1$ in time, and the estimates of Lemma 12 leading to

$$\|\bar{g}_{h,\tau} - \pi_h^0 \bar{g}\|_{L^\infty(L^\infty)} \leq Ch^{-3/2}\tau^{-1/2}(h^2 + \tau^2).$$

For $\tau = ch$, the constant C'' in Lemma 14 can thus be bounded uniformly in h and τ. We can then apply the discrete Gronwall lemma, cf. Lemma 19, similarly as in the proof of Lemma 8, to obtain

$$\mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau}|\hat{\phi}_{h,\tau}, \hat{q}_{h,\tau})\big|_{t=t^n} + c'' \int_0^{t^n} \|\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}\|_1^2 + \|\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\|_1^2 \, \mathrm{d}s \leq 0.$$

In the last step, we used that both functions $(\phi_{h,\tau}, q_{h,\tau})$ as well as $(\hat{\phi}_{h,\tau}, \hat{q}_{h,\tau})$ have the same initial values. Together with the lower bounds for the relative energy, we find that the difference between the two solutions vanishes. □

9 Numerical illustration

We complement the theoretical results by two computational tests. We consider the domain $\Omega = (0, 1)^2$, which can be extended periodically to the whole of $\mathbb{R}^2$.

The numerical scheme proposed in Problem 3 can be rewritten equivalently by choosing the standard Lagrange basis in time, i.e.

$$\begin{aligned}
\phi_{h,\tau}|_{I_n} &= \frac{t - t^{n-1}}{\tau}\phi_h^n - \frac{t - t^n}{\tau}\phi_h^{n-1}, \qquad & \bar{\phi}|_{I_n} &= \phi_h^{n-1/2} := \frac{\phi_h^n + \phi_h^{n-1}}{2}, \\
q_{h,\tau}|_{I_n} &= \frac{t - t^{n-1}}{\tau}q_h^n - \frac{t - t^n}{\tau}q_h^{n-1}, \qquad & \bar{q}|_{I_n} &= q_h^{n-1/2} := \frac{q_h^n + q_h^{n-1}}{2} \\
\bar{\mu}_{h,\tau}|_{I_n} &= \mu_h^{n-1/2}.
\end{aligned}$$

The fully discrete formulation now reads.

Problem 15 Let (A0)–(A7) hold and $\phi_{h,0}, q_{h,0} \in \mathcal{V}_h$ be given. Set $\phi_h^0 = \phi_{h,0}$ and $q_h^0 = q_{h,0}$. Find $\phi_h^n, q_h^n, \mu_h^{n-1/2} \in \mathcal{V}_h$ such that

$$\langle \phi_h^n - \phi_h^{n-1}, \psi_h\rangle = -\tau\langle b(\phi_h^{n-1/2})\nabla\mu_h^{n-1/2} - c(\phi_h^{n-1/2})\nabla(A(\phi_h^{n-1/2})q_h^{n-1/2}), \nabla\psi_h\rangle, \tag{7.1}$$

$$\langle \mu_h^{n-1/2}, \xi_h\rangle = \gamma\langle \nabla\phi_h^{n-1/2}, \nabla\xi_h\rangle + \langle \overline{f'(\phi_h^n, \phi_h^{n-1})}, \xi_h\rangle, \tag{7.2}$$

$$\begin{aligned}\langle q_h^n - q_h^{n-1}, \zeta_h\rangle = -\tau\langle d_0\nabla(A(\phi_h^{n-1/2})q_h^{n-1/2}) - c(\phi_h^{n-1/2})\nabla\mu_h^{n-1/2}, \nabla(A(\phi_h^{n-1/2})\zeta_h)\rangle \\ - \langle \kappa(\phi_h^{n-1/2})q_h^{n-1/2}, \zeta_h\rangle - \varepsilon\langle \nabla q_h^{n-1/2}\nabla\zeta_h\rangle,\end{aligned} \tag{7.3}$$

for all test functions $\psi_h, \xi_h, \zeta_h \in \mathcal{V}_h$ and all time steps $1 \le n \le N$.
To obtain the above formulation, the time integrals are directly evaluated. The exception is the time integral of the potential $f'(\phi)$, where we have applied a numerical quadrature

$$\overline{f'(\phi_h^n, \phi_h^{n-1})} := \frac{1}{\tau}\langle f'(\phi_{h,\tau}), \xi_h\rangle^n \approx \sum_{k=1}^{Q} w_k\langle f'(\phi_{h,\tau}(s_k)), \xi_h\rangle.$$

In the above equation, the pairs (w_k, s_k) denote weights and associated evaluation points of the employed quadrature rule. Note that $\phi_{h,\tau}(s_k)$ is completely determined by suitable weights of ϕ_h^n, ϕ_h^{n-1}. In the following experiments, the potential will be taken as a polynomial of fourth order. Hence, every quadrature rule with at least order three will be exact, we choose the Gauß-Legendre quadrature here. The resulting system is a nonlinear algebraic system for every time step, and we use Newton's method with an absolute tolerance of 10^{-10} in the maximum norm of the solution vector. The resulting linear system is treated by a direct LU solver.

9.1 Convergence rates

We start with evaluating the convergence rate of the proposed method. We set the time interval $[0, T], T = 10$ and choose smooth initial data

$$\phi_0(x, y) = 0.25\cos(2\pi x)\cos(2\pi y) + 0.5, \qquad q_0(x, y) = 0.01\sin(2\pi x)\sin(2\pi y), \quad (x, y) \in \Omega.$$

The parameters are set to $\gamma = \varepsilon = 10^{-3}$. For the nonlinear functions, we chose $b(\phi) = c(\phi)^2 + \varepsilon$, $c(\phi) = \frac{4}{\sqrt{10}} \cdot \phi(1-\phi)$, $d_0 = 1$, $f(\phi) = (\phi - 0.95)^2(\phi - 0.05)^2$, $\kappa(\phi) = 10^{-2}(10\phi^2 + 10^{-4})^{-1}$, and

$$A(\phi) = 5 \cdot 10^{-3} \cdot \left[1 + \tanh(5[\cot(\pi\phi^*) - \cot(\pi\phi)])\right]$$

with $\phi^* = 0.5 = \langle \phi_0, 1\rangle$ denoting the total mass. Apart from the specific choice of the initial data, the problem setting is similar to that of [46].

Table 1 Errors and experimental orders of convergence: Part I

k	$e_{h,\tau}$	eoc	$e_{\phi,h,\tau}$	eoc	$e_{q,h,\tau}$	eoc
1	$9.84 \cdot 10^{-1}$	—	$8.78 \cdot 10^{-1}$	—	$1.18 \cdot 10^{-10}$	—
2	$6.55 \cdot 10^{-2}$	3.03	$5.95 \cdot 10^{-2}$	3.88	$1.39 \cdot 10^{-11}$	3.10
3	$8.02 \cdot 10^{-3}$	3.03	$7.64 \cdot 10^{-3}$	2.96	$1.28 \cdot 10^{-12}$	3.62
4	$5.32 \cdot 10^{-4}$	3.91	$5.08 \cdot 10^{-4}$	3.91	$2.47 \cdot 10^{-14}$	5.51
5	$3.37 \cdot 10^{-5}$	3.98	$3.22 \cdot 10^{-5}$	3.98	$3.10 \cdot 10^{-16}$	6.32

Table 2 Errors and experimental orders of convergence: Part II

k	$e_{\bar{\mu},h,\tau}$	eoc	$e_{\bar{q},h,\tau}$	eoc
1	$1.04 \cdot 10^{-1}$	—	$1.17 \cdot 10^{-6}$	—
2	$5.93 \cdot 10^{-3}$	4.14	$4.04 \cdot 10^{-7}$	1.54
3	$3.78 \cdot 10^{-4}$	3.97	$1.10 \cdot 10^{-7}$	1.87
4	$2.41 \cdot 10^{-5}$	3.97	$1.13 \cdot 10^{-8}$	3.28
5	$1.52 \cdot 10^{-6}$	3.99	$5.82 \cdot 10^{-10}$	4.28

The discretization errors are estimated by comparing the computed solutions on two consecutively refined grids. The error quantities which we report in the following are defined as

$$\begin{aligned} e_{h,\tau} &= \|\phi_{h,\tau} - \phi_{h/2,\tau/2}\|^2_{L^\infty(H^1)} + \|q_{h,\tau} - q_{h/2,\tau/2}\|^2_{L^\infty(L^2)} \\ &\quad + \|\bar{\mu}_{h,\tau} - \bar{\mu}_{h/2,\tau/2}\|^2_{L^2(H^1)} + \|\bar{q}_{h,\tau} - \bar{q}_{h/2,\tau/2}\|^2_{L^2(H^1)}. \end{aligned}$$

These are the natural norms arising in the stability and error analysis of the problem. We also present the individual error components, which are denoted by $e_{\phi,h,\tau}, e_{q,h,\tau}, e_{\bar{\mu},h,\tau}, e_{\bar{q},h,\tau}$.

In the Tables 1–2, we display the results of our computations obtained on a sequence of uniformly refined meshes with mesh size $h_k = 2^{-(1+k)}$, $k = 1, \ldots, 6$, and time steps $\tau_k = h_k$.

As predicted by Theorem 5, we observe the convergence of at least the fourth order for the squared norms of the errors in all solution components. The error $e_{q,h,\tau}$ even converges with the sixth order, which can be expected as long as the temporal error is negligible. Let us finally mention that, as predicted, the discrete identities for the conservation of mass and energy dissipation are valid in our computations up to round-off errors.

To study the impact of center-of-mass diffusion coefficient ε, we repeated the same test for $\varepsilon \in \{10^{-3}, 10^{-6}, 10^{-9}, 10^{-12}, 0\}$. According to the results presented in Fig. 1, the errors $e_{\phi,h,\tau}$ and $e_{\bar{\mu},h,\tau}$ are more or less independent of ε. The convergence rates for $e_{q,h,\tau}$ and $e_{\bar{q},h,\tau}$, on the other hand, are reduced for $\varepsilon \to 0$. This can be expected since these terms are multiplied by ε in the model.

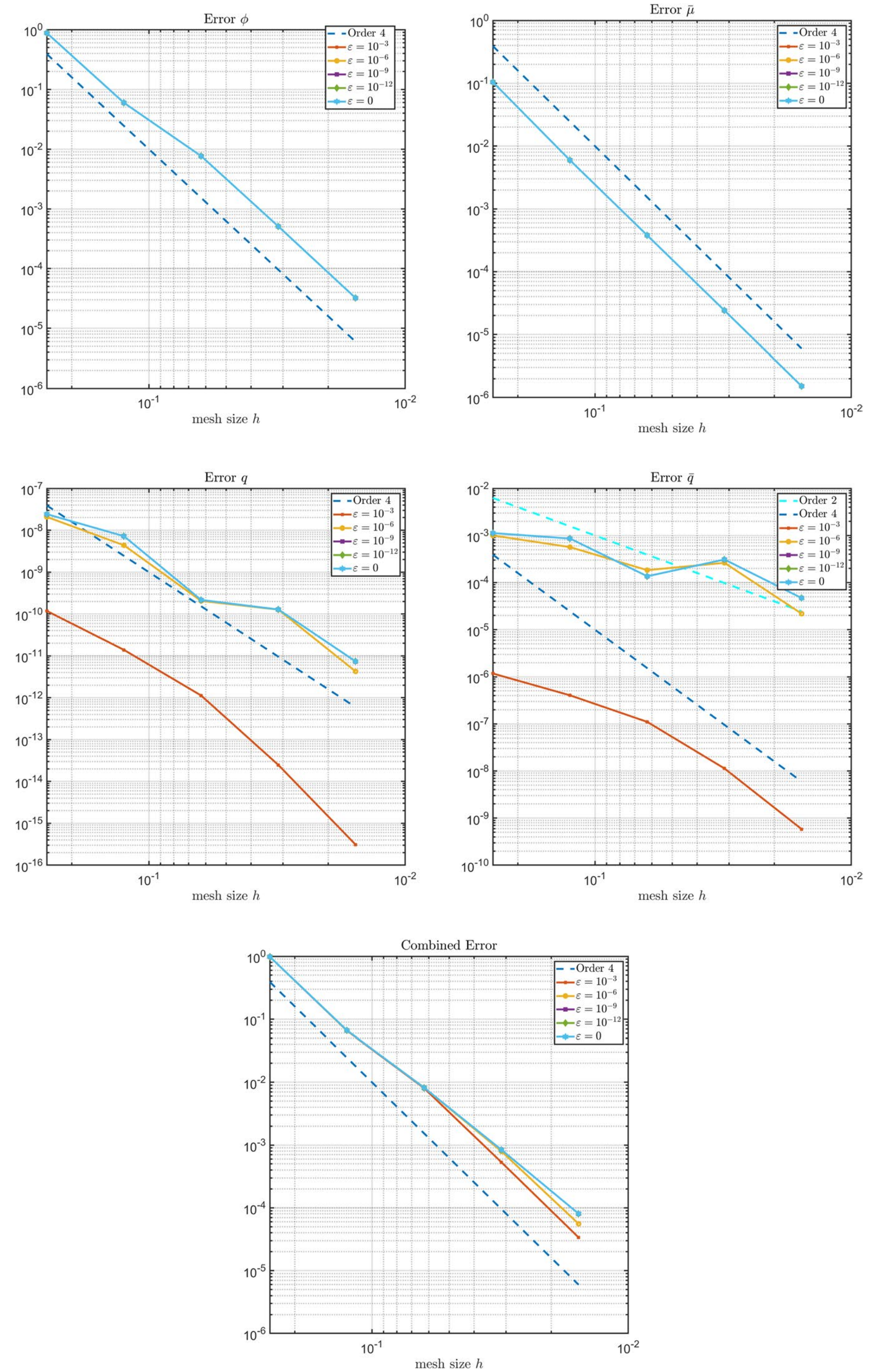

Fig. 1 Convergence rates for the errors in ϕ (top left), $\bar{\mu}$ (top right), q (middle left), $\bar{q}$ (middle right) and the combined error (bottom) for different ε

9.2 Qualitative behavior

This experiment illustrates typical features associated with viscoelastic phase separation and compares the results to the standard phase separation. Similarly to [14, 46], we choose the initial data as

$$\phi_0(x,y) = 0.4 + \xi(x,y), \qquad q_0(x,y) = 0$$

with $\xi(x,y)$ a uniform random perturbation of small amplitude, i.e. $\xi(x,y) \in [-0.0025, 0.0025]$. The model parameters are set to $\gamma = \varepsilon = 10^{-3}$ and $T = 12$. For the nonlinear functions, we chose $b(\phi) = c(\phi)^2 + \varepsilon$, $c(\phi) = \frac{1}{\sqrt{10}}\phi(1-\phi)$, $d_0 = 1$, $f(\phi) = (\phi - 0.95)^2(\phi - 0.05)^2$, $\kappa(\phi) = 10^{-3}(10\phi^2 + 10^{-4})^{-1}$, and

$$A(\phi) = \begin{cases} \frac{1}{2}\left[1 + \tanh(10[\cot(\pi\phi^*) - \cot(\pi\phi)])\right], \\ 0 \end{cases}$$

with $\phi^* = \langle \phi_0, 1\rangle$ again denoting the total mass. The first choice of $A(\phi)$ corresponds to viscoelastic phase separation, while the second choice formally decouples the equations for ϕ and q. Hence we obtain the standard Cahn-Hilliard dynamic for ϕ. We note that the nonlinear choice of $A(\phi)$ was also used in [47, 55]. The bulk stress effects are only relevant above a critical threshold ϕ^*.

In contrast to more standard systems, the phase separation here takes place at several states [49]. First, the solvent moves out of the polymer forming small droplets which grow over time. In the intermediate state, the polymer starts to form a network-like structure, which finally collapses into separate phases. Due to the small mobility of the polymers, the overall phase separation process is much slower than in symmetric binary fluid systems. The observed behaviour is typical for the demixing of systems with dynamic asymmetry and is in good agreement with the results presented in [47, 55].

In contrast, Fig. 4 shows a typical phase separation modelled by the Cahn-Hilliard equation, i.e. $A(\phi) \equiv 0$. We observe almost instantaneous separation into small bubbles and their coalescence over time. Comparing with Fig. 2, we can see that the bulk stress effectively delays phase separation and introduces an additional phase-inversion state. In the long-time limit, both systems converge to fully separated states. Here, we expect a single bubble of phase $\phi = 1$. The temporal evolution of the energy as well as the mass conservation error is depicted for both cases in the Figs. 3 and 5.

10 Conclusion & Outlook

In this work, we have proposed and analyzed a fully discrete numerical scheme for a model of viscoelastic phase separation. The proposed method is based on variational discretization strategies in space and time, which allows the preservation of important structural properties of the system, such as conservation of mass and dissipation of energy, exactly on the discrete level. Nonlinear stability analysis for the

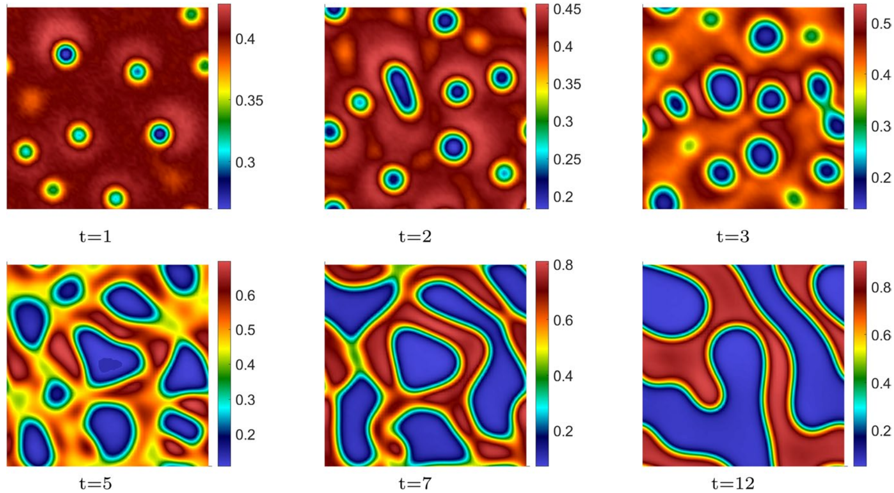

Fig. 2 Snapshots of the volume fraction ϕ with pure phases at $\phi = 0$ and $\phi = 1$ obtained for the second test case, illustrating typical states of viscoelastic phase separation

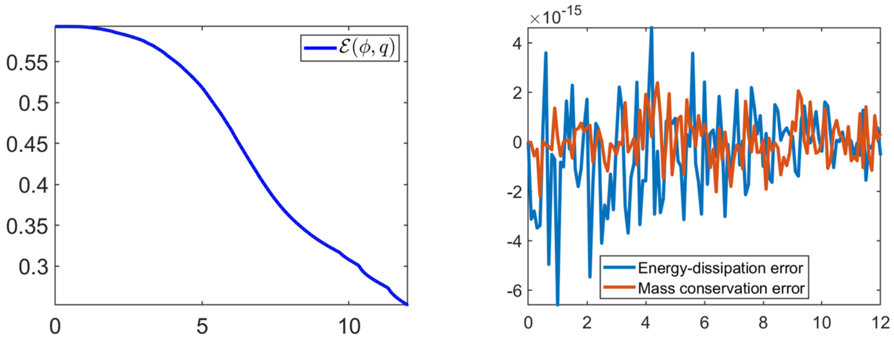

Fig. 3 Temporal evolution of the energy (left) and the conservation and energy-dissipation error (right) obtained for the viscoelastic phase separation

discrete problem was presented based on the relative energies as distance measures. This allowed us to derive order optimal convergence rates in space and time under minimal smoothness assumptions despite the presence of various strong nonlinearities. The discrete stability estimates further allowed us to derive the uniqueness of the discrete solution under a mild restriction on the time step size.

The general methodology underlying the proposed numerical method and its analysis can, in principle, be extended to a variety of related nonlinear evolution problems. The first results in these directions can be found in [14]. The rigorous error analysis in such general cases and further steps towards the efficient solution of the nonlinear systems to be solved in every time step are topics of ongoing research.

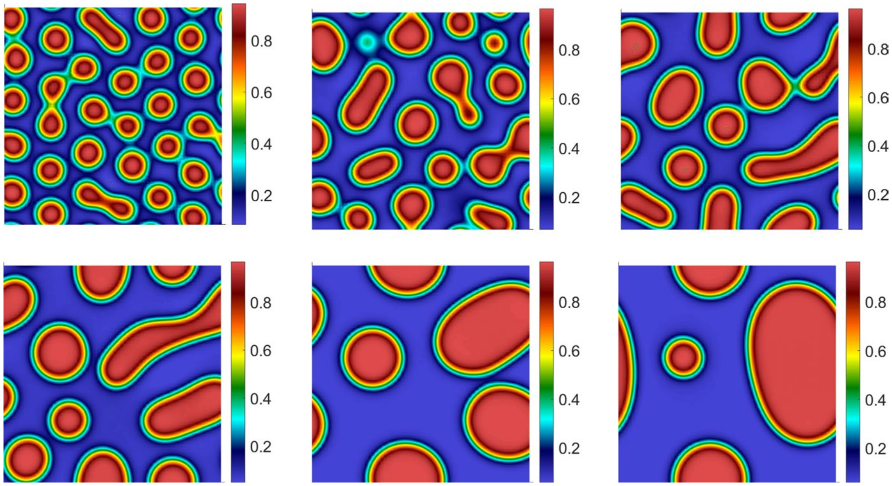

Fig. 4 Snapshots of the volume fraction ϕ with pure phases at $\phi = 0$ and $\phi = 1$ obtained for the second test case, illustrating typical states of standard phase separation

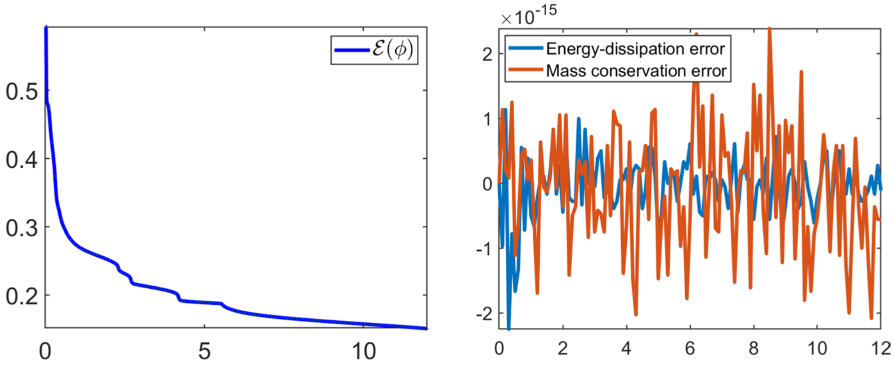

Fig. 5 Temporal evolution of the energy (left) and the conservation and energy-dissipation error (right) obtained for the standard phase separation

Appendices

For completeness of the presentation, we now provide detailed proofs for some of the technical results that were used in the error analysis of the previous sections. The appendix is divided into two sections. In Appendix A, we present the projection errors anticipated in the forthcoming estimates. These encompass familiar linear and nonlinear projection errors, along with specific estimates tailored to the errors arising in the analysis.

Appendix B and C are dedicated primarily to proving Lemma 11 and Lemma 13. Within this section, our approach focuses on appropriately estimating the residuals through the relative energy, dissipation, and projection errors. This part is notably technical due to the numerous nonlinearities involved.

Projection error estimates

In the following, we summarize some well-known results about standard projection and interpolation operators, which are used in our analysis.

Space discretization

We consider the setting of Sections 3.1 and 4.1 and, in particular, assume (A6)–(A7) to hold true. The following results then follow with standard arguments; see, e.g. [13]. The L^2-orthogonal projection $\pi_h^0 : L^2(\Omega) \to \mathcal{V}_h$, satisfies

$$\|u - \pi_h^0 u\|_{H^s} \leq C h^{r-s} \|u\|_{H^r} \qquad \forall u \in H^r(\Omega), \tag{A.1}$$

and all parameters $-1 \leq s \leq r$ and $0 \leq r \leq 4$. On quasi-uniform meshes $\mathcal{T}_h$, which we consider here, the projection π_h^0 is also stable with respect to the H^1-norm, i.e.,

$$\|\pi_h^0 u\|_{H^1} \leq C \|u\|_{H^1} \qquad \forall u \in H^1(\Omega). \tag{A.2}$$

The H^1-elliptic projection $\pi_h^1 : H^1(\Omega) \to \mathcal{V}_h$, defined in (2.2), satisfies

$$\|u - \pi_h^1 u\|_{H^s} \leq C h^{r-s} \|u\|_{H^r} \qquad \forall u \in H^r(\Omega), \tag{A.3}$$

for all parameters $-1 \leq s \leq r$ and $1 \leq r \leq 3$. Since we assumed quasi-uniformity of the mesh $\mathcal{T}_h$, we can further resort to the inverse inequalities

$$\|v_h\|_{H^1} \leq c_{inv} h^{-1} \|v_h\|_{L^2} \qquad \text{and} \qquad \|v_h\|_{L^p} \leq c_{inv} h^{d/p-d/q} \|v_h\|_{L^q} \tag{A.4}$$

which hold for all discrete functions $v_h \in \mathcal{V}_h$ and all $1 \leq q \leq p \leq \infty$.

Discrete interpolation

Let us introduce the discrete Laplacian $\Delta_h : \mathcal{V}_h \to \mathcal{V}_h$ given by

$$\langle \Delta_h v_h, w_h \rangle = -\langle \nabla v_h, \nabla w_h \rangle, \qquad \forall w_h \in \mathcal{V}_h. \tag{A.5}$$

In particular since $\Delta_h v_h \in \mathcal{V}_h$ the L^2-norm can be deduced by setting $w_h = \Delta_h v_h$, i.e,

$$\|\Delta_h v_h\|_0^2 = -\langle \nabla v_h, \nabla \Delta_h v_h \rangle.$$

For a quasi-uniform triangulation, see assumption (A6), one can obtain

$$\|\nabla v_h\|_{0,3} \leq C \|\Delta_h v_h\|_0^{1/2} \|\nabla v_h\|_0^{1/2} + C \|\nabla v_h\|_0. \tag{A.6}$$

A proof of these discrete interpolation inequalities can be found in [25, 39].

Time discretization

The piecewise linear interpolation $I_\tau^1 : H^1(0,T) \to P_1^c(\mathcal{I}_\tau)$ and the piecewise constant projection $\bar{\pi}_\tau^0 : L^2(0,T) \to P_0(I_\tau)$ in time satisfy

$$\|u - \bar{\pi}_\tau^0 u\|_{L^p(0,T)} \le C\tau^{1/p-1/q+r}\|u\|_{W^{r,q}(0,T)} \qquad \forall u \in W^{r,q}(0,T), \tag{A.7}$$

$$\|u - I_\tau^1 u\|_{L^p(0,T)} \le C\tau^{1/p-1/q+s}\|u\|_{W^{s,q}(0,T)} \qquad \forall u \in W^{s,q}(0,T) \tag{A.8}$$

with $1 \le p \le q \le \infty$ and for $0 \le r \le 1$, respectively, $1 \le s \le 2$; see again [13]. Moreover, these operators commute with differentiation in the sense that

$$\partial_t(I_\tau^1 u) = \bar{\pi}_\tau^0(\partial_t u). \tag{A.9}$$

We can now derive the following nonlinear projection error estimates as in [17].

Projection estimates for nonlinear terms

Lemma 16 *Let $\bar{a} = \pi_0 a$ denote the L^2-orthogonal projection onto $P_0(\mathcal{I}_\tau)$. Then for any $u, v \in W^{2,p}(0,T)$ with $1 \le p \le \infty$, one has*

$$\|\overline{\bar{u}\bar{v}} - \overline{uv}\|_{L^p(0,T)} \le C\tau^2\|u\|_{W^{2,p}(0,T)}\|v\|_{W^{2,p}(0,T)}, \tag{A.10}$$

with a constant C independent of u and v.

In a similar manner, we obtain the following estimate [18].

Lemma 17 *Let $\bar{a} = \pi_0 a$ denote the L^2-orthogonal projection onto $P_0(\mathcal{I}_\tau)$. Furthermore, let $\phi \in P_1(\mathcal{I}_\tau)$. Then for any $\phi \in W^{2,p}(0,T)$ with $1 \le p \le \infty$ and $g \in C^2(\mathbb{R})$ with $\|g\|_{W^{2,\infty}(\mathbb{R})} \le C$, one has*

$$\|g(\bar{\phi}) - \overline{g(\phi)}\|_{L^p(0,T)} \le C\tau^2\|g(\phi)\|_{W^{2,p}(0,T)}, \tag{A.11}$$

with a constant C depending only on the polynomial degree k.

The following nonlinear projection estimates will be required for estimating the residual terms in the following section.

Lemma 18 *Let $(\hat{\phi}_{h,\tau}, \bar{\mu}_{h,\tau}, \hat{q}_{h,\tau})$ given by (5.1). Then the following estimates hold*

$$\int_{I_n} \|A'(\bar{\hat{\phi}}_{h,\tau})^2\bar{\hat{q}}_{h,\tau}|\nabla\bar{\hat{\phi}}_{h,\tau}|^2 - \overline{A'(\phi))^2 q|\nabla\phi|^2}\|_{0,6/5}^2 \le C_1h^4 + C_2\tau^4,$$

$$\int_{I_n} \|(A\cdot A')(\bar{\hat{\phi}}_{h,\tau})\nabla\bar{\hat{q}}_{h,\tau}\nabla\bar{\hat{\phi}}_{h,\tau} - \overline{(A\cdot A')(\phi)\nabla q\nabla\phi}\|_{0,6/5}^2 \le C_3h^4 + C_4\tau^4,$$

$$\int_{I_n} \|A'(\bar{\hat{\phi}}_{h,\tau})b^{1/2}(\bar{\hat{\phi}}_{h,\tau})\nabla\bar{\mu}_{h,\tau}\nabla\bar{\hat{\phi}}_{h,\tau} - \overline{A'(\phi)b^{1/2}(\phi)\nabla\mu\nabla\phi}\|_{0,6/5}^2 \le C_5h^4 + C_6\tau^4.$$

Proof We introduce the abbreviations $B_1(\cdot) = A'(\cdot)^2, B_2(\cdot) = A'(\cdot)A(\cdot)$. We consider the first term, and by addition of suitable zeros, we estimate

$$\begin{aligned}
&\int_{I_n} \|B_1(\bar{\hat{\phi}}_{h,\tau})\bar{\hat{q}}_{h,\tau}|\nabla\bar{\hat{\phi}}_{h,\tau}|^2 - \overline{B_1(\phi))q|\nabla\phi|^2}\|_{0,6/5}^2 \\
&\leq \int_{I_n} \|(B_1(\bar{\hat{\phi}}_{h,\tau}) - \overline{B_1(\phi)})\bar{q}|\nabla\bar{\phi}|^2\|_{0,6/5}^2 + \|B_1(\bar{\hat{\phi}}_{h,\tau})|\nabla\bar{\phi}|^2(\bar{\hat{q}}_{h,\tau} - \bar{q})\|_{0,6/5}^2 \\
&\quad + \|B_1(\bar{\hat{\phi}}_{h,\tau})\bar{\hat{q}}_{h,\tau}\nabla(\bar{\hat{\phi}}_{h,\tau} + \bar{\phi})\nabla(\bar{\hat{\phi}}_{h,\tau} - \bar{\phi})\|_{0,6/5}^2 + \|\overline{B_1(\phi)}\bar{q}|\nabla\bar{\phi}|^2 - \overline{B_1(\phi)q|\nabla\phi|^2}\|_{0,6/5}^2 \\
&= (a) + (b) + (c) + (d).
\end{aligned}$$

For the first term we use Lemma 16 and estimate

$$\begin{aligned}
(a) &\leq \|\bar{q}\|_{0,\infty}^2\|\nabla\bar{\phi}\|_{0,3}^4 \int_{I_n} C\|\bar{\hat{\phi}}_{h,\tau} - \bar{\phi}\|_{0,6}^2 + \int_{I_n} \|B_1(\bar{\phi}) - \overline{B_1(\phi)}\|_{0,6}^2 \\
&\leq \|q\|_{L^\infty(L^\infty)}^2\|\nabla\phi\|_{L^\infty(L^3)}^4(\tau^4\|B_1(\phi)\|_{H^2(L^6)}^2 + h^4\|\phi\|_{L^2(H^3)}^2).
\end{aligned}$$

The second term can be bounded using (A.1) by

$$(b) \leq C\|\nabla\bar{\phi}\|_{0,3}^4 \int_{I_n} \|\bar{\hat{q}}_{h,\tau} - \bar{q}\|_{0,6}^2 \leq Ch^4\|q\|_{L^2(H^3)}^2\|\nabla\phi\|_{L^\infty(L^3)}^4.$$

For the third term, we can use using (A.3) and find

$$(c) \leq \|\nabla\bar{\phi}\|_{0,3}^2\|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^2 \int_{I_n} \|\bar{\hat{\phi}}_{h,\tau} - \bar{\phi}\|_1^2 \leq Ch^4\|\nabla\phi\|_{L^\infty(L^3)}^2\|q\|_{L^\infty(L^\infty)}^2\|\phi\|_{L^2(H^3)}.$$

The last term can again be treated by Lemma 16, which leads to

$$(d) \leq \tau^4\|B_1(\phi)q|\nabla\phi|^2\|_{H^2(L^{6/5})}^2.$$

In summary, this yields the first bound of the lemma. The second bound stated in the lemma can be rewritten and estimated, using similar arguments, by

$$\begin{aligned}
&\int_{I_n} \|B_2(\bar{\hat{\phi}}_{h,\tau})\nabla\bar{\hat{q}}_{h,\tau}\nabla\bar{\hat{\phi}}_{h,\tau} - \overline{B_2(\phi))\nabla q\nabla\phi}\|_{0,6/5}^2 \\
&\qquad \leq \int_{I_n} \|(B_2(\bar{\hat{\phi}}_{h,\tau}) - \overline{B_2(\phi)})\nabla\bar{q}\nabla\bar{\phi}\|_{0,6/5}^2 + \|B_2(\bar{\hat{\phi}}_{h,\tau})\nabla\bar{\phi}\nabla(\bar{\hat{q}}_{h,\tau} - \bar{q})\|_{0,6/5}^2 \\
&\qquad\quad + \|B_2(\bar{\hat{\phi}}_{h,\tau})\nabla\bar{\hat{q}}_{h,\tau}(\nabla\bar{\hat{\phi}}_{h,\tau} - \bar{\phi})\|_{0,6/5}^2 + \|\overline{B_2(\phi)}\nabla\bar{q}\nabla\bar{\phi} - \overline{B_2(\phi)\nabla q\nabla\phi}\|_{0,6/5}^2.
\end{aligned}$$

The individual terms can now be estimated as before. The integral in the last bound of the lemma can be treated like the second one after replacing B_2 by $A'(\cdot)b^{1/2}(\cdot)$ and q by μ. □

Proof of Lemma 11

We have now obtained all ingredients for the proof of Lemma 11. Without further mentioning, we assume the conditions of Lemma 11 to be valid. We estimate the three residuals separately.

First residual

By definition of the dual norm (1.1) and splitting the terms, we get

$$\begin{aligned}\int_{I_n} \|\bar{r}_{1,h,\tau}\|_{-1,h}^2 \,\mathrm{d}s \leq 3 \int_{I_n} & \|\partial_t(\pi_h^1\phi - \phi)\|_{-1,h}^2 + \|b(\bar{\phi}_{h,\tau})\nabla\bar{\mu}_{h,\tau} - \overline{b(\phi)\nabla\mu}\|_0^2 \\ & + \|c(\bar{\phi}_{h,\tau})\nabla(A(\bar{\phi}_{h,\tau})\bar{\hat{q}}_{h,\tau}) - \overline{c(\phi)\nabla(A(\phi)q)}\|_0^2 \,\mathrm{d}s \\ = & (i) + (ii) + (iii).\end{aligned}$$

The first term can be bounded using error estimates (A.3) by

$$(i) \leq Ch^4 \|\partial_t \phi\|_{L^2(H^1)}^2.$$

The second term can be further split into multiple parts according to

$$\begin{aligned}(ii) \leq C \int_{I_n} & \|b(\bar{\phi}_{h,\tau})\nabla(\bar{\hat{\mu}}_{h,\tau} - \nabla\bar{\mu})\|_0^2 + \|(b(\bar{\phi}_{h,\tau}) - b(\bar{\phi}))\nabla\bar{\mu}\|_0^2 \\ & + \|(b(\bar{\phi}) - \overline{b(\phi)})\nabla\bar{\mu}\|_0^2 + \|\overline{b(\phi)}\nabla\bar{\mu} - \overline{b(\phi)\nabla\mu}\|_0^2 \,\mathrm{d}s \\ = & (a) + (b) + (c) + (d).\end{aligned}$$

By the stability of the L^2-projection in time and the estimates of Lemma 9, we get

$$(a) \leq C \int_{I_n} \|\pi_h^0\mu - \mu\|_1^2 \,\mathrm{d}s \leq Ch^4 \|\mu\|_{L^2(H^3)}^2.$$

With the bounds for the derivatives of the parameter function $b(\cdot)$, cf. (A1), the Hölder inequality, the stability of the L^2-projection, and Lemma 9, we further get

$$\begin{aligned}(b) \leq C \int_{I_n} & \|\phi_{h,\tau} - \phi\|_{0,6}^2 \|\mu\|_{1,3}^2 \,\mathrm{d}s \leq Ch^4 \|\mu\|_{L^\infty(W^{1,3})}^2 \|\phi\|_{L^2(H^3)}^2 \\ & + C\tau^4 \|\mu\|_{L^\infty(W^{1,3})}^2 \|\phi\|_{H^2(H^1)}^2 + \|\mu\|_{L^\infty(W^{1,3})}^2 \int_{I_n} \mathcal{E}_\alpha^\phi(\phi_{h,\tau}|\hat{\phi}_{h,\tau}) \,\mathrm{d}s.\end{aligned}$$

The third term can be treated by Lemma A.11 and yields

$$(c) \leq C\tau^4 \|\mu\|_{L^\infty(W^{1,3})}^2 \|b(\phi)\|_{H^2(L^6)}^2.$$

The last term in the above expansion can be treated by Lemma A.10, which leads to

$$(d) \leq C\tau^4 \|b(\phi)\nabla\mu\|^2_{H^2(L^2)}.$$

The last norm can be further expanded using the product and chain rule of differentiation. All terms arising in these computations can be controlled appropriately. In summary, we thus get

$$(ii) \leq C_1(\phi,\mu)h^4 + C_2(\phi,\mu)\tau^4 + C(\|\mu\|_{L^\infty(W^{1,3})}) \int_{I_n} \mathcal{E}_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau})\,\mathrm{d}s.$$

The constants depend on norms of the solution that are bounded by our assumptions. We continue with the third term, which can be estimated by

$$\begin{aligned}(iii) \leq \int_{I_n} &\|c(\bar{\phi}_{h,\tau})A(\bar{\phi}_{h,\tau})\nabla\bar{\hat{q}}_{h,\tau} - \overline{c(\phi)A(\bar{\phi}_{h,\tau})\nabla q}\|_0^2 \\ &+ \|c(\bar{\phi}_{h,\tau})\bar{\hat{q}}_{h,\tau}A'(\bar{\phi}_{h,\tau})\nabla\bar{\phi}_{h,\tau} - \overline{c(\phi)qA'(\phi)\nabla\phi}\|_0^2\,\mathrm{d}s \\ =\ & E_1 + E_2.\end{aligned}$$

The first part can be estimated similarly to term (*i*) before, which leads to

$$E_1 \leq C_1(\phi,q)h^4 + C_2(\phi,q)\tau^4 + C(\|q\|_{L^\infty(W^{1,3})}) \int_{I_n} \mathcal{E}^\phi_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau})\,\mathrm{d}s.$$

The two constants again depend on the norms of the solution that are bounded by assumption. The second part can be further split and estimated by

$$\begin{aligned}E_2 \leq 2\int_{I_n} &\|c(\bar{\phi}_{h,\tau})A'(\bar{\phi}_{h,\tau})\nabla\bar{\phi}_{h,\tau} - \overline{c(\phi)A'(\phi)\nabla\phi}\|_0^2 \|\bar{\hat{q}}_{h,\tau}\|^2_{0,\infty} \\ &+ \|\overline{c(\phi)\bar{\hat{q}}_{h,\tau}A'(\phi)\nabla\phi} - \overline{c(\phi)qA'(\phi)\nabla\phi}\|_0^2\,\mathrm{d}s \\ \leq \int_{I_n} &C\mathcal{E}^\phi_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau}) + C_3(\phi,q)h^4 + C_4(\phi,q)\tau^4,\end{aligned}$$

where we have used similar arguments as in the previous steps. The constants again only depend on bounds for the parameters and the solutions that are available from our assumptions. Combining all estimates, we can finally bound the first residual by

$$\int_{I_n} \|\bar{r}_{1,h,\tau}\|^2_{-1,h}\,\mathrm{d}s \leq C(h^4+\tau^4) + \int_{I_n} C\mathcal{E}^\phi_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau})\,\mathrm{d}s.$$

The constants in this estimate are independent of the discretization parameters.

Second residual

The second residual can be expressed in the strong form as

$$\bar{r}_{2,h,\tau} = (\overline{\pi_h^0 \mu} - \overline{I_\tau^1 \pi_h^0 \mu}) + (\overline{I_\tau^1 \phi} - \overline{\hat{\phi}_{h,\tau}}) + (\overline{f'(\hat{\phi}_{h,\tau})} - \overline{I_\tau^1 f'(\phi)}).$$

Recall that $\overline{g} = \bar{\pi}_\tau^0 g$ is used to denote the piecewise constant projection of a function g with respect to time. This pointwise representation allows us to estimate

$$\begin{aligned}\frac{1}{3}\int_{I_n} \|\bar{r}_{2,h,\tau}\|_1^2 \,\mathrm{d}s &\leq \|\pi_h^0 \mu - I_\tau^1 \pi_h^0 \mu\|_{L^2(H^1)}^2 + \|I_\tau^1 \phi - \hat{\phi}_{h,\tau}\|_{L^2(H^1)}^2 \\ &\quad + \|f'(\hat{\phi}_{h,\tau}) - I_\tau^1 f'(\phi)\|_{L^2 H^1)}^2 \\ &= (i) + (ii) + (iii).\end{aligned}$$

Using the contraction property of the L^2-projection in space, we obtain for the first term

$$(i) \leq \|\mu - I_\tau^1 \mu\|_{L^2(H^1)}^2 \leq C\tau^4 \|\mu\|_{H^2(H^1)}^2.$$

With the error estimate for the H^1-projection π_h^1, see (A.3), we further find

$$(ii) \leq C\|\phi - \pi_h^1 \phi\|_{L^\infty(H^1)}^2 \leq Ch^4 \|\phi\|_{L^\infty(H^3)}^2.$$

For the last term we employ the uniform bounds of ϕ and $\hat{\phi}_{h,\tau}$ in $L^\infty(0,T;W^{1,\infty}(\Omega))$. Hence all terms of the form $f^{(k)}(\cdot)$ can be bounded uniformly by a constant *C*(*f*), cf. (A2), and we obtain

$$\begin{aligned}(iii) &\leq 2\|f'(\hat{\phi}_{h,\tau}) - f'(\phi)\|_{L^2(H^1)}^2 + 2\|f'(\phi) - I_\tau^1 f'(\phi)\|_{L^2(H^1)}^2 \\ &\leq C(f)\|\hat{\phi}_{h,\tau} - \phi\|_{L^2(H^2)}^2 + C\tau^4 \|f'(\phi)\|_{H^2(H^1)}^2 \\ &\leq C'(f) h^4 \|\phi\|_{L^2(H^3)}^2 + C'(f)\tau^4 \|\phi\|_{H^2(H^1)}^2 + C\tau^4 \|f'(\phi)\|_{H^2(H^1)}^2.\end{aligned}$$

The terms involving derivatives of $f(\phi)$ can all be estimated due to the regularity assumptions on *f* and ϕ. In summary, we obtain the following bound for the second residual

$$\int_{I_n} \|\bar{r}_{2,h,\tau}\|_1^2 \,\mathrm{d}s \leq C(h^4 + \tau^4).$$

The constant is again independent of the discretization parameters.

Third residual

Due to many nonlinearities, this is the most technical part of our estimates. As a preliminary step, we decompose

$$
\begin{aligned}
&d_0\langle\nabla(A(\bar\phi_{h,\tau})\bar{\hat q}_{h,\tau}),\nabla(A(\bar\phi_{h,\tau})\bar\zeta_{h,\tau})\rangle\\
&= d_0\langle A^2(\bar\phi_{h,\tau})\nabla\bar{\hat q}_{h,\tau},\nabla\bar\zeta_{h,\tau}\rangle + d_0\langle(A'(\bar\phi_{h,\tau}))^2\bar{\hat q}_{h,\tau}|\nabla\bar\phi_{h,\tau}|^2,\bar\zeta_{h,\tau}\rangle\\
&\quad + d_0\langle(A\cdot A')(\bar\phi_{h,\tau})\bar{\hat q}_{h,\tau}\nabla\bar\phi_{h,\tau},\nabla\bar\zeta_{h,\tau}\rangle + d_0\langle(A\cdot A')(\bar\phi_{h,\tau})\nabla\bar{\hat q}_{h,\tau}\nabla\bar\phi_{h,\tau},\bar\zeta_{h,\tau}\rangle,
\end{aligned}
$$

and in a similar manner, we also split

$$
\begin{aligned}
&\langle c(\bar\phi_{h,\tau})\nabla\bar{\hat\mu}_{h,\tau},\nabla(A(\bar\phi_{h,\tau})\bar\zeta_{h,\tau})\\
&= \langle A(\bar\phi_{h,\tau})c(\bar\phi_{h,\tau})\nabla\bar{\hat\mu}_{h,\tau},\nabla\bar\zeta_{h,\tau}\rangle + \langle A'(\bar\phi_{h,\tau})c(\bar\phi_{h,\tau})\nabla\bar{\hat\mu}_{h,\tau}\nabla\bar\phi_{h,\tau},\bar\zeta_{h,\tau}\rangle.
\end{aligned}
$$

From the definition of the dual norm (1.1), the binomial inequality, and the bound for the coefficient d_0, we then obtain

$$
\begin{aligned}
\int_{I_n}\|\bar r_{3,h,\tau}\|^2_{-1,h}\,\mathrm{d}s \le 8\int_{I_n} &\|\kappa^{1/2}(\bar\phi_{h,\tau})\bar{\hat q}_{h,\tau} - \overline{\kappa^{1/2}(\phi)q}\|_0^2\\
&+ \|A^2(\bar\phi_{h,\tau})\nabla\bar{\hat q}_{h,\tau} - \overline{A^2(\phi)\nabla q}\|_0^2\\
&+ \|A'(\bar\phi_{h,\tau}))^2\bar{\hat q}_{h,\tau}(\nabla\bar\phi_{h,\tau})^2 - \overline{A'(\phi))^2q(\nabla\phi)^2}\|^2_{0,6/5}\\
&+ \|(A\cdot A')(\bar\phi_{h,\tau})\bar{\hat q}_{h,\tau}\nabla\bar\phi_{h,\tau} - \overline{(A\cdot A')(\phi)q\nabla\phi}\|_0^2\\
&+ \|(A\cdot A')(\bar\phi_{h,\tau})\nabla\bar{\hat q}_{h,\tau}\nabla\bar\phi_{h,\tau} - \overline{(A\cdot A')(\phi)\nabla q\nabla\phi}\|^2_{0,6/5}\\
&+ \|A(\bar\phi_{h,\tau})c(\bar\phi_{h,\tau})\nabla\bar{\hat\mu}_{h,\tau} - \overline{A(\phi)c(\phi)\nabla\mu}\|_0^2\\
&+ \|A'(\bar\phi_{h,\tau})c(\bar\phi_{h,\tau})\nabla\bar{\hat\mu}_{h,\tau}\nabla\bar\phi_{h,\tau} - \overline{A'(\phi)c(\phi)\nabla\mu\nabla\phi}\|^2_{0,6/5} + \|\nabla(\bar{\hat q}_{h,\tau}-\bar q)\|_0^2\,\mathrm{d}s\\
= (i) + (ii) + (iii) + (iv) + (v) + (vi) + (vii) + (viii).
\end{aligned}
$$

With similar arguments as used for bounding the first residual above, we obtain

$$
(i) \le C_1h^4 + C_2\tau^4 + C(\|q\|_{L^\infty(W^{1,3})},\|\mu\|_{L^\infty(W^{1,3})})\int_{I_n}\mathcal{E}^\phi_\alpha(\phi_{h,\tau}|\hat\phi_{h,\tau})\,\mathrm{d}s.
$$

The constants C_1, C_2 again only depend on quantities that can be controlled by our assumptions. The terms (*ii*), (*iv*), and (*vi*) can be estimated in the same manner as the terms (*ii*) and (*iii*) in the first residual and term (*viii*) is bounded by the projection error Lemma 9; the details are therefore omitted. For the first term containing the $L^{6/5}$-norm, we have

$$
\begin{aligned}
(iii) \le 2\int_{I_n} &\|A'(\bar\phi_{h,\tau})^2(|\nabla\bar\phi_{h,\tau}|^2 - |\nabla\bar{\hat\phi}_{h,\tau}|^2)\|^2_{0,6/5}\|\bar{\hat q}_{h,\tau}\|^2_{0,\infty}\\
&+ \|A'(\bar\phi_{h,\tau})^2\bar{\hat q}_{h,\tau}|\nabla\bar{\hat\phi}_{h,\tau}|^2 - \overline{A'(\phi))^2q|\nabla\phi|^2}\|^2_{0,6/5}\,\mathrm{d}s = (a) + (b).
\end{aligned}
$$

With the bounds for A' and the discrete interpolation inequality (A.6), we obtain

$$
\begin{aligned}
(a) &\leq C \int_{I_n} \|\nabla\bar{\phi}_{h,\tau} - \nabla\bar{\hat{\phi}}_{h,\tau}\|_{0,3}^2 \|\nabla\bar{\phi}_{h,\tau} + \nabla\bar{\hat{\phi}}_{h,\tau}\|_{0,2}^2 \|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^2 \\
&\leq C \int_{I_n} \left(\|\nabla\bar{\phi}_{h,\tau} - \nabla\bar{\hat{\phi}}_{h,\tau}\|_{0,2} \|\Delta_h(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})\|_{0,2} + \mathcal{E}_\alpha^\phi(\phi_{h,\tau}|\hat{\phi}_{h,\tau})\right) \|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^2 \\
&\leq C(\delta) \int_{I_n} \mathcal{E}_\alpha^\phi(\phi_{h,\tau}|\hat{\phi}_{h,\tau}) \|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^4 \, \mathrm{d}s + \delta \int_{I_n} \|\Delta_h(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})\|_{0,2}^2.
\end{aligned}
$$

The second term in the first line is controlled by the uniform bounds for $\phi_{h,\tau}$, $\hat{\phi}_{h,\tau}$ in $L^\infty(H^1)$. The parameter $\delta > 0$ will be chosen later as needed. Using (2.6), (4.2), and the definition of the discrete Laplacian, we further find

$$
\begin{aligned}
\int_{I_n} \|\Delta_h(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})\|_{0,2}^2 &\leq \int_{I_n} \|\overline{f'(\phi_{h,\tau}) - f'(\hat{\phi}_{h,\tau})}\|_0^2 + \|\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}\|_0^2 + \|\bar{r}_{2,h,\tau}\|_0^2 \, \mathrm{d}s \\
&\leq \int_{I_n} C(f)\mathcal{E}_\alpha^\phi(\phi_{h,\tau}|\hat{\phi}_{h,\tau}) + \delta\mathcal{D}_{\bar{\phi}_{h,\tau}}(\bar{\mu}_{h,\tau} - \bar{\hat{\mu}}_{h,\tau}) + C\|\bar{r}_{2,h,\tau}\|_1^2 \, \mathrm{d}s.
\end{aligned}
\tag{B.1}
$$

In summary, this leads to the bound for (*a*). For the second term, we use Lemma 18 to see that

$$
\begin{aligned}
(b) &\leq \int_{I_n} \|[A'(\bar{\phi}_{h,\tau})^2 - A'(\bar{\hat{\phi}}_{h,\tau})^2]\bar{\hat{q}}_{h,\tau}|\nabla\bar{\hat{\phi}}_{h,\tau}|^2\|_{0,6/5}^2 \\
&\quad + \|A'(\bar{\hat{\phi}}_{h,\tau})^2\bar{\hat{q}}_{h,\tau}|\nabla\bar{\hat{\phi}}_{h,\tau}|^2 - \overline{A'(\phi))^2 q|\nabla\phi|^2}\|_{0,6/5}^2 \\
&\leq \int_{I_n} \|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^2 \|\nabla\bar{\hat{\phi}}_{h,\tau}\|_{0,3}^4 \mathcal{E}_\alpha^\phi(\phi_{h,\tau}|\hat{\phi}_{h,\tau}) + C_1 h^4 + C_2\tau^4.
\end{aligned}
$$

For the fifth term in the above error decomposition, we again use Lemma 18 to get

$$
\begin{aligned}
(v) &\leq \int_{I_n} \|(A\cdot A')(\bar{\phi}_{h,\tau})\nabla\bar{q}_{h,\tau}\nabla\bar{\phi}_{h,\tau} - (A\cdot A')(\bar{\phi}_{h,\tau})\nabla\bar{q}_{h,\tau}\nabla\bar{\hat{\phi}}_{h,\tau}\|_{0,6/5}^2 \\
&\quad + \|(A\cdot A')(\bar{\phi}_{h,\tau})\nabla\bar{q}_{h,\tau}\nabla\bar{\hat{\phi}}_{h,\tau} - \overline{(A\cdot A')(\phi)\nabla q\nabla\phi}\|_{0,6/5}^2 \\
&\leq C\|\nabla\bar{q}_{h,\tau}\|_{0,3}^2 \|\nabla(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})\|_{0,2}^2 + C\|\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_{0,6}^2 \|\nabla\bar{q}_{h,\tau}\nabla\bar{\hat{\phi}}_{h,\tau}\|_{0,3/2}^2 \\
&\quad + \|(A\cdot A')(\bar{\hat{\phi}}_{h,\tau})\nabla\bar{q}_{h,\tau}\nabla\bar{\hat{\phi}}_{h,\tau} - \overline{(A\cdot A')(\phi)\nabla q\nabla\phi}\|_{0,6/5}^2 \\
&\leq C(\|\nabla\bar{q}_{h,\tau}\|_{0,3}^2 + \|\nabla\bar{q}_{h,\tau}\nabla\bar{\hat{\phi}}_{h,\tau}\|_{0,3/2}^2)\mathcal{E}_\alpha^\phi(\phi_{h,\tau}|\hat{\phi}_{h,\tau}) + C_3 h^4 + C_4\tau^4.
\end{aligned}
$$

For the remaining term, we obtain in a similar manner

$$
\begin{aligned}
(vii) \leq \int_{I_n} & \|(A \cdot A')(\bar{\phi}_{h,\tau}) \nabla \bar{\mu}_{h,\tau} \nabla \bar{\phi}_{h,\tau} - (A \cdot A')(\bar{\phi}_{h,\tau}) \nabla \bar{\mu}_{h,\tau} \nabla \bar{\hat{\phi}}_{h,\tau}\|_{0,6/5}^2 \\
& + \|(A \cdot A')(\bar{\phi}_{h,\tau}) \nabla \bar{\mu}_{h,\tau} \nabla \bar{\hat{\phi}}_{h,\tau} - \overline{(A \cdot A')(\phi) \nabla \mu \nabla \phi}\|_{0,6/5}^2 \\
\leq{}& C \|\nabla \bar{\mu}_{h,\tau}\|_{0,3}^2 \|\nabla(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})\|_{0,2}^2 + C \|\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_{0,6}^2 \|\nabla \bar{\mu}_{h,\tau} \nabla \bar{\hat{\phi}}_{h,\tau}\|_{0,3/2}^2 \\
& + \|(A \cdot A')(\bar{\hat{\phi}}_{h,\tau}) \nabla \bar{\mu}_{h,\tau} \nabla \bar{\hat{\phi}}_{h,\tau} - \overline{(A \cdot A')(\phi) \nabla \mu \nabla \phi}\|_{0,6/5}^2 \\
\leq{}& C(\|\nabla \bar{\mu}_{h,\tau}\|_{0,3}^2 + \|\nabla \bar{\mu}_{h,\tau} \nabla \bar{\hat{\phi}}_{h,\tau}\|_{0,3/2}^2) \mathcal{E}_\alpha^\phi(\phi_{h,\tau} | \hat{\phi}_{h,\tau}) + C_3 h^4 + C_4 \tau^4.
\end{aligned}
$$

In total the third residual can therefore be estimated by

$$
\int_{I_n} \|\bar{r}_{3,h,\tau}\|_{-1,h}^2 \, \mathrm{d}s \leq C(h^4 + \tau^4) + \int_{I_n} C \mathcal{E}_\alpha(\phi_{h,\tau}, q_{h,\tau} | \hat{\phi}_{h,\tau}, \hat{q}_{h,\tau}) \, \mathrm{d}s.
$$

□

Proof of Lemma 14

We assume the conditions of Lemma 14 to hold and again estimate the two relevant residuals separately.

First residual

With similar arguments as used in the previous section, we obtain

$$
\begin{aligned}
\int_{I_n} \|\bar{r}_{1,h,\tau}\|_{-1,h}^2 \, \mathrm{d}s \leq C \int_{I_n} & \|b'\|_{0,\infty}^2 \|\hat{\mu}\|_{1,3}^2 \|\hat{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_{0,6}^2 \\
& + \|(cA)'\|_{0,\infty}^2 \|\bar{\hat{q}}_{h,\tau}\|_{1,3} \|\hat{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_{0,6}^2 \\
& + \|cA'\|_{0,\infty}^2 \|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^2 \|\hat{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_1^2 \\
& + \|(cA')'\|_{0,\infty}^2 \|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^2 \|\hat{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_{0,6}^2 \|\bar{\hat{\phi}}_{h,\tau}\|_{1,3}^2 \\
\leq C_1 \int_{I_n} & \mathcal{E}_\alpha^\phi(\phi_{h,\tau} | \hat{\phi}_{h,\tau}) \, \mathrm{d}s
\end{aligned}
$$

with constant C_1 depending on $\|\bar{\hat{\mu}}_{h,\tau}\|_{L^\infty(W^{1,3})}$, $\|\bar{\hat{q}}_{h,\tau}\|_{L^\infty(W^{1,3})}$, and $\|\bar{\hat{\phi}}_{h,\tau}\|_{L^\infty(W^{1,3})}$.

Third residual

In a similar manner, we can estimate

$$
\begin{aligned}
\int_{I_n} \|\bar{r}_{3,h,\tau}\|_{-1,h}^2 \,\mathrm{d}s \le C \int_{I_n} & \|\kappa'\|_{0,\infty}^2 \|\bar{q}_{h,\tau} - \bar{\hat{q}}_{h,\tau}\|_0^2 + \|cA'\|_{0,\infty}^2 \|\bar{\hat{\mu}}_{h,\tau}\|_{1,3}^2 \|\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_{0,6}^2 \\
& + \|cA'\|_{0,\infty}^2 \|\bar{\hat{\mu}}_{h,\tau}\|_{1,3}^2 \|\nabla(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})\|_0^2 \\
& + \|cA'\|_{0,\infty}^2 \|\bar{\hat{\mu}}_{h,\tau}\|_{1,3}^2 \|\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_{0,6}^2 \|\bar{\hat{\phi}}_{h,\tau}\|_{1,3}^2 \\
& + \|(A^2)'\|_{0,\infty}^2 \|\bar{\hat{q}}_{h,\tau}\|_{1,3}^2 \|\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_{0,6}^2 \\
& + \|(A')^2\|_{0,\infty} \|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^2 \|\nabla(\bar{\phi}_{h,\tau} + \bar{\hat{\phi}}_{h,\tau})\|_0^2 \|\nabla(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})\|_{0,3}^2 \\
& + \|((A')^2)'\|_{0,\infty} \|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^2 \|\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_{0,6}^2 \|\nabla \bar{\hat{\phi}}_{h,\tau}\|_0^2 \\
& + \|AA'\|_{0,\infty}^2 (\|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^2 + \|\bar{\hat{q}}_{h,\tau}\|_{1,3}^2) \|\nabla(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})\|_0^2 \\
& + \|(AA')'\|_{0,\infty}^2 (\|\bar{\hat{q}}_{h,\tau}\|_{0,\infty}^2 + \|\bar{\hat{q}}_{h,\tau}\|_{1,3}^2) \|\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau}\|_0^2 \|\nabla \bar{\hat{\phi}}_{h,\tau}\|_{0,3}^2 \\
\le C_2 \int_{I_n} \mathcal{E}_\alpha(z_{h,\tau} | \hat{z}_{h,\tau}) \,\mathrm{d}s & + C_3 \int_{I_n} \|\nabla(\bar{\phi}_{h,\tau} - \bar{\hat{\phi}}_{h,\tau})\|_{0,3}^2 \,\mathrm{d}s.
\end{aligned}
$$

The constants C_2, C_3 depend on $\|\bar{\hat{\mu}}_{h,\tau}\|_{L^\infty(W^{1,3})}$, $\|\bar{\hat{q}}_{h,\tau}\|_{L^\infty(W^{1,3})}$, $\|\bar{\hat{q}}_{h,\tau}\|_{L^\infty(L^\infty)}$, $\|\bar{\hat{\phi}}_{h,\tau}\|_{L^\infty(W^{1,3})}$ and $\|\bar{\hat{q}}_{h,\tau}\|_{L^\infty(L^\infty)}^2$, $\|\nabla(\bar{\phi}_{h,\tau} + \bar{\hat{\phi}}_{h,\tau})\|_{L^\infty(L^2)}^2$, respectively. The last term in the above estimate can again be estimated by the discrete interpolation inequality (A.6) and estimates for the discrete Laplacian, which finally can be absorbed in the dissipation terms; compare with (B.1). In summary, we thus have obtained the required estimates for the two residuals of Lemma 14. □

Discrete Gronwall lemma

For completeness, let us recall the following version of the discrete Gronwall lemma.

Lemma 19 *Let $(u_n)_n$, $(b_n)_n$, $(c_n)_n$, and $(\lambda_n)_n$ be given positive sequences, satisfying the inequality $u_n + b_n \le e^{\lambda_n} u_{n-1} + c_n$ for all $n \ge 0$. Then*

$$
u_n + \sum_{k=1}^{n} e^{\sum_{j=k+1}^{n} \lambda_j} b_k \le e^{\sum_{j=1}^{n} \lambda_j} u_0 + \sum_{k=0}^{n} e^{\sum_{j=k+1}^{n} \lambda_j} c_k, \quad n > 0. \tag{D.1}
$$

Proof The result follows applying mathematical induction. □

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