A posteriori error analysis for time-dependent Ginzburg-Landau type equations

Sören Bartels

Department of Mathematics, University of Maryland, College Park, MD 20742, USA

Abstract. This work presents an a posteriori error analysis for the finite element approximation of time-dependent Ginzburg-Landau type equations in two and three space dimensions. The solution of an elliptic, self-adjoint eigenvalue problem as a post-processing procedure in each time step of a finite element simulation leads to a fully computable upper bound for the error. Theoretical results for the stability of degree one vortices in Ginzburg-Landau equations and of generic interfaces in Allen-Cahn equations indicate that the error estimate only depends on the inverse of a small parameter in a low order polynomial. The actual dependence of the error estimate upon this parameter is explicitly determined by the computed eigenvalues and can therefore be monitored within an approximation scheme. The error bound allows for the introduction of local refinement indicators which may be used for adaptive mesh and time step size refinement and coarsening. Numerical experiments underline the reliability of this approach.

Key Words. Ginzburg-Landau equations, Allen-Cahn equations, error analysis, eigenvalue approximation, finite element method, adaptive mesh refinement.

AMS Subject Classification: 65M15, 65M60, 65M50.

Date: April 15, 2004.

1. INTRODUCTION

Given a bounded Lipschitz domain $\Omega \subseteq \mathbb{R}^n$, $n = 2, 3$, a subset $\Gamma_{\rm D} \subseteq \partial\Omega$ which is either empty or of positive surface measure, a positive integer m, a small number $\varepsilon > 0$, a parameter $T > 0$, initial data $u_0^\varepsilon \in H^1(\Omega; \mathbb{R}^m)$, and boundary data $g^\varepsilon = u_0^\varepsilon|_{\Gamma_{\rm D}} \in H^{1/2}(\Gamma_{\rm D}; \mathbb{R}^m)$, we aim to approximate the problem:

$$(\mathfrak{P}) \qquad \begin{cases} \textit{Find } u^\varepsilon \in Z := H^1(0,T;Y') \cap L^2(0,T;H^1(\Omega;\mathbb{R}^m)) \textit{ such that} \\ \textit{for almost all } t \in (0,T) \textit{ and all } v \in Y \textit{ there holds} \\ \quad \begin{aligned} \langle u_t^\varepsilon; v\rangle + (\nabla u^\varepsilon; \nabla v) + \varepsilon^{-2}(f(u^\varepsilon); v) &= 0, \\ u^\varepsilon|_{\Gamma_{\rm D}} &= g^\varepsilon, \\ u^\varepsilon(0) &= u_0^\varepsilon. \end{aligned} \end{cases}$$

Here, $Y := \{v \in H^1(\Omega; \mathbb{R}^m) : v|_{\Gamma_{\rm D}} = 0\}$, $f(a) = (|a|^2 - 1)a$ for $a \in \mathbb{R}^m$, $(\cdot;\cdot)$ stands for the scalar product in $L^2(\Omega; \mathbb{R}^m)$, $\langle\cdot;\cdot\rangle$ denotes the duality pairing of Y and Y', and u_t^ε is the time derivative of u^ε. Throughout this work $a \cdot b$ denotes the scalar product of two vectors $a, b \in \mathbb{R}^m$.

Existence and uniqueness of a solution u^ε for $(\mathfrak{P})$ follow from standard techniques. Throughout this work we abbreviate

$$u = u^\varepsilon, \quad u_0 = u_0^\varepsilon, \quad \text{and} \quad g = g^\varepsilon$$

but stress that the dependence of the error of numerical approximation schemes upon the parameter ε is the main focus of this work.

The model problem $(\mathfrak{P})$ reduces to Allen-Cahn equations [1] for the description of melting processes in binary alloys if $m = 1$ and $\Gamma_\mathrm{D} = \emptyset$ and to (simplified) Ginzburg-Landau equations [13] as a mathematical model for certain superconducting materials if $n = m = 2$, $\Gamma_\mathrm{D} = \partial\Omega$, and $|g(x)| \approx 1$. Since solutions for these problems develop interfaces of thickness ε or evolve vortices with large gradients of order ε^{-1} in a small neighborhood, optimal approximation schemes require locally refined meshes which resolve such topological effects. Adaptive finite element methods based on a posteriori error estimates are known to allow for very efficient approximations when features on small scales have to be resolved. It is the aim of this work to prove robust a posteriori error estimates which lead to local refinement and coarsening indicators that allow for an automatic mesh and time-step size refinement and coarsening.

Standard error estimates for the numerical approximation of $(\mathfrak{P})$ depend exponentially on ε^{-2} and are useless if ε is small. We establish an a posteriori error estimate which depends on ε^{-1} only in a low order polynomial if no critical topological effects take place. Otherwise, the error estimate localizes critical times at which such effects occur. In particular, let $U(t) \in \mathcal{S}$ be the output of an approximation scheme and which serves as an approximation of $u(t)$ for some $t \in (0, T)$. We then approximate the self-adjoint, elliptic (after introduction of a constant shift) eigenvalue problem

$$-\Delta w + \varepsilon^{-2} f'(U(t))w = -\lambda w \qquad \text{in } \Omega$$

and the value λ determines the stability of the solution of $(\mathfrak{P})$ at time t and enters error estimates exponentially. Theoretical results in [5, 6] for Allen-Cahn equations and in [17] for Ginzburg-Landau equations indicate that λ is bounded ε-independently from above if the zero level set of u is smooth and if zeros of u are of topological degree one, respectively.

Our analysis is inspired by recent work by Feng and Prohl [9, 10] on the a priori error analysis for the approximation of Allen-Cahn and Cahn-Hilliard equations and by Kessler, Nochetto, and Schmidt [14, 15] on the a posteriori error analysis for the approximation of Allen-Cahn equations. Here, we do not restrict the analysis to initial conditions and parameters $T > 0$ that allow for an ε-independent upper bound for λ but propose its approximation in each time step of a numerical simulation and thereby avoid the use of any a priori information. Numerical experiments indicate that this approach is reliable. We remark that our analysis is still valid if outer body forces or inhomogeneous Neumann boundary conditions on $\partial\Omega \setminus \Gamma_\mathrm{D}$ are included in $(\mathfrak{P})$. Moreover, the function f may be replaced by any function that satisfies the estimates of Lemma 3.1 below. For related numerical aspects of Allen-Cahn and Ginzburg-Landau equations we refer the reader to [7, 8] and references therein.

The outline of this article is as follows. We present the main result in an abstract setting in Section 2 employing a continuation argument from [14]. The abstract framework allows for a posteriori error estimates that are method independent. Section 3 is devoted to the derivation of an error equation that is needed in the proof of the main result. We then specify notation in finite element spaces in Section 4 and state estimates that control the influence of approximated boundary data on the global approximation error. Error estimates for the approximation of eigenvalue problems are discussed in Section 5 and their combination with explicit bounds for the residual of a lowest order finite element approximation of u in Section 6 make the abstract result of Section 2 practically applicable. The fully computable error estimate then motivates an adaptive mesh and time step size coarsening and refining algorithm which is stated in Section 7. Numerical experiments that show the necessity of approximating λ and thereby underline the relevance of the theoretical results of this contribution are reported in Section 8.

2. Derivation of the main result

Given an approximation $U \in Z \cap L^\infty(0,T;L^\infty(\Omega;\mathbb{R}^m))$ of the solution u of $(\mathfrak{P})$ such that $U|_{\Gamma_{\rm D}}$ is time-independent, we define its residual $\mathcal{R}_U \in L^2(0,T;Y')$ for almost all $t \in (0,T)$ and all $v \in Y$ by

$$\langle U_t; v\rangle + (\nabla U;\nabla v) + \varepsilon^{-2}(f(U);v) = -\langle \mathcal{R}_U; v\rangle. \tag{2.1}$$

We solve eigenvalue problems to obtain functions Λ and $\eta_{\rm EV}$ such that for a constant $c_1 > 0$, for almost all $t \in (0,T)$, and $\kappa := \max\{0, \Lambda + c_1\eta_{\rm EV}\}$ there holds

$$-\kappa \le -\Lambda - c_1\eta_{\rm EV} \le \inf_{0\neq v\in Y} \frac{(\nabla v;\nabla v) + \varepsilon^{-2}(f'(U(t))v;v)}{||v||^2_{L^2(\Omega)}}. \tag{2.2}$$

One can then show (cf. Proposition 3.2) that for almost all $t \in (0,T)$ and $e := u - U$ there holds

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}||e||^2_{L^2(\Omega)} + \varepsilon^2||\nabla e||^2_{L^2(\Omega)} &\le \varepsilon^{-2}||\mathcal{R}_U||^2_{Y'} + c_2(1+\kappa)||e||^2_{L^2(\Omega)} + 2\frac{\mathrm{d}}{\mathrm{d}t}(e;w) \\ &\quad + c_3\varepsilon^{-2}\big(||U||_{L^\infty(\Omega)} + ||w||_{L^\infty(\Omega)}\big)||e||^3_{L^3(\Omega)} + c_4\eta_{\rm D}^2,\end{aligned} \tag{2.3}$$

where $w \in H^1(\Omega;\mathbb{R}^m)$ extends (the time-independent) $e|_{\Gamma_{\rm D}}$ and $\eta_{\rm D} = 0$ if $e|_{\Gamma_{\rm D}} = 0$. Integrating this equation over $(0,t)$ for any $0 \le t \le T$, using a Sobolev inequality to estimate

$$||e||^3_{L^3(\Omega)} \le ||e||_{L^2(\Omega)}||e||^2_{L^4(\Omega)} \le c_5||e||_{L^2(\Omega)}\big(||e||^2_{L^2(\Omega)} + ||\nabla e||^2_{L^2(\Omega)}\big), \tag{2.4}$$

and setting $\overline{\kappa} := \operatorname{ess\,sup}_{s\in(0,T)}\kappa(s)$ yields

$$\begin{aligned}&\frac{1}{2}||e(t)||^2_{L^2(\Omega)} + \varepsilon^2\int_0^t ||\nabla e||^2_{L^2(\Omega)}\,\mathrm{d}s \\ &\qquad \le 2||e(0)||^2_{L^2(\Omega)} + \varepsilon^{-2}\int_0^t ||\mathcal{R}_U||^2_{Y'}\,\mathrm{d}s + c_2(1+\overline{\kappa})\int_0^t ||e||^2_{L^2(\Omega)}\,\mathrm{d}s \\ &\qquad\quad + c_4\int_0^t \eta_{\rm D}^2\,\mathrm{d}s + 3\int_0^t ||w||^2_{L^2(\Omega)}\,\mathrm{d}s \\ &\qquad\quad + c_3c_5\varepsilon^{-2}\big(||U||_{L^\infty(0,T;L^\infty(\Omega))} + ||w||_{L^\infty(\Omega)}\big) \\ &\qquad\qquad \times \operatorname{ess\,sup}_{s\in(0,t)}||e||_{L^2(\Omega)}\Big(t\operatorname{ess\,sup}_{s\in(0,t)}||e||^2_{L^2(\Omega)} + \int_0^t ||\nabla e||^2_{L^2(\Omega)}\,\mathrm{d}s\Big).\end{aligned} \tag{2.5}$$

We choose η and a constant $c_6 > 0$ such that

$$2||e(0)||^2_{L^2(\Omega)} + \varepsilon^{-2}\int_0^T ||\mathcal{R}_U||^2_{Y'}\,\mathrm{d}s + c_4\int_0^T \eta_{\rm D}^2\,\mathrm{d}s + 3\int_0^T ||w||^2_{L^2(\Omega)}\,\mathrm{d}s \le c_6\eta^2. \tag{2.6}$$

Since the left-hand side of (2.5) depends continuously on t, we may conclude that the set

$$I := \Big\{ t \in [0,T] : \operatorname{ess\,sup}_{s\in(0,t)} \frac{1}{2}||e(s)||^2_{L^2(\Omega)} + \varepsilon^2 \int_0^t ||\nabla e||^2_{L^2(\Omega)}\,\mathrm{d}s \le 4c_6\eta^2 \exp\big(c_2(1+\overline{\kappa})T\big) \Big\}$$

is non-empty and we aim to prove that $I = [0,T]$. Let $t^* := \max I$ and suppose that $t^* < T$. We use the definition of I and (2.6) to derive from (2.5) that for all $0 \le t \le t^*$ we have

$$\frac{1}{2}||e(t)||^2_{L^2(\Omega)} + \varepsilon^2 \int_0^t ||\nabla e||^2_{L^2(\Omega)}\,\mathrm{d}s \le c_6\eta^2 + c_2(1+\overline{\kappa}) \int_0^t ||e||^2_{L^2(\Omega)}\,\mathrm{d}s$$
$$+ c_3c_5\varepsilon^{-2}\big(||U||_{L^\infty(0,T;L^\infty(\Omega))} + ||w||_{L^\infty(\Omega)}\big)2^3\sqrt{2}c_6^{3/2}\eta^3 C^3_{T,\overline{\kappa}}(2T+\varepsilon^{-2}),$$

where $C^2_{T,\overline{\kappa}} := \exp\big(c_2(1+\overline{\kappa})T\big)$. If

$$c_3c_5\varepsilon^{-2}\big(||U||_{L^\infty(0,T;L^\infty(\Omega))} + ||w||_{L^\infty(\Omega)}\big)2^3\sqrt{2}c_6^{3/2}\eta^3 C^3_{T,\overline{\kappa}}(2T+\varepsilon^{-2}) \le c_6\eta^2,$$

or equivalently

$$(2.7)\quad ||U||_{L^\infty(0,T;L^\infty(\Omega))} + ||w||_{L^\infty(\Omega)} = 0 \quad \text{or} \quad \eta \le \varepsilon^4 \frac{\big(||U||_{L^\infty(0,T;L^\infty(\Omega))} + ||w||_{L^\infty(\Omega)}\big)^{-1}}{8\sqrt{2}c_3c_5c_6^{1/2}(2\varepsilon^2 T + 1)} C^{-3}_{T,\overline{\kappa}},$$

then we have for all $0 \le t \le t^*$ that

$$\frac{1}{2}||e(t)||^2_{L^2(\Omega)} + \varepsilon^2 \int_0^t ||\nabla e||^2_{L^2(\Omega)}\,\mathrm{d}s \le 2c_6\eta^2 + c_2(1+\overline{\kappa}) \int_0^t ||e||^2_{L^2(\Omega)}\,\mathrm{d}s.$$

Gronwall's inequality yields

$$\operatorname{ess\,sup}_{s\in(0,t^*)} \frac{1}{2}||e(s)||^2_{L^2(\Omega)} + \varepsilon^2 \int_0^{t^*} ||\nabla e||^2_{L^2(\Omega)}\,\mathrm{d}s \le 2c_6\eta^2 \exp\big(c_2(1+\overline{\kappa})T\big)$$

which by continuity of the left-hand side contradicts $t^* < T$ and therefore proves $I = [0,T]$. The argumentation leads to the following theorem.

Theorem 2.1. *Suppose that* (2.7) *holds. Then there holds*

$$\operatorname{ess\,sup}_{s\in(0,T)} \frac{1}{2}||e(s)||^2_{L^2(\Omega)} + \varepsilon^2 \int_0^T ||\nabla e||^2_{L^2(\Omega)}\,\mathrm{d}s \le 4c_6\eta^2 \exp\big(c_2(1+\overline{\kappa})T\big).$$

In order to make the proof of the theorem complete we only need to prove (2.3). In order to make it applicable we need to define a strategy to compute Λ and η_{EV} in (2.2) and we need to establish a computable estimator η in (2.6).

Remark. *The error estimate of Theorem 2.1 is useful only if $\overline{\kappa} \le C$ for some ε-independent constant $C > 0$. Supposing that $||u-U||_{L^\infty((0,T);L^\infty(\Omega))} \le C'\varepsilon^2$ for some ε-independent constant $C' > 0$ then a uniform bound for $\overline{\kappa}$ may be deduced from* [5] *if $m = 1$ and the zero level set of u is smooth, and from* [17] *if $n = m = 2$ and the zeros of u are of topological degree one.*

3. Proof of the error equation (2.3)

We employ the following estimates which relate the first equation in $(\mathfrak{P})$ to its linearization.

Lemma 3.1. *For all $a, b, c \in \mathbb{R}^m$ there holds*

$$(f(a) - f(b))\cdot(a-b-c) \ge f'(b)(a-b-c)\cdot(a-b-c)$$
$$+ f'(b)c\cdot(a-b-c) - (5|b| + |c|)|a-b|^3 - |b||c|^3,$$
$$f'(b)(a-b-c)\cdot(a-b-c) \ge -|a-b-c|^2,$$

where $f' : \mathbb{R}^m \to \mathbb{R}^{m\times m}$ *denotes the total derivative of* f.

Proof. For all $d \in \mathbb{R}^m$ there holds

$$f''(b)(d,d) = 4(b\cdot d)d + 2|d|^2 b \quad \text{and} \quad f'''(b)(d,d,d) = 6|d|^2 d$$

and a Taylor expansion of the cubic function f shows

$$f(a) - f(b) = f'(b)(a-b) + 2(b\cdot(a-b))(a-b) + |a-b|^2 b + |a-b|^2(a-b).$$

We thus have

$$\begin{aligned}(f(a)-f(b))\cdot(a-b-c) &= f'(b)(a-b-c)\cdot(a-b-c) + f'(b)c\cdot(a-b-c)\\ &\quad + 2(b\cdot(a-b))(a-b)\cdot(a-b-c) + |a-b|^2 b\cdot(a-b-c)\\ &\quad + |a-b|^2(a-b)\cdot(a-b-c)\\ &\geq f'(b)(a-b-c)\cdot(a-b-c) + f'(b)c\cdot(a-b-c)\\ &\quad - 3|b||a-b|^2|a-b-c| - |a-b|^3|c|.\end{aligned}$$

We employ the triangle inequality and Young's inequality to estimate

$$3|b||a-b|^2|a-b-c| \leq 3|b||a-b|^3 + 3|b||a-b|^2|c| \leq 5|b||a-b|^3 + |b||c|^3.$$

The combination of the last two estimates proves the first assertion. For all $d \in \mathbb{R}^n$ we have

$$f'(b)d\cdot d = (|b|^2-1)|d|^2 + 2(b\cdot d)^2 \geq -|d|^2$$

and this proves the second assertion of the lemma. □

If $\varepsilon \leq 1$ then the following proposition proves (2.3) with $c_2 = 8$, $c_3 = 10$, $c_4 = 2$, and $\eta_{\rm D} = \tilde\eta_{\rm D}$.

Proposition 3.2. *Let* $w \in H^1(\Omega;\mathbb{R}^m)$ *satisfy* $w|_{\Gamma_{\rm D}} = e|_{\Gamma_{\rm D}}$ *for almost all* $t\in(0,T)$. *For almost all* $t \in (0,T)$ *there holds*

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}||e||^2_{L^2(\Omega)} + \varepsilon^2||\nabla e||^2_{L^2(\Omega)} &\leq \varepsilon^{-2}||\mathcal{R}_U||^2_{Y'} + 2\big(\varepsilon^2 + 2(1-\varepsilon^2)\kappa + 3\big)||e||^2_{L^2(\Omega)} + 2\frac{\mathrm{d}}{\mathrm{d}t}(e;w)\\ &\quad + 2\varepsilon^{-2}(5||U||_{L^\infty(\Omega)} + ||w||_{L^\infty(\Omega)})||e||^3_{L^3(\Omega)} + 2\tilde\eta_{\rm D},\end{aligned}$$

where

$$\begin{aligned}\tilde\eta_{\rm D} = \big(&\varepsilon^2 + 2(1-\varepsilon^2)\kappa + 3 + (\varepsilon^{-4}/2)||f'(U)||^2_{L^\infty(\Omega)}\big)||w||^2_{L^2(\Omega)}\\ &+ \varepsilon^{-2}||U||_{L^\infty(\Omega)}||w||^3_{L^3(\Omega)} + 3\varepsilon^{-2}\big((1-\varepsilon^2)^2 + 5/9\big)||\nabla w||^2_{L^2(\Omega)}.\end{aligned}$$

Proof. The governing equations in $(\mathfrak{P})$ for u and the definition of the residual $\mathcal{R}_U$ in (2.1) lead to

$$\langle e_t; v\rangle + (\nabla e;\nabla v) + \varepsilon^{-2}(f(u)-f(U);v) = \langle\mathcal{R}_U; v\rangle$$

for all $v \in Y$. The choice $v = e - w$ implies

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}||e||^2_{L^2(\Omega)} + ||\nabla e||^2_{L^2(\Omega)} + \varepsilon^{-2}(f(u)-f(U);e-w) = \langle\mathcal{R}_U; e-w\rangle + \langle e_t; w\rangle + (\nabla e;\nabla w).$$

We employ the first estimate of Lemma 3.1 with $a = u$, $b = U$, and $c = w$ to verify

$$\begin{aligned}-\varepsilon^{-2}(f(u)-f(U);e-w) &= -\varepsilon^{-2}(f(u)-f(U);u-U-w)\\ &\leq -\varepsilon^{-2}(f'(U)(e-w);e-w) - \varepsilon^{-2}(f'(U)w;e-w)\\ &\quad + \varepsilon^{-2}(5||U||_{L^\infty(\Omega)} + ||w||_{L^\infty(\Omega)})||e||^3_{L^3(\Omega)} + \varepsilon^{-2}||U||_{L^\infty(\Omega)}||w||^3_{L^3(\Omega)}.\end{aligned}$$

Given any $\theta \in [0,1]$ we split the first term on the right-hand side into two contributions weighted by θ and $1-\theta$ and use the second estimate of Lemma 3.1 to deduce

$$-\theta\varepsilon^{-2}(f'(U)(e-w);e-w) \le \theta\varepsilon^{-2}||e-w||^2_{L^2(\Omega)}$$

while (2.2) yields

$$-(1-\theta)\varepsilon^{-2}(f'(U)(e-w);e-w) \le (1-\theta)||\nabla(e-w)||^2_{L^2(\Omega)} + (1-\theta)\kappa||e-w||^2_{L^2(\Omega)}.$$

Hölder inequalities allow us to derive

$$-\varepsilon^{-2}(f'(U)w;e-w) \le \frac{\varepsilon^{-4}}{2}||f'(U)||^2_{L^\infty(\Omega)}||w||^2_{L^2(\Omega)} + \frac{1}{2}||e-w||^2_{L^2(\Omega)}.$$

Young's inequality with some positive α proves

$$\langle \mathcal{R}_U; e-w\rangle \le ||\mathcal{R}_U||_{Y'}||e-w||_Y \le \frac{1}{4\alpha}||\mathcal{R}_U||^2_{Y'} + \alpha||e-w||^2_{L^2(\Omega)} + \alpha||\nabla(e-w)||^2_{L^2(\Omega)}$$

and

$$(\nabla e;\nabla w) \le \frac{\alpha}{2}||\nabla e||^2_{L^2(\Omega)} + \frac{1}{2\alpha}||\nabla w||^2_{L^2(\Omega)}$$

The combination of the estimates results in

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}||e||^2_{L^2(\Omega)} + ||\nabla e||^2_{L^2(\Omega)} &\le \frac{1}{4\alpha}||\mathcal{R}_U||^2_{Y'} + \big(\alpha + \theta\varepsilon^{-2} + (1-\theta)\kappa + 1/2\big)||e-w||^2_{L^2(\Omega)}\\ &+ (1-\theta+\alpha)||\nabla(e-w)||^2_{L^2(\Omega)} + \langle e_t; w\rangle + \varepsilon^{-2}(5||U||_{L^\infty(\Omega)} + ||w||_{L^\infty(\Omega)})||e||^3_{L^3(\Omega)}\\ &+ \frac{1}{2}\varepsilon^{-4}||f'(U)||^2_{L^\infty(\Omega)}||w||^2_{L^2(\Omega)} + \varepsilon^{-2}||U||_{L^\infty(\Omega)}||w||^3_{L^3(\Omega)} + \frac{\alpha}{2}||\nabla e||^2_{L^2(\Omega)} + \frac{1}{2\alpha}||\nabla w||^2_{L^2(\Omega)}.\end{aligned}$$

We abbreviate $\delta := \theta - \alpha$ and set $\varrho := 2(1-\delta)/\delta$ to deduce with the help of Young's inequality

$$\begin{aligned}(1-\theta+\alpha)||\nabla(e-w)||^2_{L^2(\Omega)} &= (1-\delta)||\nabla(e-w)||^2_{L^2(\Omega)}\\ &\le (1-\delta)||\nabla e||^2_{L^2(\Omega)} + \frac{1-\delta}{\varrho}||\nabla e||^2_{L^2(\Omega)} + \varrho(1-\delta)||\nabla w||^2_{L^2(\Omega)} + (1-\delta)||\nabla w||^2_{L^2(\Omega)}\\ &= (1-\delta/2)||\nabla e||^2_{L^2(\Omega)} + 2\frac{(1-\delta)^2}{\delta}||\nabla w||^2_{L^2(\Omega)} + (1-\delta)||\nabla w||^2_{L^2(\Omega)}\\ &= (1-\theta/2+\alpha/2)||\nabla e||^2_{L^2(\Omega)} + \frac{1}{\delta}(\delta^2 - 3\delta + 2)||\nabla w||^2_{L^2(\Omega)}.\end{aligned}$$

This, the choices $\theta = 2\varepsilon^2$ and $\alpha = \varepsilon^2/2$, and the identity $\langle e_t; w\rangle = \frac{\mathrm{d}}{\mathrm{d}t}(e;w)$ lead to

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}||e||^2_{L^2(\Omega)} + \varepsilon^2||\nabla e||^2_{L^2(\Omega)} \le\ & \varepsilon^{-2}||\mathcal{R}_U||^2_{Y'} + \big(\varepsilon^2 + 2(1-\varepsilon^2)\kappa + 3\big)||e-w||^2_{L^2(\Omega)} + 2\frac{\mathrm{d}}{\mathrm{d}t}(e;w)\\ &+ 2\varepsilon^{-2}(5||U||_{L^\infty(\Omega)} + ||w||_{L^\infty(\Omega)})||e||^3_{L^3(\Omega)} + \varepsilon^{-4}||f'(U)||^2_{L^\infty(\Omega)}||w||^2_{L^2(\Omega)}\\ &+ 2\varepsilon^{-2}||U||_{L^\infty(\Omega)}||w||^3_{L^3(\Omega)} + 3\varepsilon^{-2}\big((1-\varepsilon^2)^2 + 5/9\big)||\nabla w||^2_{L^2(\Omega)}\end{aligned}$$

which proves the proposition. □

4. Finite element spaces and bounds for η_{D} in (2.3)

4.1. **Notation in finite element spaces.** We suppose that Ω is polygonal or polyhedral if $n=2$ or $n=3$, respectively. Given a regular triangulation $\mathcal{T}$ of Ω into tetrahedra and quadrilaterals or triangles and parallelograms if $n=2$ or $n=3$, respectively, we let $\mathcal{S}^1(\mathcal{T})^m$ denote the discrete space of $\mathbb{R}^m$ valued, continuous functions which are $\mathcal{T}$-elementwise affine or bilinear and we set $\mathcal{S}^1_{\mathrm{D}}(\mathcal{T})^m := \mathcal{S}^1(\mathcal{T})^m \cap Y$. We specify a $\mathcal{T}$-elementwise constant function $h_{\mathcal{T}} \in L^\infty(\Omega)$ by requiring $h_\mathcal{T}|_S = h_S := \operatorname{diam}(S)$ for all $S \in \mathcal{T}$. The set $\mathcal{F}$ consists of all faces of elements (edges of elements if $n = 2$) and we assume that Γ_D is matched exactly by the union of all elements in $\mathcal{F}_\mathrm{D} := \{F \in \mathcal{F} : F \subseteq \Gamma_\mathrm{D}\}$. The function $h_\mathcal{F} \in L^\infty(\cup\mathcal{F})$ is defined by $h_\mathcal{F}|_F := \operatorname{diam}(F)$ for all $F \in \mathcal{F}$.

For a function $\psi \in C(\Gamma_\mathrm{D};\mathbb{R}^m)$ such that $\psi|_F \in H^2(F;\mathbb{R}^m)$ for all $F \in \mathcal{F}$ we let $D^2_\mathcal{F}\psi|_F$ denote the second weak derivative of $\psi|_F$ with respect to a proper coordinate system on $F \in \mathcal{F}$.

The operator $\Delta_\mathcal{T}$ satisfies $\Delta_\mathcal{T} V|_S = \Delta(V|_S)$ for all functions $V \in \mathcal{S}^1(\mathcal{T})^m$ and all $S \in \mathcal{T}$. Given a $\mathcal{T}$-elementwise smooth function $\phi \in L^\infty(\Omega;\mathbb{R}^{m\times n})$ let

$$[\phi \cdot n_\mathcal{F}]|_F := \big(\phi|_{S_2} - \phi|_{S_1}\big) n_F$$

if $F \in \mathcal{F}$ is such that $F = S_1 \cap S_2$ for distinct $S_1, S_2 \in \mathcal{T}$ and $n_F \in \mathbb{R}^n$ is the unit vector which is perpendicular to F and which points from S_1 into S_2. For $F \in \mathcal{F}$ such that $F \subseteq \partial\Omega$ we set

$$[\phi \cdot n_\mathcal{F}]|_F := \begin{cases} 0 & \text{for } F \subseteq \Gamma_\mathrm{D}, \\ -\phi\, n_{\partial\Omega} & \text{for } F \subseteq \overline{\partial\Omega \setminus \Gamma_\mathrm{D}}, \end{cases}$$

where $n_{\partial\Omega}$ denotes the outer unit normal to Ω on $\partial\Omega$.

Given a function $\phi \in C(\Omega;\mathbb{R}^m)$ we let $\mathcal{I}_\mathcal{T}\phi \in \mathcal{S}^1(\mathcal{T})^m$ denote the nodal interpolant of ϕ on $\mathcal{T}$.

4.2. **Estimates for** η_D**.** The construction of a function $w \in H^1(\Omega;\mathbb{R}^m)$ with $w|_{\Gamma_\mathrm{D}} = e|_{\Gamma_\mathrm{D}}$ in [3] allows to estimate $||w||_{L^\infty(\Omega)}$, $||\nabla w||_{L^2(\Omega)}$, $||w||_{L^2(\Omega)}$, and $\tilde\eta_\mathrm{D}$ occurring in Proposition 3.2. We thereby obtain a computable quantity (or an upper bound for) η_D in the main result of Section 2.

Lemma 4.1 ([3])**.** *(i) Let $\mathcal{T}$ be a regular triangulation of Ω, assume $g \in C(\Gamma_\mathrm{D};\mathbb{R}^m)$ with $g|_F \in H^2(F;\mathbb{R}^m)$ for all $F \in \mathcal{F}_\mathrm{D}$, and set $G := \mathcal{I}_\mathcal{T} u_0|_{\Gamma_\mathrm{D}}$. There exists $w \in H^1(\Omega;\mathbb{R}^m) \cap C(\Omega;\mathbb{R}^m)$ such that $w|_{\Gamma_\mathrm{D}} = g - G$, supp $w \subseteq \{S \in \mathcal{T} : S \cap \Gamma_\mathrm{D} \neq \emptyset\}$, and*

$$||w||_{L^\infty(\Omega)} = ||g - G||_{L^\infty(\Gamma_\mathrm{D})} \quad \textit{and} \quad \|\nabla w\|_{L^2(\Omega)} \le c_\mathrm{D} \|h_\mathcal{F}^{3/2} D^2_\mathcal{F} g\|_{L^2(\Gamma_\mathrm{D})},$$

where $c_\mathrm{D} > 0$ is an $(h_\mathcal{T}, h_\mathcal{F})$-independent constant.
(ii) Under the assumptions in (i) and with w as in (i) there holds

$$||w||_{L^2(\Omega)} \le c'_\mathrm{D} \|h_\mathcal{F}||_{L^\infty(\Gamma_\mathrm{D})} \|h_\mathcal{F}^{3/2} D^2_\mathcal{F} g\|_{L^2(\Gamma_\mathrm{D})}$$

and

$$||w||_{L^3(\Omega)} \le c'_\mathrm{D} \|h_\mathcal{F}||^{1/3}_{L^\infty(\Gamma_\mathrm{D})} \|h_\mathcal{F}^{3/2} D^2_\mathcal{F} g\|_{L^2(\Gamma_\mathrm{D})},$$

where $c'_\mathrm{D} > 0$ is an $(h_\mathcal{T}, h_\mathcal{F})$-independent constant.

Proof. A proof for (i) can be found in [3]. In order to verify (ii) we use Poincaré inequalities (on patches of elements) to estimate with an $(h_\mathcal{T}, h_\mathcal{F})$-independent constant $C > 0$

$$||w||^2_{L^2(\Omega)} = \sum_{S \in \mathcal{T},\, S\cap\Gamma_\mathrm{D} \neq \emptyset} ||w||^2_{L^2(S)} \le C \sum_{S \in \mathcal{T},\, S\cap\Gamma_\mathrm{D} \neq \emptyset} h_S^2 ||\nabla w||^2_{L^2(S)} \le C \|h_\mathcal{F}||^2_{L^\infty(\Gamma_\mathrm{D})} ||\nabla w||^2_{L^2(\Omega)}.$$

A proof for the second estimate in (ii) then follows from (2.4) with e replaced by w. □

5. Error control for the computation of Λ in (2.2)

This section discusses practical realizations of (2.2). For more details on the approximation of eigenvalue problems we refer the reader to [2, 16]. Given $t \in [0,T]$ we set

$$-\lambda(t) := \inf_{0\neq v\in Y} \frac{(\nabla v;\nabla v) + \varepsilon^{-2}\big(f'(U(t))v;v\big)}{||v||^2_{L^2(\Omega)}}. \tag{5.1}$$

We remark that a minimizing w in (5.1) exists and satisfies for all $v \in Y$

$$(\nabla w;\nabla v) + \varepsilon^{-2}\big(f'(U(t))w;v\big) = -\lambda(t)(w;v). \tag{5.2}$$

Let $P_{\lambda(t)}$ denote the L^2 projection onto the subspace of all $w \in Y$ that satisfy (5.2). The following lemma states an abstract version of (2.2) under the assumption that an approximation of a minimizer in (5.2) is not L^2-orthogonal to the exact eigenspace.

Lemma 5.1 ([16])**.** *Let $(W,\Lambda) \in Y \times \mathbb{R}$ satisfy $(W; P_{\lambda(t)}W) \neq 0$ and let $r_{W,\Lambda} \in Y'$ be such that*

$$\langle r_{W;\Lambda}; v\rangle = -\Lambda(W;v) - (\nabla W;\nabla v) - \varepsilon^{-2}\big(f'(U(t))W;v\big)$$

for all $v \in Y$. Then there holds

$$-\Lambda - \frac{\langle r_{W,\Lambda}; P_{\lambda(t)}W\rangle}{(W;P_{\lambda(t)}W)} = -\lambda(t).$$

Proof. Abbreviate $p := \varepsilon^{-2} f'(U(t))$ and $w := P_{\lambda(t)}W$. There holds

$$(w;W)\big(\lambda(t)-\Lambda\big) = -(\nabla w;\nabla W) - (pw;W) + (\nabla W;\nabla w) + (pW;w) + \langle r_{W,\Lambda};w\rangle = \langle r_{W,\Lambda};w\rangle$$

which proves the lemma. □

We derive computable upper bounds for the residual $r_{W,\Lambda}$ in Lemma 5.1 for the case that (W,Λ) is obtained from the following lowest order finite element scheme.

$$\big(\mathfrak{EV}_h^{(t)}\big) \quad \begin{cases} \text{Let } (W,\Lambda) \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T})^m \times \mathbb{R} \text{ satisfy } ||W||_{L^2(\Omega)} = 1 \text{ and for all } V \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T})^m \\ (\nabla W;\nabla V) + \varepsilon^{-2}\big(f'(U(t))W;V\big) = \Lambda(W;V). \end{cases}$$

The nonlinear problem $\big(\mathfrak{EV}_h^{(t)}\big)$ can be recast as: Find $(x,\Lambda) \in \mathbb{R}^\ell \times \mathbb{R}$ such that $Ax = \Lambda Bx$ and $x\cdot(Bx) = 1$. Since we may introduce a constant shift, i.e., a term $\varepsilon^{-2}||f'(U(t))||_{L^\infty(\Omega)}(W;V)$ in the left-hand side of the equation in $\big(\mathfrak{EV}_h^{(t)}\big)$, we may assume that A and B are positive definite. A solution (x,Λ) can then be obtained from classical vector iterations.

Lemma 5.2 ([16])**.** *Let $(W,\Lambda) \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T})^m \times \mathbb{R}$ solve $\big(\mathfrak{EV}_h^{(t)}\big)$ and assume that*

$$||W - P_{\lambda(t)}W||^2_{L^2(\Omega)} \le 1/2. \tag{5.3}$$

For $k = 1,2$ set

$$\tilde\eta^{(k)}_{\mathrm{EV}} := ||h^k_{\mathcal{T}}\big(\Delta_{\mathcal{T}}W - \varepsilon^{-2}f'(U(t))W + \Lambda W\big)||_{L^2(\Omega)} + ||h_{\mathcal{F}}^{k-1/2}[\nabla W\cdot n_{\mathcal{F}}]||_{L^2(\cup\mathcal{F})}.$$

Let $k \in \{1,2\}$ and suppose that $||D^2\phi||_{L^2(\Omega)} \le c_{2,0}||\Delta\phi||_{L^2(\Omega)}$ for all $\phi \in H^2(\Omega;\mathbb{R}^m)\cap Y$ if $k=2$. There holds

$$\frac{\langle r_{W,\Lambda}; P_{\lambda(t)}W\rangle}{(W;P_{\lambda(t)}W)} \le c_{\mathrm{EV}}\,\tilde\eta^{(k)}_{\mathrm{EV}} \times \begin{cases} (\varepsilon^{-2}||f'(U(t))||_{L^\infty(\Omega)} - \Lambda)^{1/2} & \text{for } k=1, \\ (2\varepsilon^{-2}||f'(U(t))||_{L^\infty(\Omega)} + c_Y) & \text{for } k=2, \end{cases}$$

where $c_Y := \inf_{0\neq v\in Y}\frac{||\nabla v||_{L^2(\Omega)}}{||v||_{L^2(\Omega)}}$ and $c_{\mathrm{EV}} > 0$ is an $(\varepsilon, h_{\mathcal{T}}, h_{\mathcal{F}})$-independent constant.

Proof. Abbreviate $p := \varepsilon^{-2} f'(U(t))$ and $w := P_{\lambda(t)} W$. Since $\langle r_{W,\Lambda}; V\rangle = 0$ for all $V \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T})^m$ there holds

$$\langle r_{W,\Lambda}; w\rangle = \langle r_{W,\Lambda}; w - V\rangle = -\Lambda(W; w - V) - (\nabla W; \nabla(w - V)) - (pW; w - V).$$

A $\mathcal{T}$-elementwise integration by parts and Hölder inequalities show for $k = 1$ and $k = 2$,

$$\langle r_{W,\Lambda}; w\rangle \le \sum_{S\in\mathcal{T}} ||h_{\mathcal{T}}^k(-\Delta_{\mathcal{T}} W + pW + \Lambda W)||_{L^2(S)} ||h_{\mathcal{T}}^{-k}(w - V)||_{L^2(S)} \\ + \sum_{F\in\mathcal{F}} ||h_{\mathcal{F}}^{k-1/2}[\nabla W \cdot n_{\mathcal{F}}]||_{L^2(F)} ||h_{\mathcal{F}}^{1/2-k}(w - V)||_{L^2(F)}.$$

Let V be the Clément interpolant of w if $k = 1$ and its nodal interpolant if $k = 2$. Standard estimates imply with an $(\varepsilon, h_{\mathcal{T}}, h_{\mathcal{F}})$-independent constant $C > 0$

$$\langle r_{W,\Lambda}; w\rangle \le C\big(||h_{\mathcal{T}}^k(\Delta_{\mathcal{T}} W - pW + \Lambda W)||_{L^2(\Omega)} + ||h_{\mathcal{F}}^{k-1/2}[\nabla W \cdot n_{\mathcal{F}}]||_{L^2(\mathcal{F})}\big) ||D^k w||_{L^2(\Omega)}.$$

Notice that $W \in Y$ so that $-\lambda(t) \le -\Lambda$. Since $||w||_{L^2(\Omega)} \le ||W||_{L^2(\Omega)} = 1$ we have

$$||Dw||^2_{L^2(\Omega)} = ||\nabla w||^2_{L^2(\Omega)} = -\lambda(t)(w; w) - (pw; w) \le -\Lambda + ||p||_{L^\infty(\Omega)}. \tag{5.4}$$

If $k = 2$ then we have

$$||D^2 w||_{L^2(\Omega)} \le c_{2,0} ||\Delta w||_{L^2(\Omega)} \le c_{2,0} ||(\lambda + p) w||_{L^2(\Omega)} \le c_{2,0}\big(|\lambda| + ||p||_{L^\infty(\Omega)}\big). \tag{5.5}$$

We estimate $|\lambda|$ in the right-hand side by noting that

$$-||p||_{L^\infty(\Omega)} \le -\lambda(t) \le c_Y + ||p||_{L^\infty(\Omega)}.$$

Since $||W - w||^2_{L^2(\Omega)} \le 1/2$ and $||W||^2_{L^2(\Omega)} = 1$ we have

$$2(w; W) = ||w||^2_{L^2(\Omega)} + ||W||^2_{L^2(\Omega)} - ||w - W||^2_{L^2(\Omega)} \ge 1/2,$$

and the combination of the estimates with Lemma 5.1 concludes the proof of the lemma. □

Remark. *If $n = 2$, Ω is convex, and $\Gamma_{\mathrm{D}} = \partial\Omega$ then there exists a constant $c_{2,0} > 0$ such that $||D^2\phi||_{L^2(\Omega)} \le c_{2,0} ||\Delta\phi||_{L^2(\Omega)}$ for all $\phi \in H^2(\Omega; \mathbb{R}^m) \cap Y$, cf.* [12].

The following proposition shows that if U is piecewise affine in $[0, T]$ then it suffices to approximate λ at a finite number of times.

Proposition 5.3. *Let $0 \le t_j < t < t_{j+1} \le T$ be such that $t = t_j + \theta(t_{j+1} - t_j)$ for some $\theta \in (0, 1)$ and assume that $U(t) = (1 - \theta)U(t_j) + \theta U(t_{j+1})$. We then have*

$$-(1 - \theta)\lambda(t_j) - \theta\lambda(t_{j+1}) - \frac{5}{4}\varepsilon^{-2} ||U(t_j) - U(t_{j+1})||^2_{L^\infty(\Omega)} \le -\lambda(t).$$

Proof. For all $v \in Y$ there holds

$$\begin{aligned}
&(1 - \theta)\big((\nabla v; \nabla v) + (f'(U(t_j))v; v)\big) + \theta\big((\nabla v; \nabla v) + (f'(U(t_{j+1}))v; v)\big) \\
&\quad = (\nabla v; \nabla v) + \big(f'(U(t))v; v\big) + \big([(1 - \theta)f'(U(t_j)) + \theta f'(U(t_{j+1})) - f'(U(t))]v; v\big) \\
&\quad \le (\nabla v; \nabla v) + \big(f'(U(t))v; v\big) + ||(1 - \theta)f'(U(t_j)) + \theta f'(U(t_{j+1})) - f'(U(t))||_{L^\infty(\Omega)} (v; v)
\end{aligned}$$

so that

$$(1 - \theta)(-\lambda(t_j)) + \theta(-\lambda(t_{j+1})) \le -\lambda(t) + ||(1 - \theta)f'(U(t_j)) + \theta f'(U(t_{j+1})) - f'(U(t))||_{L^\infty(\Omega)}.$$

Therefore, it suffices to verify that

$$||(1-\theta)f'(U(t_j))+\theta f'(U(t_{j+1}))-f'(U(t))||_{L^\infty(\Omega)} \le \frac{5}{4}||U(t_j)-U(t_{j+1})||^2_{L^\infty(\Omega)}.$$

Taylor expansions of the quadratic function f' show for $a,b\in\mathbb{R}^m$

$$\begin{aligned}f'((1-\theta)a+\theta b) &= (1-\theta)f'(a+\theta(b-a))+\theta f'(b-(1-\theta)(b-a))\\ &= (1-\theta)f'(a)+\theta f'(b)+(1-\theta)\theta(f''(a)-f''(b))(b-a)/2\\ &\quad+(1-\theta)\theta\big(\theta f'''(a)(b-a,b-a)+(1-\theta)f'''(b)(b-a,b-a)\big)/6.\end{aligned}$$

This, explicit formula for f'' and f''', and the estimate $\theta(1-\theta)\le 1/4$ imply the assertion. $\square$

Given any $W\in\mathcal{S}^1_{\rm D}(\mathcal{T})^m$ with $||W||_{L^2(\Omega)}=1$ there holds $||W-P_{\lambda(t)}W||^2_{L^2(\Omega)}\le 2$. Therefore, the assumption (5.3) does not seem to be restrictive. Since it is however not clear how to verify it in practice we include an explicit a priori error estimate for the difference $\lambda(t)-\Lambda$ in case that the Laplace operator is H^2 regular in Ω. We let $c_{\mathcal{I}_\mathcal{T}}$ be the smallest constant such that for all $\phi\in H^2(\Omega;\mathbb{R}^m)\cap Y$ there holds

$$||\phi-\mathcal{I}_\mathcal{T}\phi||_{L^2(\Omega)}+h||\nabla(\phi-\mathcal{I}_\mathcal{T}\phi)||_{L^2(\Omega)}\le c_{\mathcal{I}_\mathcal{T}}h^2||D^2\phi||_{L^2(\Omega)},$$

where $h:=||h_\mathcal{T}||_{L^\infty(\Omega)}$.

Lemma 5.4. *Suppose that there exists a constant* $c_{2,0}>0$ *such that* $||D^2\phi||_{L^2(\Omega)}\le c_{2,0}||\Delta\phi||_{L^2(\Omega)}$ *for all* $v\in Y\cap H^2(\Omega;\mathbb{R}^m)$. *Let* $(W,\Lambda)\in\mathcal{S}^1_0(\mathcal{T})^m\times\mathbb{R}$ *solve* $\big(\mathfrak{EV}^{(t)}_h\big)$ *and assume that*

$$c_{\mathcal{I}_\mathcal{T}}c_{2,0}(c_Y+2\varepsilon^{-2}||f'(U(t))||_{L^\infty(\Omega)})\,h^2\le 1/2.$$

Then there holds

$$0\le\lambda(t)-\Lambda\le c_9\big(c_Y+2\varepsilon^{-2}||f'(U(t))||_{L^\infty(\Omega)}\big)^{3/2}\,h,$$

where the constant $c_9>0$ *only depends on* $c_{\mathcal{I}_\mathcal{T}}$ *and* $c_{2,0}$.

Proof. Throughout this proof C denotes a generic (ε,h)-independent constant. Let $w\in Y$ satisfy (5.2) and $||w||_{L^2(\Omega)}=1$. We abbreviate $\lambda:=\lambda(t)$ and $p:=\varepsilon^{-2}f'(U(t))$ and define $q:=p+||p||_{L^\infty(\Omega)}I_m$ where I_m is the identity matrix in $\mathbb{R}^{m\times m}$. Then $q\in L^\infty(\Omega;\mathbb{R}^{m\times m})$ is positive definite and symmetric almost everywhere in Ω. Since W is minimal for

$$V\mapsto(\nabla V;\nabla V)+(pV;V)$$

among all $V\in\mathcal{S}^1_{\rm D}(\mathcal{T})^m$ with $||V||_{L^2(\Omega)}=1$ there holds for all such V

$$\begin{aligned}0\le\lambda-\Lambda &\le -||\nabla w||^2_{L^2(\Omega)}-||p^{1/2}w||^2_{L^2(\Omega)}+||\nabla V||^2_{L^2(\Omega)}+||p^{1/2}V||^2_{L^2(\Omega)}\\ &= -||\nabla w||^2_{L^2(\Omega)}-||q^{1/2}w||^2_{L^2(\Omega)}+||\nabla V||^2_{L^2(\Omega)}+||q^{1/2}V||^2_{L^2(\Omega)}\\ &\le 2\big(\nabla V;\nabla(V-w)\big)+2(qV;V-w)\\ &\le 2\big(||\nabla V||^2_{L^2(\Omega)}+||q^{1/2}V||^2_{L^2(\Omega)}\big)^{1/2}\big(||\nabla(V-w)||^2_{L^2(\Omega)}+||q^{1/2}(V-w)||^2_{L^2(\Omega)}\big)^{1/2}.\end{aligned}$$

Let $\tilde W:=\mathcal{I}_\mathcal{T}w$. The estimate (cf. (5.5))

$$||D^2w||_{L^2(\Omega)}\le c_{2,0}||\Delta w||_{L^2(\Omega)}\le c_{2,0}(c_Y+2||p||_{L^\infty(\Omega)})=:c_{2,0}\gamma$$

and the assumption on h imply

$$\big|1-||\tilde W||_{L^2(\Omega)}\big|=\big|||w||_{L^2(\Omega)}-||\tilde W||_{L^2(\Omega)}\big|\le||w-\tilde W||_{L^2(\Omega)}\le c_{\mathcal{I}_\mathcal{T}}c_{2,0}\gamma h^2\le 1/2$$

and hence $||\tilde{W}||_{L^2(\Omega)} \geq 1/2$. Set $V := \tilde{W}/||\tilde{W}||_{L^2(\Omega)}$. Employing the estimate (cf. (5.4))

$$||\nabla w||_{L^2(\Omega)} \leq \gamma^{1/2}$$

and using that by assumption on h there holds $\gamma^{1/2}h + \gamma h^2 \leq C$, we deduce that

$$\begin{aligned}
||\nabla(V-w)||_{L^2(\Omega)} &\leq \frac{\big|1-||\tilde{W}||_{L^2(\Omega)}\big|}{||\tilde{W}||_{L^2(\Omega)}}||\nabla\tilde{W}||_{L^2(\Omega)} + ||\nabla(\tilde{W}-w)||_{L^2(\Omega)} \\
&\leq 2c_{\mathcal{I}_\mathcal{T}}c_{2,0}\gamma h^2||\nabla\tilde{W}||_{L^2(\Omega)} + ||\nabla(\tilde{W}-w)||_{L^2(\Omega)} \\
&\leq 2c_{\mathcal{I}_\mathcal{T}}c_{2,0}\gamma h^2||\nabla w||_{L^2(\Omega)} + (1+2c_{\mathcal{I}_\mathcal{T}}c_{2,0}\gamma h^2)||\nabla(\tilde{W}-w)||_{L^2(\Omega)} \\
&\leq 2c_{\mathcal{I}_\mathcal{T}}c_{2,0}\gamma^{3/2}h^2 + (1+2c_{\mathcal{I}_\mathcal{T}}c_{2,0}\gamma h^2)c_{\mathcal{I}_\mathcal{T}}c_{2,0}\gamma h \leq C\gamma h.
\end{aligned}$$

and

$$||\nabla V||_{L^2(\Omega)} \leq ||\nabla(V-w)||_{L^2(\Omega)} + ||\nabla w||_{L^2(\Omega)} \leq C\gamma h + \gamma^{1/2} \leq C\gamma^{1/2}.$$

Similarly, there holds

$$\begin{aligned}
||q^{1/2}(V-w)||_{L^2(\Omega)} &\leq \frac{\big|1-||\tilde{W}||_{L^2(\Omega)}\big|}{||\tilde{W}||_{L^2(\Omega)}}||q^{1/2}\tilde{W}||_{L^2(\Omega)} + ||q^{1/2}(\tilde{W}-w)||_{L^2(\Omega)} \\
&\leq c_{\mathcal{I}_\mathcal{T}}c_{2,0}\gamma h^2||q^{1/2}||_{L^\infty(\Omega)} + ||q^{1/2}||_{L^\infty(\Omega)}c_{\mathcal{I}_\mathcal{T}}c_{2,0}\gamma h^2 \\
&\leq C\gamma h^2||q^{1/2}||_{L^\infty(\Omega)}
\end{aligned}$$

and

$$||q^{1/2}V||_{L^2(\Omega)} \leq ||q^{1/2}(V-w)||_{L^2(\Omega)} + ||q^{1/2}w||_{L^2(\Omega)} \leq ||q^{1/2}||_{L^\infty(\Omega)}\big(C\gamma h^2+1\big) \leq C||q^{1/2}||_{L^\infty(\Omega)}.$$

A combination of the estimates with $||q^{1/2}||^2_{L^\infty(\Omega)} \leq C\gamma$ results in

$$0 \leq \lambda - \Lambda \leq Ch\gamma^{1/2}(||q^{1/2}||^2_{L^\infty(\Omega)} + \gamma) \leq Ch\gamma^{3/2}$$

which proves the lemma. □

6. Approximation of $(\mathfrak{P})$ and estimation of $||\mathcal{R}_U||_{Y'}$ in (2.6)

In this section we derive a computable upper bound for the residual $\mathcal{R}_U$ for a semi-implicit finite difference in time and finite element in space discretization of $(\mathfrak{P})$ with a linearized treatment of the nonlinear term. We follow the argumentation of [14].

$(\mathfrak{P}_{\tau,h})$ *Given $0 = t_0 < t_1 < ... < t_N = T$, regular triangulations $\mathcal{T}_0, \mathcal{T}_1, ..., \mathcal{T}_N$ of Ω, $U_0 \in \mathcal{S}^1(\mathcal{T}_0)^m$, set $\tau_j := t_j - t_{j-1}$ for $j = 1, 2, ..., N$. For $j = 1, 2, ..., N$ and for all $V \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_j)^m$ let $U_j \in \mathcal{S}^1(\mathcal{T}_j)^m$ satisfy*

$$\begin{aligned}
&\tau_j^{-1}(U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}; V) + (\nabla U_j; \nabla V) \\
&\qquad + \varepsilon^{-2}\big(f(\mathcal{I}_{\mathcal{T}_j}U_{j-1}) + f'(\mathcal{I}_{\mathcal{T}_j}U_{j-1})(U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}); V\big) = 0, \\
&\qquad\qquad U_j|_{\Gamma_\mathrm{D}} = U_0|_{\Gamma_\mathrm{D}}.
\end{aligned}$$

Given $1 \leq j \leq N$ and some $U_{j-1} \in \mathcal{S}^1(\mathcal{T}_{j-1})^m$, existence of a unique solution $U_j \in \mathcal{S}^1(\mathcal{T}_j)^m$ of the first equation in $(\mathfrak{P}_{\tau,h})$ is guaranteed if $\tau_j \leq \varepsilon^2||f'(\mathcal{I}_{\mathcal{T}_j}U_{j-1})||^{-1}_{L^\infty(\Omega)}$. A function $U \in Z \cap L^\infty(0,T;L^\infty(\Omega;\mathbb{R}^m))$ is defined through a sequence $(U_j : j = 0, 1, ..., N) \subseteq H^1(\Omega;\mathbb{R}^m)$ by setting, for $s \in [t_{j-1}, t_j]$ for $1 \leq j \leq N$ and $\theta \in [0,1]$ such that $s = t_{j-1} + \theta(t_j - t_{j-1})$,

$$U(s) := U(t_{j-1}) + \theta\big(U(t_j) - U(t_{j-1})\big). \tag{6.1}$$

For an approximation of u resulting from the solution of $(\mathfrak{P}_{\tau,h})$ and a subsequent linear interpolation in time, the residual $\mathcal{R}_U$ can be estimated by fully computable quantities. The combination of the next lemma with the estimates for $\eta_{\rm D}$ and $||w||_{L^2(\Omega)}$ in Lemma 4.1 leads to a computable η in (2.6).

Lemma 6.1. *Let $U \in Z \cap L^\infty(0,T;L^\infty(\Omega;\mathbb{R}^m))$ be defined through a solution $(U_j : j = 0,1,...,N)$ of $(\mathfrak{P}_{\tau,h})$ and* (6.1)*. There holds*

$$\int_0^T ||\mathcal{R}_U||_{Y'}^2 \,{\rm d}s \le \sum_{j=1}^N \tau_j \big(c_{\rm Cl}\,\eta_{\rm h}^{(j)} + \eta_{\rm t}^{(j)} + \eta_{\rm c}^{(j)} + \eta_\ell^{(j)}\big)^2,$$

where for $j = 1,2,...,N$,

$$\begin{aligned}
\eta_{\rm h}^{(j)} &:= \big\|h_{\mathcal{T}_j}\Big(\big(\tau_j^{-1} + \varepsilon^{-2} f'(\mathcal{I}_{\mathcal{T}_j}U_{j-1})\big)(U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}) - \Delta_{\mathcal{T}_j}U_j + \varepsilon^{-2} f(\mathcal{I}_{\mathcal{T}_j}U_{j-1})\Big)\big\|_{L^2(\Omega)} \\
&\qquad + ||h_{\mathcal{F}_j}^{1/2}[\nabla U_j \cdot n_{\mathcal{F}_j}]||_{L^2(\cup\mathcal{F}_j)}, \\
\eta_{\rm t}^{(j)} &:= ||\nabla(U_{j-1} - U_j)||_{L^2(\Omega)} + \varepsilon^{-2}\Big(||f'(U_j)||_{L^\infty(\Omega)}||U_{j-1} - U_j||_{L^2(\Omega)} \\
&\qquad + \frac{1}{2}||f''(U_j)||_{L^\infty(\Omega)}||U_{j-1} - U_j||_{L^4(\Omega)}^2 + \frac{1}{6}||f'''(U_j)||_{L^\infty(\Omega)}||U_{j-1} - U_j||_{L^6(\Omega)}^3\Big), \\
\eta_{\rm c}^{(j)} &:= \tau_j^{-1}||\mathcal{I}_{\mathcal{T}_j}U_{j-1} - U_{j-1}||_{L^2(\Omega)}, \\
\eta_\ell^{(j)} &:= \varepsilon^{-2}\Big(\frac{1}{2}||f''(\mathcal{I}_{\mathcal{T}_j}U_{j-1})||_{L^\infty(\Omega)}||U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}||_{L^4(\Omega)}^2 \\
&\qquad + \frac{1}{6}||f'''(\mathcal{I}_{\mathcal{T}_j}U_{j-1})||_{L^\infty(\Omega)}||U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}||_{L^6(\Omega)}^3\Big),
\end{aligned}$$

and $c_{\rm Cl} > 0$ is an $(\varepsilon, h_{\mathcal{T}_j}, h_{\mathcal{F}_j})$-independent constant.

Proof. For almost all $s \in (t_{j-1}, t_j)$ and all $v \in Y$ there holds

$$\begin{aligned}
\langle \mathcal{R}_U(s); v\rangle &= \tau_j^{-1}(U_j - U_{j-1}; v) + (\nabla U(s); \nabla v) + \varepsilon^{-2}(f(U); v) \\
&= \tau_j^{-1}\big(U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}; v\big) + (\nabla U_j; \nabla v) \\
&\quad + \varepsilon^{-2}(f(\mathcal{I}_{\mathcal{T}_j}U_{j-1}); v) + \varepsilon^{-2}\big(f'(\mathcal{I}_{\mathcal{T}_j}U_{j-1}))(U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}); v\big) \\
&\quad + \big(\nabla(U(s) - U_j); \nabla v\big) + \varepsilon^{-2}\big(f(U(s)) - f(U_j); v\big) \\
&\quad + \tau_j^{-1}(\mathcal{I}_{\mathcal{T}_j}U_{j-1} - U_{j-1}; v) \\
&\quad + \varepsilon^{-2}\big(f(U_j) - f(\mathcal{I}_{\mathcal{T}_j}U_{j-1}) - f'(\mathcal{I}_{\mathcal{T}_j}U_{j-1})(U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}); v\big).
\end{aligned}$$

Let $\langle r_{\rm h}; v\rangle$ be defined by the first four terms, $\langle r_{\rm t}; v\rangle$ by the fifth and sixth term, $\langle r_{\rm c}; v\rangle$ by the seventh term, and $\langle r_\ell; v\rangle$ by the last two terms on the right-hand side of the equation. The first equation in $(\mathfrak{P}_{\tau,h})$ allows to insert the Clément interpolant $V \in \mathcal{S}^1_{\rm D}(\mathcal{T})^m$ of v in $\langle r_{\rm h}; v\rangle$. An elementwise integration by parts and standard estimates for $v - V$ yield

$$\langle r_{\rm h}; v\rangle = \langle r_{\rm h}; v - V\rangle \le c_{\rm Cl}\,\eta_{\rm h}^{(j)}||\nabla v||_{L^2(\Omega)}.$$

Hölder inequalities, a Taylor expansion of f about U_j, and linearity of U in s lead to

$$\begin{aligned}
\langle r_{\rm t}; v\rangle &\le ||\nabla(U(s) - U_j)||_{L^2(\Omega)}||\nabla v||_{L^2(\Omega)} + \varepsilon^{-2}\big(||f'(U_j)||_{L^\infty(\Omega)}||U(s) - U_j||_{L^2(\Omega)} \\
&\quad + \frac{1}{2}||f''(U_j)||_{L^\infty(\Omega)}||U(s) - U_j||_{L^4(\Omega)}^2 + \frac{1}{6}||f'''(U_j)||_{L^\infty(\Omega)}||U(s) - U_j||_{L^6(\Omega)}^3\big)||v||_{L^2(\Omega)} \\
&\le \eta_{\rm t}^{(j)}||v||_Y.
\end{aligned}$$

Hölder's inequality proves

$$\langle r_{\rm c}; v\rangle \le \tau_j^{-1}||\mathcal{I}_{\mathcal{T}_j}U_{j-1} - U_{j-1}||_{L^2(\Omega)}||v||_{L^2(\Omega)} = \eta_{\rm c}^{(j)}||v||_{L^2(\Omega)}.$$

A Taylor expansion of f about $\mathcal{I}_{\mathcal{T}_j}U_{j-1}$ gives

$$\langle r_\ell; v\rangle \le \varepsilon^{-2}\big(\frac{1}{2}||f''(\mathcal{I}_{\mathcal{T}_j}U_{j-1})||_{L^\infty(\Omega)}||U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}||^2_{L^4(\Omega)} + \frac{1}{6}||f'''(\mathcal{I}_{\mathcal{T}_j}U_{j-1})||_{L^\infty(\Omega)}||U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}||^3_{L^6(\Omega)}\big)||v||_{L^2(\Omega)} = \eta_\ell^{(j)}||v||_{L^2(\Omega)}.$$

The combination of the estimates proves the lemma. □

Remarks. *(i) The quantities $\eta_{\rm h}^{(j)}$, $\eta_{\rm t}^{(j)}$, $\eta_{\rm c}^{(j)}$, and $\eta_\ell^{(j)}$, $j = 1, 2, ..., N$, represent space discretization, time discretization, coarsening, and linearization residuals, respectively.*
(ii) A sharper version of Theorem 2.1 can be deduced from the observation in [14] *that*

$$\langle \mathcal{R}_U(s); v\rangle \le c_{\rm Cl}\,\eta_{\rm h}^{(j)}||\nabla v||_{L^2(\Omega)} + \big(\eta_{\rm t}^{(j)} + \eta_{\rm c}^{(j)} + \eta_\ell^{(j)}\big)||v||_{L^2(\Omega)}$$

where $s \in [t_{j-1}, t_j]$ and $v \in Y$. This estimate avoids an additional factor ε^{-2} for $\eta_{\rm t}^{(j)}$, $\eta_{\rm c}^{(j)}$, and $\eta_\ell^{(j)}$.
(iii) A presumably smaller coarsening estimator $\tilde\eta_{\rm c}^{(j)} = \tau_j^{-1}||h_{\mathcal{T}_j}(U_{j-1} - \Pi_{\mathcal{T}_j}U_{j-1})||_{L^2(\Omega)}$, where $\Pi_{\mathcal{T}_j}$ denotes the L^2 projection onto $\mathcal{S}^1(\mathcal{T}_j)^m$ subject to certain boundary conditions, than $\eta_{\rm c}^{(j)}$ can be obtained if $\mathcal{I}_{\mathcal{T}_j}$ is replaced by $\Pi_{\mathcal{T}_j}$ in $(\mathfrak{P}_{\tau,h})$.

7. Adaptive Algorithm

The error estimate of Theorem 2.1 and the local character of the computable quantities $\eta_{\rm D}$ and η allows for the definition of local refinement and coarsening indicators in space and time. The following algorithm follows ideas in [18] and aims to simultaneously solve $(\mathfrak{P}_{\tau,h})$ and automatically generate optimal time step sizes $\tau_1, \tau_2, ..., \tau_N$ and triangulations $\mathcal{T}_0, \mathcal{T}_1, ..., \mathcal{T}_N$ if $\Theta_{\rm h} = 1$ and $\Theta_{\rm t} = 1$. For $\Theta_{\rm h} = 0$ or $\Theta_{\rm t} = 0$ the algorithm employs the same triangulation $\mathcal{T}_j = \mathcal{T}_0$ for all $j = 1, 2, ..., N$ or the same time-step step size $\tau_j = \tau_1$ for all $j = 1, 2, ..., N$, respectively. Given $S \in \mathcal{T}_j$ we set

$$\eta_{\rm h}^{(j)}(S)^2 := \big\|h_{\mathcal{T}_j}\Big(\big(\tau_j^{-1} + \varepsilon^{-2}f'(\mathcal{I}_{\mathcal{T}_j}U_{j-1})\big)(U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}) - \Delta_{\mathcal{T}_j}U_j + \varepsilon^{-2}f(\mathcal{I}_{\mathcal{T}_j}U_{j-1})\Big)\big\|^2_{L^2(S)} + ||h_{\mathcal{F}_j}^{1/2}[\nabla U_j \cdot n_{\mathcal{F}_j}]||^2_{L^2(\partial S)}.$$

Adaptive Algorithm $(\mathcal{A}_{\Theta_{\rm h},\Theta_{\rm t}})$**.** Input: A regular triangulation $\mathcal{T}_0$ of Ω, an initial time step size $\tau_1 > 0$, and a termination criterion $\delta > 0$.

(a) Set $t_0 := 0$, $U_0 := \mathcal{I}_{\mathcal{T}_0}u_0$, and $j := 1$.
(b) Set $\mathcal{T}_j := \mathcal{T}_{j-1}$ and if $\Theta_{\rm t} = 1$ coarsen $\mathcal{T}_j$ so that $\eta_{\rm c}^{(j)} \le \delta$ and $\mathcal{T}_j|_{\Gamma_{\rm D}} = \mathcal{T}_{j-1}|_{\Gamma_{\rm D}}$.
(c) Set $t_j := \min\{t_{j-1} + \tau_j, T\}$ and compute $U_j \in \mathcal{S}^1(\mathcal{T}_j)^m$ such that $U_j|_{\Gamma_{\rm D}} = U_0|_{\Gamma_{\rm D}}$ and

$$\tau_j^{-1}(U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}; V) + (\nabla U_j; \nabla V) + \varepsilon^{-2}\big(f(\mathcal{I}_{\mathcal{T}_j}U_{j-1}) + f'(\mathcal{I}_{\mathcal{T}_j}U_{j-1})(U_j - \mathcal{I}_{\mathcal{T}_j}U_{j-1}); V\big) = 0$$

for all $V \in \mathcal{S}^1_{\rm D}(\mathcal{T}_j)^m$.
(c) If $\eta_{\rm t}^{(j)} > \delta$ and $\Theta_{\rm t} = 1$ set $\tau_j := \frac{1}{2}\tau_j$ and go to (b).

(d) If $\eta_{\mathrm{h}}^{(j)} > \varepsilon^2\delta$ and $\Theta_{\mathrm{h}} = 1$ then refine each $S \in \mathcal{T}_j$ for which $\eta_{\mathrm{h}}^{(j)}(S) \geq \frac{1}{2}\max_{S' \in \mathcal{T}_j} \eta_{\mathrm{h}}^{(j)}(S')$ to obtain a refined regular triangulation $\mathcal{T}_j$ and go to (c).
(e) Stop if $t_j = T$.
(f) Choose a regular triangulation $\hat{\mathcal{T}}$ of Ω.
 (i) Compute $(W, \Lambda^{(j)}) \in \mathcal{S}^1_{\mathrm{D}}(\hat{\mathcal{T}})^m \times \mathbb{R}$ such that $||W||_{L^2(\Omega)} = 1$ and

$$(\nabla W; \nabla V) + \varepsilon^{-2}\big(f'(U(t_j))W; V\big) = \Lambda^{(j)}(W; V)$$

 for all $V \in \mathcal{S}^1_{\mathrm{D}}(\hat{\mathcal{T}})^m$.
 (ii) If $\Theta_{\mathrm{t}} = 1$, $\Theta_{\mathrm{h}} = 1$ and $\eta_{\mathrm{EV}} \geq 1$ refine $\hat{\mathcal{T}}$ and go to (i).
(g) Set $j := j + 1$, $\tau_j := 2\tau_{j-1}$, and go to (b).

If $\mathcal{T}_0$ and U_0 are such that $||e(0)||_{L^2(\Omega)} \leq \delta$ and $||w||_{L^2(\Omega)} + \eta_{\mathrm{D}} \leq \delta$, if the algorithm terminates, and if $\delta \leq C\varepsilon^4$ then Theorem 2.1 implies

$$\operatorname{ess\,sup}_{s \in (0,T)} \frac{1}{2}||e(s)||_{L^2(\Omega)} + \varepsilon \int_0^T ||\nabla e||_{L^2(\Omega)} \,\mathrm{d}s \leq C\delta$$

provided that $\big(\Lambda^{(j)}\big)$ is uniformly bounded from above.

8. Numerical Experiments

In this section we discuss the practical applicability of the error estimate of Theorem 2.1 by specifying $(\mathfrak{P})$ through the following three examples.

Example 1 (Allen-Cahn equations)**.** *Given* $\varepsilon > 0$ *set* $n := 2$, $m := 1$, $\Omega := (-2, 2)^2$, $\Gamma_{\mathrm{D}} := \emptyset$, $T := 1$, *and for* $x \in \Omega$ *let*

$$u_0(x) := -\tanh\big((|x| - 1)/\varepsilon\big).$$

Example 2 (Ginzburg-Landau equations I)**.** *Given* $\varepsilon > 0$ *set* $n = m := 2$, $\Omega := (-1, 1)^2$, $\Gamma_{\mathrm{D}} := \partial\Omega$, $T := 5/2$, *and* $u_{\mathrm{D}} := \tilde{u}_{\mathrm{D}}|_{\partial\Omega}$ *for* $\tilde{u}_{\mathrm{D}}(x) := x/|x|$. *Set* $a := (1, 1)/4$ *and for* $x \in \Omega$ *let*

$$u_0(x) := \theta\big(\mathrm{dist}(x, \partial\Omega)\big)\tilde{u}_{\mathrm{D}}(x) + \big(1 - \theta\big(\mathrm{dist}(x, \partial\Omega)\big)\big)\frac{x - a}{\big(|x - a|^2 + \varepsilon^2\big)^{1/2}},$$

where $\theta(s) = 1 - 48s^2 + 128s^3$ *for* $s \leq 1/4$ *and* $\theta(s) = 0$ *for* $s \geq 1/4$.

Example 3 (Ginzburg-Landau equations II)**.** *Given* $\varepsilon > 0$ *set* $n = m := 2$, $\Omega := (-1, 1)^2$, $\Gamma_{\mathrm{D}} := \partial\Omega$, *and* $T := 1$. *We identify* $\mathbb{R}^2$ *with the complex plane, define for* $x \in \Omega$

$$u_0(x) := \frac{x^2}{|x|^2 + \varepsilon^2},$$

and set $u_{\mathrm{D}} := u_0|_{\partial\Omega}$.

Algorithm $(\mathcal{A}_{\Theta_{\mathrm{h}},\Theta_{\mathrm{t}}})$ was implemented in Matlab with a direct solution of linear systems of equations and an assemblation of stiffness matrices in C. The adaptive refinement strategy was realized by standard bisection approaches and the mesh coarsening was achieved as follows: given a (locally refined) triangulation $\mathcal{T}_f$, $U \in \mathcal{S}^1(\mathcal{T}_f)$, $\delta > 0$, and a coarse triangulation $\mathcal{T}_c$, locally refine $\mathcal{T}_c$ until $||\mathcal{I}_{\mathcal{T}}U - U||_{L^2(\Omega)} \leq \delta$. This approach may be suboptimal but worked reliably in practice. In all the experiments reported below, the overall CPU time (on a node of a Compaq SC-Cluster with four Alpha-EV68 processors (1 GHz, 8 MB Cache/CPU) and 32 GB RAM) of Algorithm $(\mathcal{A}_{\Theta_{\rm h},\Theta_{\rm t}})$ was at most one week.

8.1. **Validity and failure of a uniform upper bound for Λ in (2.2).** The following numerical experiments reveal practical limitations of the error estimate of Theorem 2.1 in the sense that Λ may not be uniformly bounded from above ε-independently if critical topological effects occur.

We ran Algorithm $(\mathcal{A}_{0,0})$ in Example 1 for $\varepsilon = 1/4, 1/8, 1/16$, initial uniform triangulations $\mathcal{T}_0$ of $\Omega = (-2, 2)^2$ with maximal meshsizes $h = 1/8, 1/16, 1/32$, respectively, and with $\tau_1 := \varepsilon^4$. Figure 1 shows the numerical solution $U(t)$ for $\varepsilon = 1/8$ and $t = 0.0488,\ 0.2930,\ 0.3906,\ 0.4639$. We observe that the phases $U \approx 1$ and $U \approx -1$ are separated by a sharp interface, that the region in which $U \approx 1$ becomes smaller and that the interface finally collapses for $t \approx 0.48$. Figure 2 displays for $\varepsilon = 1/4, 1/8, 1/16$ the eigenvalues Λ_j computed in step (f) of Algorithm $(\mathcal{A}_{\Theta_{\rm h},\Theta_{\rm t}})$ with $\hat{\mathcal{T}} = \mathcal{T}_0$ as functions of $t \in [0, 1]$. The eigenvalues are uniformly bounded for $t \le 0.3$ and grow proportionally to ε^{-2} for $t \in (0.3, 0.5)$. For $t \ge 0.5$ we see that Λ_j is bounded from above by 0, corresponding to the stable solution $u \equiv -1$. Theorem 2.1 may therefore be employed for $t \le 0.3$ provided that $\eta \le C\varepsilon^4$. In the region $t \in (0.3, 0.5)$ we would have to ensure that $\eta \le C/\exp(C'\varepsilon^{-2})$, which can only be expected to hold if h and τ_1 are unrealistically small, i.e., satisfy $h, \tau_1 \le C/\exp(C'\varepsilon^{-2})$.

We chose $\varepsilon = 1/4, 1/8, 1/16$, uniform triangulations $\mathcal{T}_0$ of $\Omega = (-1, 1)^2$ with maximal meshsizes $h = 1/8, 1/16, 1/32$, respectively, and $\tau_1 = \varepsilon^4$ in order to approximate $(\mathfrak{P})$ specified through Example 2 with Algorithm $(\mathcal{A}_{0,0})$. We see in Figure 5 that the vortex, initially located at $(1/2, 1/2)$, moves to the origin and the solution reaches a stable state. For all choices of ε we plotted the eigenvalues Λ_j as functions of $t \in [0, 2.5]$ in Figure 4. As in the previous experiment, the same triangulation $\hat{\mathcal{T}} = \mathcal{T}_0$ was used to compute Λ_j in each time step. In this example the eigenvalues are uniformly bounded from above by 3. This is in good agreement with theoretical results in [17] which state that degree-one vortices in Ginzburg-Landau equations are stable. Therefore, in this example Theorem 2.1 can be used in practice to control the discretization error.

A theoretical result in [4] states that higher degree vortices in Ginzburg-Landau equations are unstable. This is numerically confirmed by simulations for Example 3 where the function u_0 has a degree-2 vortex at the origin. The snapshots of the numerical solutions generated by Algorithm $(A_{0,0})$ for $\varepsilon = 1/8$, $h = 1/16$, and $\tau_1 = \varepsilon^4$, and displayed in Figure 5 for $t = 0, 0.1953, 0.3906, 0.5859$ show that the degree-2 vortex immediately splits into two degree one vortices which repulse each other and reach a steady state for $t \ge 1$. The computed eigenvalues Λ_j calculated in step (f) of Algorithm $(\mathcal{A}_{0,0})$ in Example 3 with $\varepsilon = 1/4, 1/8, 1/16$, uniform triangulations with maximal mesh-sizes $h = 1/8, 1/16, 1/32$, respectively, and $\tau_1 = \varepsilon^4$, are shown in Figure 6. We observe that the eigenvalues satisfy $\Lambda(t) \approx \varepsilon^{-2}$ for $t \le 0.3$ and are uniformly bounded from above when the two degree-one vortices are well-separated for $t \ge 0.3$.

8.2. **Performance of the automatic mesh refinement and coarsening strategy.** Figure 7 displays the triangulations $\mathcal{T}_j$ for $j = 0, 800, 1600$ automatically generated by Algorithm $(\mathcal{A}_{1,0})$ with an initial uniform triangulation $\mathcal{T}_0$ with maximal mesh-size $h = 1/16$ and a (uniform) time-step size $\tau_1 = \varepsilon^4$ in Example 1 with $\varepsilon = 1/8$. The algorithm efficiently resolves the interface of the numerical solution and employs a coarse mesh in the remaining part of Ω. Moreover, the refined region moves together with the interface towards the origin.

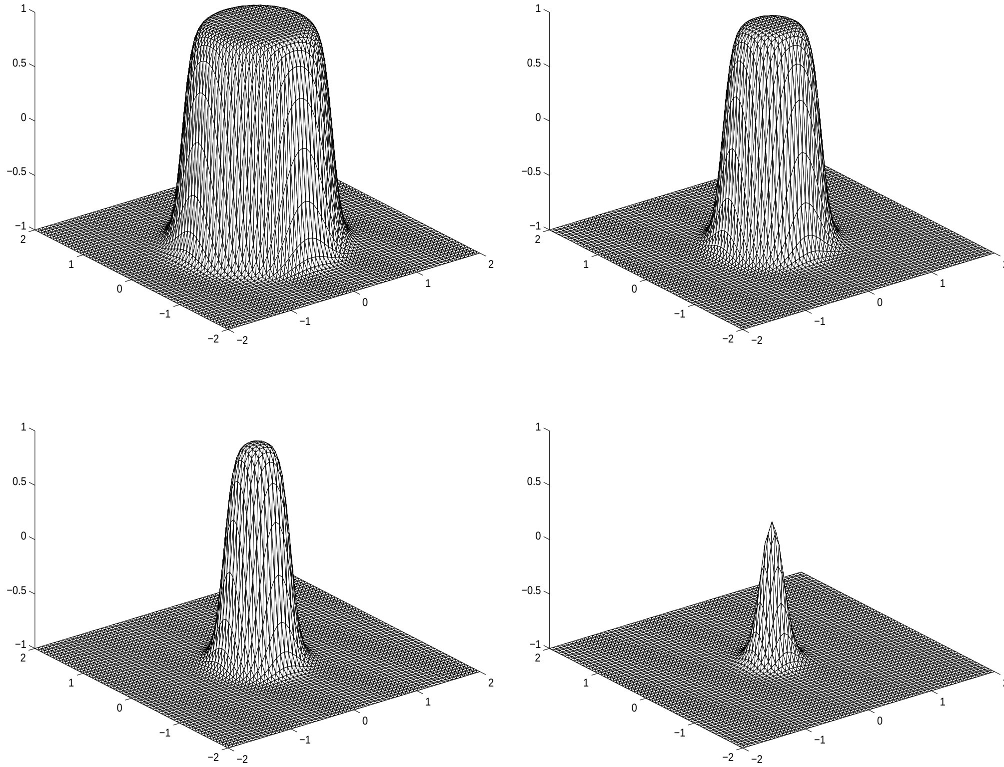

FIGURE 1. Numerical solution $U(t_j)$ for $j = 200, 1200, 1600, 1900$ in Example 1 with $\varepsilon = 1/8$. The zero level set of U is a circle which becomes smaller and vanishes for $t \approx 0.48$.

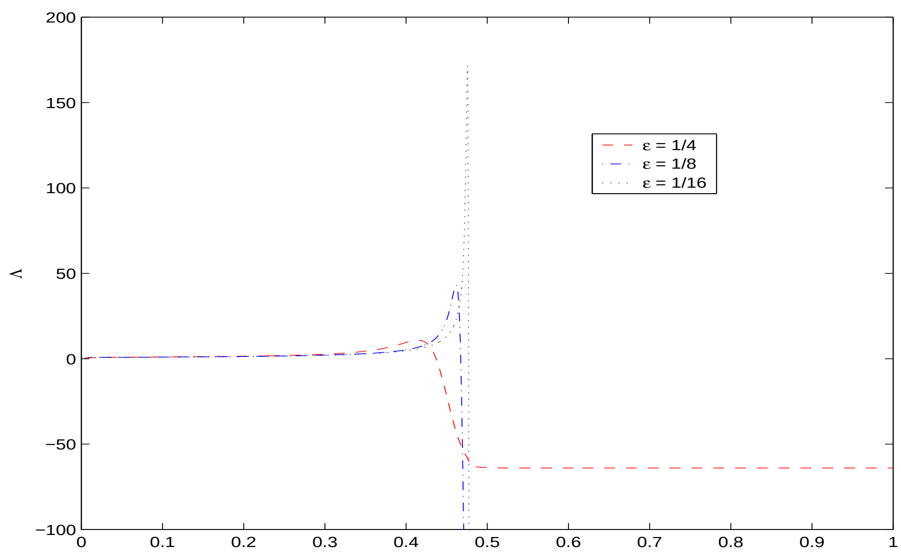

FIGURE 2. Computed eigenvalue Λ in Example 1. As the interface collapses Λ grows proportionally to ε^{-2}.

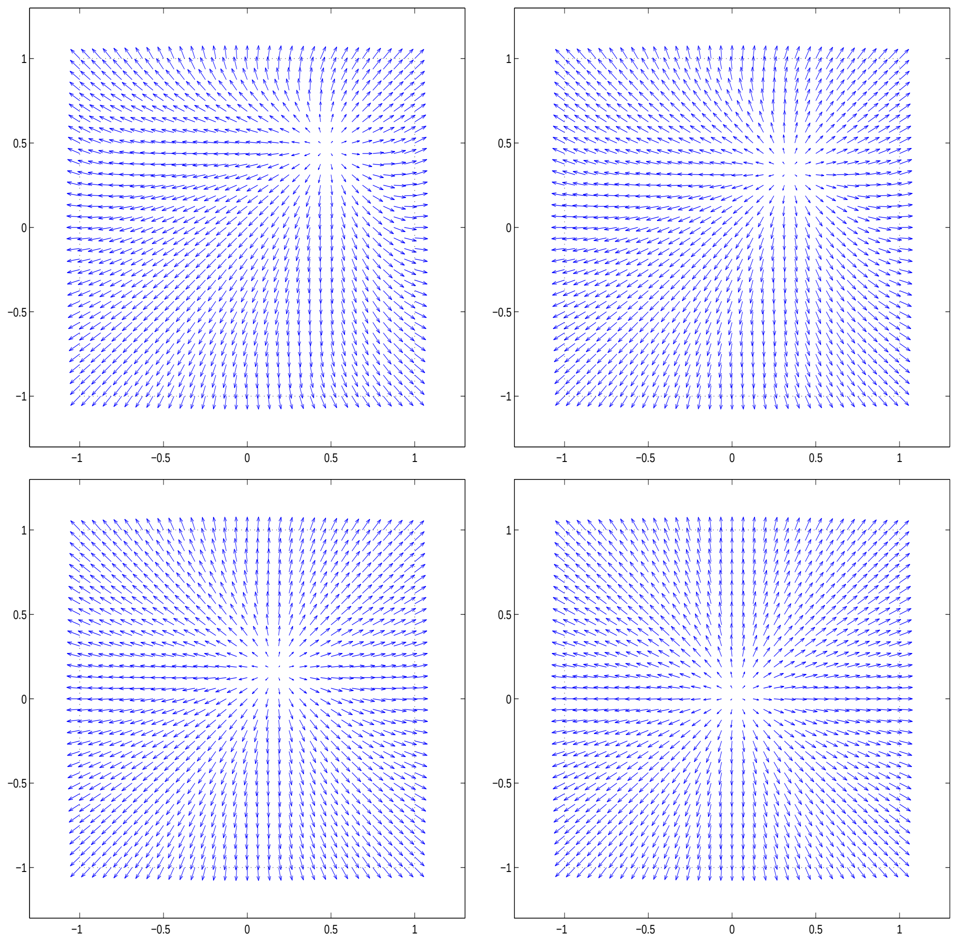

FIGURE 3. Numerical solution $U(t_j)$ for $j = 200, 1000, 3000, 10000$ in Example 2 with $\varepsilon = 1/8$. The vortex is initially located at $(1/2, 1/2)$ and moves to the origin.

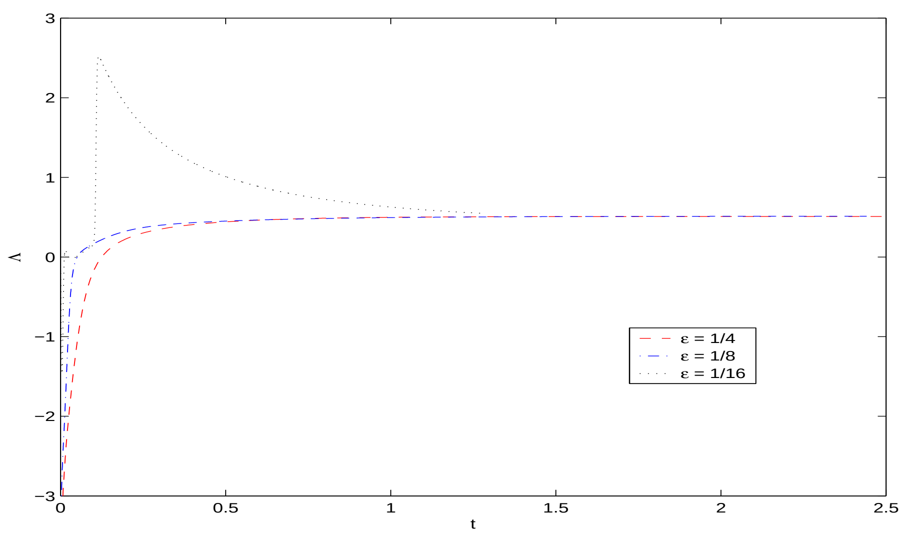

FIGURE 4. Computed eigenvalue Λ in Example 2. A uniform upper bound holds.

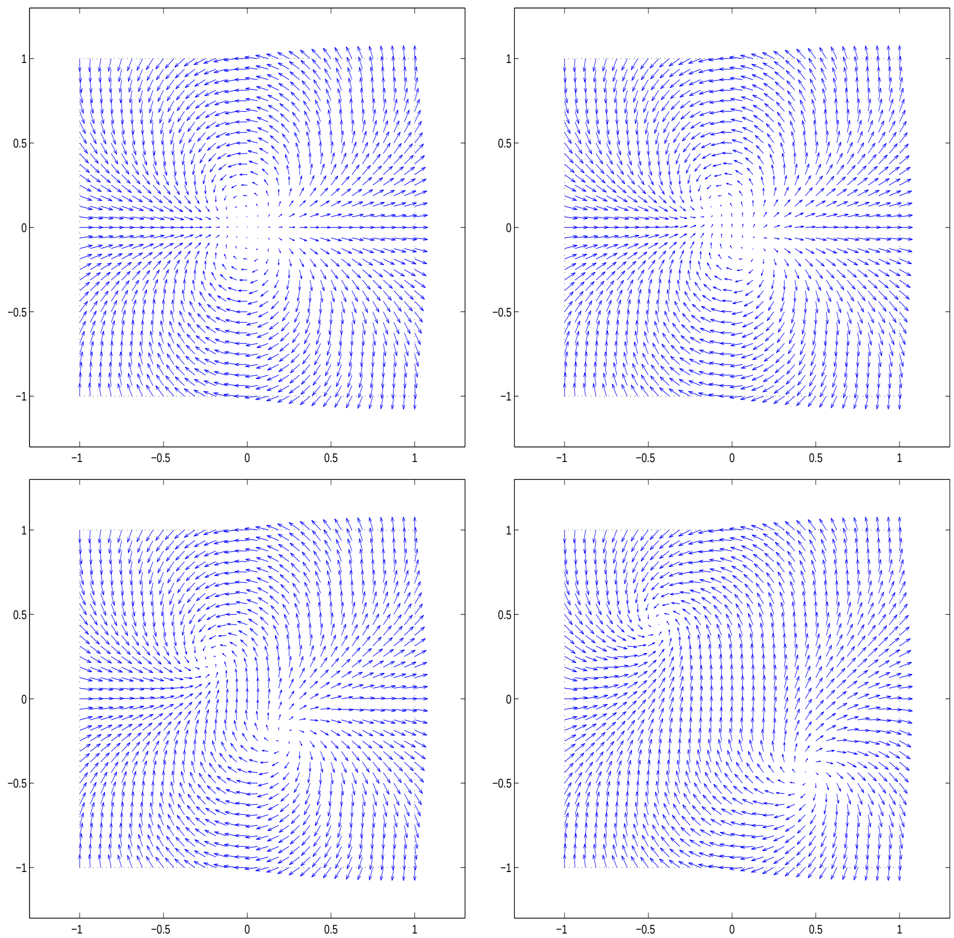

FIGURE 5. Numerical solution $U(t_j)$ for $j = 200, 500, 800, 2000$ in Example 3 with $\varepsilon = 1/8$. The initial degree-2 vortex splits into two degree-1 vortices.

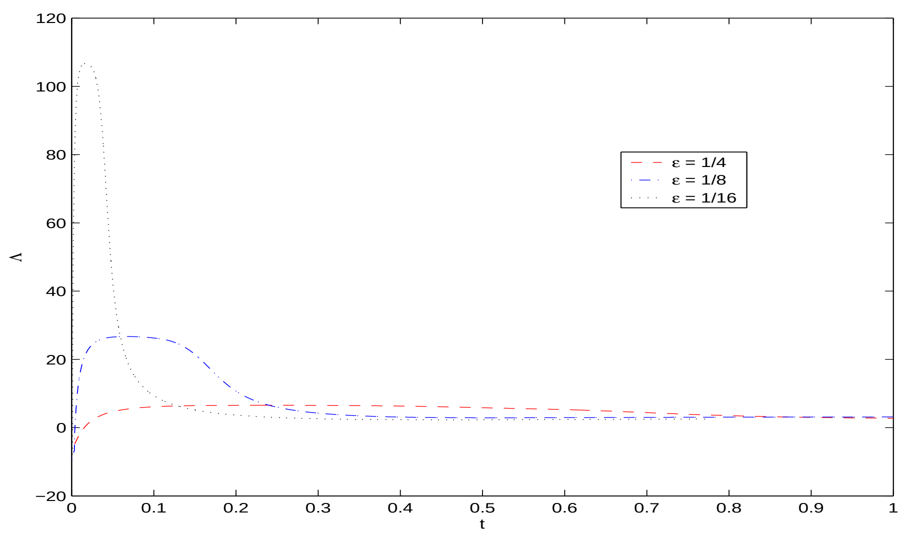

FIGURE 6. Computed eigenvalue Λ in Example 3. We observe a significant dependence on ε for $t \leq 0.3$ while a uniform upper bound for Λ holds once the two degree-1 vortices are well-separated.

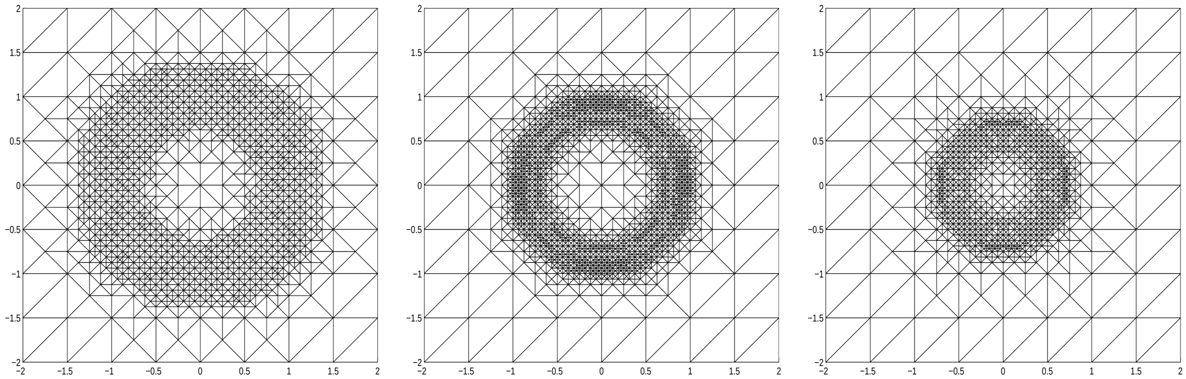

FIGURE 7. Adaptively refined and coarsened triangulations $\mathcal{T}_j$ for $j = 0, 800, 1600$ in Example 1 with $\varepsilon = 1/8$. An automatic refinement towards the zero level set of U and a coarsening in the remaining part of the domain are observable.

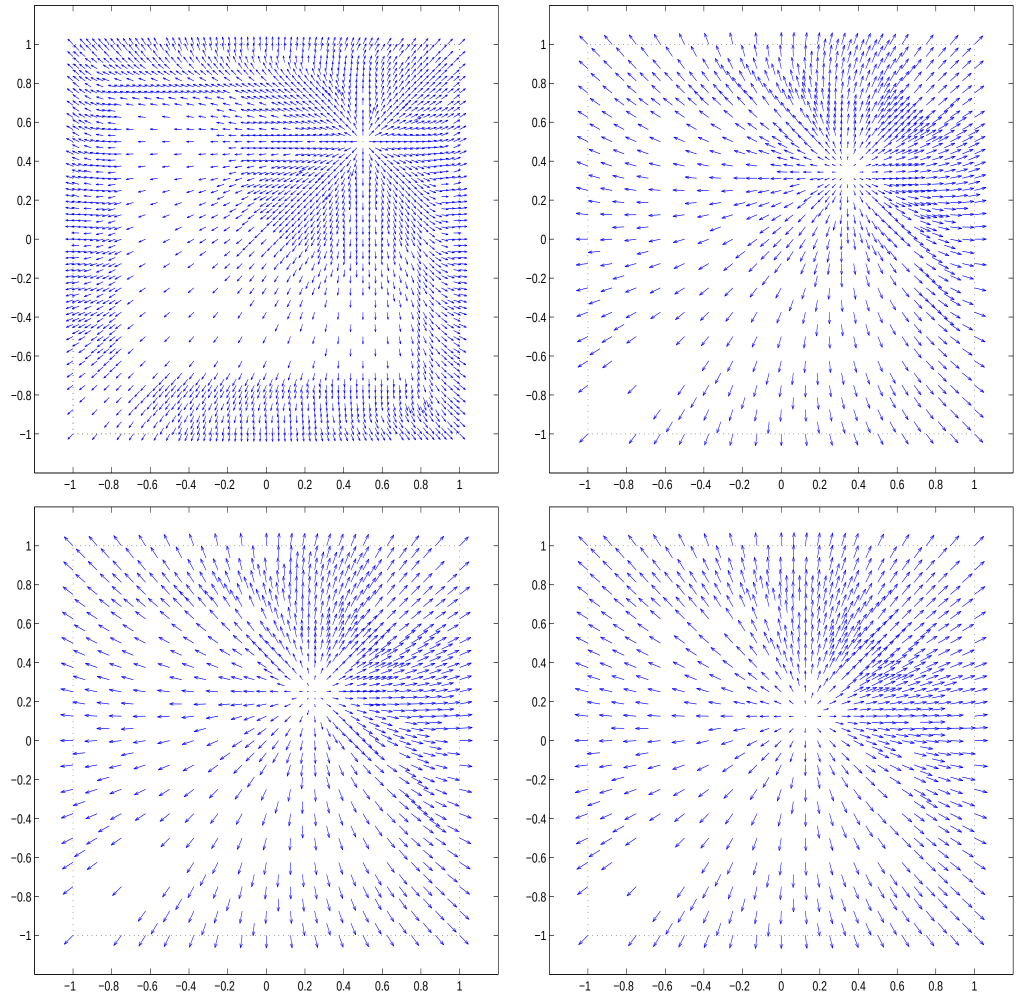

FIGURE 8. Numerical solution and adaptively refined and coarsened triangulations $\mathcal{T}_j$ for $j = 0, 1000, 2000, 4000$ in Example 2 with $\varepsilon = 1/8$. Each arrow corresponds to a vertex in the triangulation.

The automatically refined and coarsened triangulations $\mathcal{T}_j$ together with the numerical solution $U(t_j)$ for $j = 0, 1000, 2000, 4000$ as outputs of Algorithm $(\mathcal{A}_{1,0})$ in Example 2 with $\varepsilon = 1/8$, an initial uniform triangulation with maximal mesh-size $h = 1/32$, and a uniform time step size $\tau_1 = \varepsilon^4$ are displayed in Figure 8. The coarsened triangulation $\mathcal{T}_0$ shows a higher resolution in a boundary layer which stems from a practically non-smooth u_0. In all displayed solutions we observe a smaller local mesh-size around the moving vortex.

For numerical evidence of improved experimental convergence rates obtained by a related automatic mesh refining strategy we refer the reader to [14].

Acknowledgments. S.B. is thankful to G. Dolzmann and R.H. Nochetto for stimulating discussions. This work was supported by a fellowship within the Postdoc-Programme of the German Academic Exchange Service (DAAD).

REFERENCES

[1] S. ALLEN, J. W. CAHN: A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening. *Acta. Metall.* **27** (1979), 1084-1095.

[2] I. BABUŠKA, J. OSBORN: Eigenvalue problems. In *Handbook of numerical analysis II*, North-Holland (1991), 641–787.

[3] S. BARTELS, C. CARSTENSEN, G. DOLZMANN: Inhomogeneous Dirichlet conditions in a priori and a posteriori finite element error analysis. *Berichtsreihe des Mathematischen Seminars Kiel*, Technical report **02-1**, Christian–Albrechts–Universität zu Kiel, Kiel (2002).

[4] A. BEAULIEU: Some remarks on the linearized operator about the radial solution for the Ginzburg-Landau equation. *Nonlinear Anal.* **54** (2003), 1079–1119.

[5] X. CHEN: Spectrum for the Allen-Cahn, Cahn-Hilliard, and phase-field equations for generic interfaces. *Comm. Partial Differential Equations* **19** (1994), 1371–1395.

[6] P. DE MOTTONI, M. SCHATZMAN: Geometrical evolution of developed interfaces. *Trans. Amer. Math. Soc.* **347** (1995), 1533–1589.

[7] Q. DU, M. GUNZBURGER, J. PETERSON: Analysis and approximation of the Ginzburg-Landau model of superconductivity. *SIAM Rev.* **34** (1992), 54–81.

[8] C. M. ELLIOTT: Approximation of curvature dependent interface motion. *The state of the art in numerical analysis*, Inst. Math. Appl. Conf. Ser. New Ser., 63, Oxford Univ. Press (1997), 407–440.

[9] X. FENG, A. PROHL: Numerical analysis of the Allen-Cahn equation and approximation for mean curvature flows. *Numer. Math.* **94** (2003), 33–65.

[10] X. FENG, A. PROHL: Numerical analysis of the Cahn-Hilliard equation and approximation of the Hele-Shaw problem. Part I: Error analysis under minimum regularities. *SIAM J. Numer. Anal.* (to appear).

[11] X. FENG, A. PROHL: Analysis of a fully discrete finite element method for the phase field model and approximation of its sharp interface limits. *Math. Comp.* **73** (2004), 541-567.

[12] D. GILBARG, N. S. TRUDINGER: *Elliptic partial differential equations of second order.* Springer, Berlin (2001).

[13] V. GINZBURG, L. LANDAU: On the theory of superconductivity. *Zh. Èksper. Teoret. Fiz.* **20** (1950), 1064–1082. In *Men of Physics: L.D. Landau*, D. TER HAAR, ed. Pergamon, Oxford (1965), 138–167.

[14] D. KESSLER, R. H. NOCHETTO, A. SCHMIDT: A posteriori error control for the Allen-Cahn problem: circumventing Gronwall's inequality. *M2AN* (to appear) (2004).

[15] D. KESSLER, R. H. NOCHETTO, A. SCHMIDT: A duality approach to a posteriori error control for the Allen-Cahn problem. Preprint (2003).

[16] M. G. LARSON: A posteriori and a priori error analysis for finite element approximations of self-adjoint elliptic eigenvalue problems. *SIAM J. Numer. Anal.* **38** (2000), 608–625.

[17] E. H. LIEB, M. LOSS: Symmetry of the Ginzburg-Landau minimizer in a disc. *Math. Res. Lett.* **1** (1994), 701–715.

[18] R. H. NOCHETTO, A. SCHMIDT, C. VERDI: A posteriori error estimation and adaptivity for degenerate parabolic problems. *Math. Comp.* **69** (1999), 1–24.