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A POSTERIORI ERROR CONTROL FOR THE ALLEN–CAHN PROBLEM: CIRCUMVENTING GRONWALL'S INEQUALITY

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Abstract. Phase-field models, the simplest of which is Allen–Cahn's problem, are characterized by a small parameter ε that dictates the interface thickness. These models naturally call for mesh adaptation techniques, which rely on *a posteriori* error control. However, their error analysis usually deals with the underlying non-monotone nonlinearity via a Gronwall argument which leads to an exponential dependence on ε^{-2}. Using an energy argument combined with a topological continuation argument and a spectral estimate, we establish an *a posteriori* error control result with only a low order polynomial dependence in ε^{-1}. Our result is applicable to any conforming discretization technique that allows for a posteriori residual estimation. Residual estimators for an adaptive finite element scheme are derived to illustrate the theory.

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1. Introduction

Phase-field models, the simplest of which is Allen-Cahn's problem, describe the evolution of a diffuse phase boundary, concentrated in a small region of size ε. They naturally call for adaptive mesh discretization techniques, which rely on error control based on *a posteriori* estimators. However, if Gronwall's lemma is used extensively, as is usually done in numerical analysis, the non-monotone nonlinearity used to model phase separation leads to error estimates that grow exponentially as ε becomes small. The following paradox arises: the thinnest the interface region, the worst are the error estimators justifying the use of mesh adaptation!

The problem of the dependence on ϵ is already fully present in the Allen–Cahn equation [1]:

$$\epsilon\frac{\partial u}{\partial t} - \epsilon\triangle u + \frac{1}{\epsilon}(u^3 - u) = 0.$$

In this paper, we derive new improved *a posteriori* error estimates for the Allen–Cahn equation, in which the dependence on ϵ^{-1} is no longer exponential, only polynomial. The main ingredient is the use of a spectral estimate established by de Mottoni and Schatzman [7] and Chen [4]. Our work was inspired by recent results of Caginalp and Chen [3] and Feng and Prohl [9]. Our result is presented in terms of error control to a

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given tolerance, and is directly applicable to any mesh adaptation strategy that is formulated in terms of error tolerance. For *a posteriori* error analysis, we work in the continuous setting, which has two distinctive advantages. On the one hand, it allows us to present the main argument in a clear analytical way, isolating the crucial step of the proof, which is based on a topological continuation argument. On the other hand, as we present it, this procedure could actually be extended to any conforming approximation method, in a transparent way clearly separated from the method-dependent *a posteriori* control of the residual.

This paper is organized as follows. In Section 2, we define the functional setting and main lemmas for the Allen-Cahn problem. We also introduce a finite element discretization, and give a general definition of the residual, applicable to any conforming method. In Section 3, we will assume that there is an *a posteriori* estimation of the residual, and obtain error control criteria under this assumption. The results of Section 3 are therefore applicable to any conforming method which permits the derivation of *a posteriori* residual estimators. In Section 4, residual estimators will be derived for the finite element discretization introduced in Section 2. Together with the results from Section 3, we will then have a complete *a posteriori* error control criterion for a finite element method, which can be directly used for implementing adaptive mesh computations. Some illustrative simulations are finally presented in Section 5.

2. Setting: Continuous and discrete problems

2.1. Continuous problem

Let $\Omega \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, be a convex domain and let T be a positive constant. We introduce the short notation Q_t for space-time domains $\Omega \times (0,t)$, for times $t \in [0,T]$. Let $\mathbb{V}$ be the Sobolev space $\mathrm{H}^1(\Omega)$, and $\mathbb{V}'$ its dual. We will denote by $\langle\, .|.\, \rangle$ the duality pairing between $\mathbb{V}'$ and $\mathbb{V}$, by $(.,.)$ the $\mathrm{L}^2(\Omega)$ scalar product, and by $\|.\|$ the $\mathrm{L}^2(\Omega)$ norm.

Let us recall an important embedding result from Dautrey and Lions [6] that will be useful later:

Lemma 2.1 (Dautrey-Lions)**.** *The following properties are valid.*

(1) $\mathrm{L}^2(0,T;\mathbb{V}) \cap \mathrm{H}^1(0,T;\mathbb{V}') \subset \mathrm{C}^0(0,T;\mathrm{L}^2(\Omega))$*;*
(2) *If* $v \in \mathrm{L}^2(0,T;\mathbb{V}) \cap \mathrm{H}^1(0,t;\mathbb{V}')$*, then* $\langle\, v_t | v\, \rangle = \frac{1}{2}\frac{d}{dt}\|v\|^2$.

Let $\varepsilon > 0$ be a given parameter, which can be thought of as the characteristic width of the transition layer whose evolution is described by the Allen–Cahn problem. Let $u_0 \in \mathrm{L}^2(\Omega)$ be given initial data such that $u_0 \in [-1,+1]$ *a.e.* in Ω. Let $f : \mathbb{R} \longrightarrow \mathbb{R}$ be given by $s \mapsto f(s) = s^3 - s$. This is the nonlinearity defining the Allen-Cahn problem:

Problem 2.2 (Allen–Cahn problem)**.** Find $u \in \mathrm{L}^2(0,T;\mathbb{V}) \cap \mathrm{H}^1(0,t;\mathbb{V}')$ such that $u|_{t=0} = u_0$ and that *a.e.* in $(0,T)$,

$$\varepsilon \langle\, u_t | v\, \rangle + \varepsilon (\nabla u, \nabla v) + \frac{1}{\varepsilon}(f(u), v) = 0, \quad \forall v \in \mathbb{V}. \tag{1}$$

It is known that this problem is well posed and admits a unique solution. Furthermore, this solution satisfies a maximum principle, which is also valid for more complex phase-field models [11].

Lemma 2.3 (Maximum principle)**.** *If* $u_0 \in [-1,+1]$ *a.e. in* Ω*, then* $u \in [-1,+1]$ *a.e. in* Q_T*.*

Hence, for adequate initial data, Problem 2.2 is strictly equivalent to an analogous problem in which f is replaced by

$$\tilde{f}(s) = \begin{cases} 2s+2, & s < -1, \\ f(s) & s \in [-1,+1], \\ 2s-2, & s > +1. \end{cases} \tag{2}$$

This function $\tilde{f}$ is Lipschitz continuous, with Lipschitz constant $L_f = 2$. Its first derivative is Lipschitz continuous as well, with Lipschitz constant $L_{f'} = 6$. For practical purposes, we will always be considering the problem formulated with this substitute function $\tilde{f}$, but omit the tilde in the notation.

To obtain a finer estimate on the error, we will need to use a spectral estimate established by de Mottoni and Schatzman [7] and Chen [4]:

Lemma 2.4 (Spectral estimate)**.** *Let the initial condition u_0 have a "compatible profile" with the Allen–Cahn equation, i.e. already describe bulk phase regions separated by transition zones of width $O(\varepsilon)$. Then there exists a constant λ_0 independent of ε such that for all $\varepsilon > 0$, the solution u of Problem 2.2 satisfies*

$$\varepsilon \|\nabla v\|^2_{\mathrm{L}^2(\Omega)} + \frac{1}{\varepsilon}\left(f'(u)v, v\right) \geq -\lambda_0 \varepsilon \|v\|^2_{\mathrm{L}^2(\Omega)}. \tag{3}$$

2.2. **Discrete problem**

Let $0 = t_0 < t_1 < \cdots < t_N = T$ be a partition of $[0, T]$ and $\tau_n = t_n - t_{n-1}$ be the time steps, for $n = 0, \ldots, N$.

Let $\mathcal{T}_n$, $0 = 1, \ldots, N$, be conforming shape-regular meshes on Ω, and let $\mathbb{V}_n \in \mathbb{V}$ be piecewise polynomial (of at least degree one) finite element spaces on these meshes. We denote by $I_n : \mathbb{V} \cap C^0(\bar{\Omega}) \longrightarrow \mathbb{V}_n$ the Lagrange interpolation operators into these spaces.

We can define an approximation of the Allen–Cahn problem by the following semi-implicit finite difference in time, finite element in space numerical scheme:

Problem 2.5 (Discrete problem)**.** Given $U_0 \in \mathbb{V}_0$, find $U_n \in \mathbb{V}_n$, $n = 1, \ldots, N$, s.t. for $n = 1, \ldots, N$ we have

$$\varepsilon\left(\frac{U_n - I_n U_{n-1}}{\tau_n}, V\right) + \varepsilon\left(\nabla U_n, \nabla V\right) + \frac{1}{\varepsilon}\left(f(I_n U_{n-1}), V\right) + \frac{1}{\varepsilon}\left(f'(I_n U_{n-1})(U_n - I_n U_{n-1}), V\right) = 0, \tag{4}$$

for all V in $\mathbb{V}_n$. The last two terms are the linearization of an implicit discretization of $f(u)$; the reason for this choice is given in Section 5.

Out of the sequence of functions U_n defined pointwise in time, we build a function continuous in time by piecewise $\mathbb{P}_1$ interpolation as follows:

$$U(t) = \frac{t - t_{n-1}}{\tau_n} U_n + \frac{t_n - t}{\tau_n} U_{n-1}, \quad t \in [t_{n-1}, t_n], \quad n = 1, \ldots, N. \tag{5}$$

With this definition, the time derivative of U is a function defined for *a.e.* $t \in (0, T)$ as

$$U_t = \frac{U_n - U_{n-1}}{\tau_n}, \quad t \in (t_{n-1}, t_n), \quad n = 1, \ldots, N. \tag{6}$$

Notice that $U \in \mathrm{H}^1(Q_T) \subset \mathrm{L}^2(0, T; \mathbb{V}) \cap \mathrm{H}^1(0, t; \mathbb{V}')$, so this interpretation of the discrete solution is conforming with the continuous problem.

2.3. **Residual**

We define the discrete equation residual $r \in \mathrm{L}^2(0, T; \mathbb{V}')$ by requiring that for almost every t in $(0, T)$,

$$\langle r | v \rangle = \varepsilon\left(U_t, v\right) + \varepsilon\left(\nabla U, \nabla v\right) + \frac{1}{\varepsilon}\left(f(U), v\right), \quad \forall v \in \mathbb{V}. \tag{7}$$

Such a residual can be defined for the solution of the discrete Problem 2.5, or for the solution of any other conforming approximation of the Continuous problem 2.2. Therefore, the concept of residual r is method independent.

Throughout Section 3, we will assume that *a posteriori* residual estimators η_0 and η_1 can be built, such that

$$\int_0^T \langle r | v \rangle \leq \eta_0 \|v\|_{\mathrm{L}^2(Q_T)} + \eta_1 \|\nabla v\|_{\mathrm{L}^2(Q_T)}, \quad \forall v \in \mathbb{V}. \tag{8}$$

In Section 4, residual estimators will eventually be derived for Discrete problem 2.5.

3. Error: Coarse and fine estimates

Let $e = U - u$ be the error at a generic time $t \in (0,T)$ and $e_0 = U_0 - u_0$ be the initial error, where u is the solution of continuous problem 2.2 satisfying (1) with initial condition $u_0 \in \mathrm{L}^2(\Omega)$, and U is the solution of a conforming approximate problem. We assume that the residual of U defined by (7) can be estimated by (8). By the definition of u, and the assumption that U comes from a conforming discretization, we know that

$$e \in \mathrm{L}^2(0,T;\mathbb{V}) \cap \mathrm{H}^1(0,t;\mathbb{V}'). \tag{9}$$

We want to estimate the error $\|e\|_{\mathrm{L}^\infty(0,T;\mathrm{L}^2(\Omega))}$, which makes sense thanks to Lemma 2.1. To this end, we resort to an *energy argument* combined with a *topological argument*, as explained below.

3.1. **Error equation**

Subtracting equation (1) from equation (7), we get *a.e.* in $(0,T)$

$$\varepsilon\,(e_t, v) + \varepsilon\,(\nabla e, \nabla v) + \frac{1}{\varepsilon}\,(f(U) - f(u), v) = \langle r | v \rangle, \quad \forall v \in \mathbb{V}. \tag{10}$$

Thanks to (9), this is true in particular for $v = e$. Therefore, using also Lemma 2.1, we get the error equation

$$\frac{\varepsilon}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\|e\|^2 + \varepsilon\,\|\nabla e\|^2 + \frac{1}{\varepsilon}\,(f(U) - f(u), e) = \langle r | e \rangle, \qquad a.e. \quad t \in (0,T). \tag{11}$$

3.2. **Coarse estimate**

Integrating (11) in time and using the Lipschitz continuity of f, we obtain for all $t \in [0,T]$

$$\frac{\varepsilon}{2}\,\|e(t)\|^2_{\mathrm{L}^2(\Omega)} + \varepsilon\,\|\nabla e\|^2_{\mathrm{L}^2(Q_t)} \le \frac{\varepsilon}{2}\,\|e_0\|^2_{\mathrm{L}^2(\Omega)} + \frac{L_f}{\varepsilon}\,\|e\|^2_{\mathrm{L}^2(Q_t)} + \eta_0\,\|e\|_{\mathrm{L}^2(Q_t)} + \eta_1\,\|\nabla e\|_{\mathrm{L}^2(Q_t)}, \tag{12}$$

where η_0 and η_1 are residual estimators satisfying (8).

Using Young's inequality, we can then establish that

$$\|e(t)\|^2_{\mathrm{L}^2(\Omega)} + \|\nabla e\|^2_{\mathrm{L}^2(Q_t)} \le \|e_0\|^2_{\mathrm{L}^2(\Omega)} + \frac{4L_f}{\varepsilon^2}\,\|e\|^2_{\mathrm{L}^2(Q_t)} + \frac{\eta_0^2}{2L_f} + \frac{\eta_1^2}{\varepsilon^2}, \quad \forall t \in [0,T]. \tag{13}$$

In particular, one may immediately conclude by Gronwall's lemma that

$$\|e\|^2_{\mathrm{L}^\infty(0,T;\mathrm{L}^2(\Omega))} \le \left(\|e_0\|^2_{\mathrm{L}^2(\Omega)} + \frac{\eta_0^2}{2L_f} + \frac{\eta_1^2}{\varepsilon^2}\right)\exp\left(\frac{4L_f}{\varepsilon^2}T\right). \tag{14}$$

This is a coarse *a posteriori* estimate of the error, which is not satisfactory because of the exponential dependence in ε. However, this estimate is sharp without further assumptions on u, because the Allen–Cahn equation typically exhibits an exponentially fast initial transient regime for times of order $O(\varepsilon)$, until interfaces develop [7].

3.3. **Thought experiment**

Let's imagine for a moment that inequality (13) could somehow be replaced by the following inequality:

$$\|e(t)\|^2_{\mathrm{L}^2(\Omega)} \le \|e_0\|^2_{\mathrm{L}^2(\Omega)} + \eta^2 + \frac{C}{\varepsilon^2}\,\|e\|^3_{\mathrm{L}^2(Q_t)}, \tag{15}$$

where η is some residual estimator, and C a constant independent of ε. The main difference with (13) is the cubic power in the last term. We will show that this apparently minor difference is in fact really significant.

Let us now define the time interval

$$I_\theta = \left\{ t \in [0,T] \quad \middle| \quad \|e\|_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \leq \theta \right\} \cdot \tag{16}$$

Notice that if a subinterval of $[0,T]$ is open, closed and non-empty, then it is the full interval $[0,T]$. Since by Lemma 2.1 $e \in \mathrm{C}^0(0,T;\mathrm{L}^2(\Omega))$, then the interval I_θ is closed. Furthermore, if we make sure that $\|e_0\|_{\mathrm{L}^2(\Omega)} \leq \theta$, then I_θ is non-empty. To conclude that $I_\theta = [0,T]$, it is therefore sufficient to have conditions ensuring that if $t \in I_\theta$ then $\|e\|_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} < \theta$ (for $t < T$). Again, this relies on the knowledge that $\|e\|_{\mathrm{L}^2(\Omega)} \in \mathrm{C}^0[0,T]$. Notice for instance that for t in I_θ,

$$\frac{C}{\varepsilon^2} \|e\|^3_{\mathrm{L}^2(Q_t)} \leq \frac{C}{\varepsilon^2} T\theta^3.$$

We want this quantity, as well as the other right-hand terms of (15), to be smaller than a fraction of θ^2.

Using (15), we can therefore conclude that the following conditions are sufficient to ensure that the $\mathrm{L}^2(\Omega)$ norm of the error remains below a tolerance θ up to time T:

$$\theta \leq \frac{\varepsilon^2}{4CT}, \tag{17}$$

$$\|e_0\|_{\mathrm{L}^2(\Omega)} \leq \frac{\theta}{2}, \tag{18}$$

$$\eta \leq \frac{\theta}{2} \cdot \tag{19}$$

What this tells us is that under a tight restriction on the permitted choice of the tolerance θ (it must be small enough relative to ε), if both the initial error and the residual estimator are below a fraction of the tolerance, then the error will be below the tolerance. More precisely, conditions (17)–(19) together with (15) ensure that if $t \in I_\theta$, then $\|e\|^2_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \leq \frac{3}{4}\theta^2 < \theta^2$, so the interval I_θ is open, closed and non-empty as desired.

Such a result is directly applicable to a mesh adaptation algorithm, where the user wants to set a tolerance for the error, and guarantee this tolerance by adapting the initial mesh to sufficiently resolve the initial condition, and the next meshes to sufficiently reduce the computed residual estimators.

Next we will show how the spectral estimate of Lemma 2.4 allows us to infer an inequality somewhat similar to (15). The real problem is not as nice as a thought experiment, though, and we will loose a couple of orders in ε in the process.

3.4. **Fine estimate**

To obtain a finer estimate on the error, we will need to use Lemma 2.4. Notice that $f(U) - f(u) = \int_0^e f'(u+\xi)\,\mathrm{d}\xi$. Thus, (11) with (3) applied to $v = e$ result in

$$\frac{\varepsilon}{2}\frac{\mathrm{d}}{\mathrm{d}t} \|e\|^2_{\mathrm{L}^2(\Omega)} \leq \lambda_0 \varepsilon \|e\|^2_{\mathrm{L}^2(\Omega)} + \frac{1}{\varepsilon}\left(\int_0^e (f'(u) - f'(u+\xi))\,\mathrm{d}\xi, e \right) + \langle r|e \rangle, \quad \textit{a.e. in } (0,T). \tag{20}$$

However,

$$\left| \int_0^e (f'(u) - f'(u+\xi))\,\mathrm{d}\xi \right| \leq L_{f'} \int_0^e \xi\,\mathrm{d}\xi = \frac{L_{f'}}{2} e^2, \tag{21}$$

whence we get

$$\frac{\varepsilon}{2}\frac{\mathrm{d}}{\mathrm{d}t} \|e\|^2_{\mathrm{L}^2(\Omega)} \leq \lambda_0 \varepsilon \|e\|^2_{\mathrm{L}^2(\Omega)} + \frac{L_{f'}}{2\varepsilon} \|e\|^3_{\mathrm{L}^3(\Omega)} + \langle r|e \rangle, \quad \textit{a.e. in } (0,T). \tag{22}$$

We are close to the assumptions of Section 3.3, but the norm that appears cubed is the $\mathrm{L}^3(\Omega)$ norm, instead of the $\mathrm{L}^2(\Omega)$ norm. Since the only norm stronger than $\mathrm{L}^2(\Omega)$ at our disposal is the $\mathrm{H}^1(\Omega)$ norm, which is not under control after using the spectral theorem, we will need to go back to a coarser version of the error inequality to gain complete control of the $\mathrm{L}^3(\Omega)$ norm and finally be able to perform an argument similar to the one outlined in the Section 3.3. The idea is to use interpolation between $\mathrm{L}^2(\Omega)$ and $\mathrm{H}^1(\Omega)$.

By Cauchy–Schwarz inequality, we know that

$$\|e\|^3_{\mathrm{L}^3(\Omega)} \leq \|e\|^2_{\mathrm{L}^4(\Omega)} \|e\|_{\mathrm{L}^2(\Omega)} . \tag{23}$$

For space dimensions $d \leq 4$, $\mathrm{H}^1(\Omega)$ is continuously embedded into $\mathrm{L}^4(\Omega)$ (see [2]). Hence, denoting by C_{S} the Sobolev embedding constant, we deduce

$$\|e\|^3_{\mathrm{L}^3(\Omega)} \leq C_{\mathrm{S}} \|e\|^2_{\mathrm{H}^1(\Omega)} \|e\|_{\mathrm{L}^2(\Omega)} . \tag{24}$$

Therefore, integrating (22) in time and using (8), we infer that for all t in $[0,T]$,

$$\begin{aligned} \sup_{s\in(0,t)} \|e(s)\|^2_{\mathrm{L}^2(\Omega)} \leq \|e_0\|^2_{\mathrm{L}^2(\Omega)} + 2\lambda_0 \|e\|^2_{\mathrm{L}^2(Q_t)} + \frac{L_{f'}C_{\mathrm{S}}}{\varepsilon^2} \|e\|^2_{\mathrm{L}^2(0,t;\mathrm{H}^1(\Omega))} \|e\|_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \\ + \frac{2}{\varepsilon}\eta_0 \|e\|_{\mathrm{L}^2(Q_t)} + \frac{2}{\varepsilon}\eta_1 \|\nabla e\|_{\mathrm{L}^2(Q_t)} . \end{aligned} \tag{25}$$

Using Young's inequality twice, with some arbitrary positive number δ,

$$\begin{aligned} \|e\|^2_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \leq \|e_0\|^2_{\mathrm{L}^2(\Omega)} + 4\lambda_0 \|e\|^2_{\mathrm{L}^2(Q_t)} + \frac{1}{2\lambda_0}\left(\frac{\eta_0}{\varepsilon}\right)^2 + \frac{L_{f'}C_{\mathrm{S}}T}{\varepsilon^2} \|e\|^3_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \\ + \left(\frac{L_{f'}C_{\mathrm{S}}}{\varepsilon^2} \|e\|_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} + \delta\right) \|\nabla e\|^2_{\mathrm{L}^2(Q_t)} + \frac{1}{\delta}\left(\frac{\eta_1}{\varepsilon}\right)^2 . \end{aligned} \tag{26}$$

This last inequality, combined with (13) for the evaluation of $\|\nabla e\|^2_{\mathrm{L}^2(Q_t)}$, gives a finer error estimate than the evaluation of $\sup_{s\in(0,t)} \|e(s)\|^2_{\mathrm{L}^2(\Omega)}$ from (13). It is finer in the sense that $\varepsilon^{-2} \|e\|^2_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))}$ never appears by itself, but always multiplied by some other quantity susceptible of being controlled. There is thus hope of doing better than Gronwall's inequality, namely using a continuation argument similar to the one presented in Section 3.3.

3.5. **Continuation argument**

As in Section 3.3, let

$$I_\theta = \left\{ t \in [0,T] \;\middle|\; \|e\|_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \leq \theta \right\} . \tag{27}$$

We are again looking for conditions ensuring that if $t \in I_\theta$, then $\|e\|_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} < \theta$ (for $t \leq T$). Then if also $\|e_0\|_{\mathrm{L}^2(\Omega)} \leq \theta$, the interval I_θ is open, closed and non-empty and therefore equal to the full interval $[0,T]$. In other words, $\|e\|_{\mathrm{L}^\infty(0,T;\mathrm{L}^2(\Omega))} \leq \theta$, and we thus control the L^2 error throughout the time interval $[0,T]$. The main difference with Section 3.3 lies in the sufficient conditions for I_θ to be an open interval.

By definition of I_θ, $\|e\|_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \leq \theta$ and therefore $\|e\|^2_{\mathrm{L}^2(Q_t)} \leq T\theta^2$ when $t \in I_\theta$. Hence, we infer from inequalities (13) and (26) that for all t in I_θ,

$$\|\nabla e\|^2_{\mathrm{L}^2(Q_t)} \leq \|e_0\|^2_{\mathrm{L}^2(\Omega)} + 4TL_f\frac{\theta^2}{\varepsilon^2} + \frac{\eta_0^2}{2L_f} + \frac{\eta_1^2}{\varepsilon^2} \tag{28}$$

and

$$\|e\|^2_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \leq \|e_0\|^2_{\mathrm{L}^2(\Omega)} + 4\lambda_0 \|e\|_{\mathrm{L}^2(Q_t)} + \frac{1}{2\lambda_0}\left(\frac{\eta_0}{\varepsilon}\right)^2 + L_{f'}C_{\mathrm{S}}T\frac{\theta^3}{\varepsilon^2} + \left(L_{f'}C_{\mathrm{S}}\frac{\theta}{\varepsilon^2} + \delta\right) \|\nabla e\|^2_{\mathrm{L}^2(Q_t)} + \frac{1}{\delta}\left(\frac{\eta_1}{\varepsilon}\right)^2 . \tag{29}$$

However, we still need to use Gronwall's lemma on (29) to handle the second term of its right-hand side, which we would not be able to control otherwise; this results in the following inequality:

$$\|e\|^2_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \le \left(\|e_0\|^2_{\mathrm{L}^2(\Omega)} + \frac{1}{2\lambda_0}\left(\frac{\eta_0}{\varepsilon}\right)^2 + L_{f'}C_{\mathrm{S}}T\frac{\theta^3}{\varepsilon^2} + \left(L_{f'}C_{\mathrm{S}}\frac{\theta}{\varepsilon^2} + \delta\right)\|\nabla e\|^2_{\mathrm{L}^2(Q_t)} + \frac{1}{\delta}\left(\frac{\eta_1}{\varepsilon}\right)^2 \right) \mathrm{e}^{4\lambda_0 T}. \tag{30}$$

Notice that now Gronwall's lemma did not introduce an exponential dependence on ε, since the spectral Lemma 2.4 precisely ensures that λ_0 is independent of ε.

Following the same line of proof as in Section 3.3, we want to find sufficient conditions on $\|e_0\|_{\mathrm{L}^2(\Omega)}$, η_0, η_1 and θ such that inequalities (30) and (28) enforce that $\|e\|_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \le C\theta$ for some C lower than 1. In the thought experiment in Section 3.3, θ had to be controlled by ε^2, as in condition (17). Now in the real problem, however, by careful observation of the fourth term of the right-hand side of (30) combined with the second term of the right-hand side of (28), one should be persuaded that θ *must* now be controlled by ε^4 for the product to be of order $\theta^2\varepsilon^0$. We therefore impose the condition

$$\theta \le \Lambda_0 \varepsilon^4, \tag{31}$$

and define

$$\Lambda_0 = \frac{\mathrm{e}^{-4\lambda_0 T}}{8L_f L_{f'} C_{\mathrm{S}}\alpha T}, \tag{32}$$

where α remains to be chosen later. We also choose

$$\delta = \frac{\mathrm{e}^{-4\lambda_0 T}}{8L_f\alpha T}\varepsilon^2. \tag{33}$$

This choice of δ, combined with (31), simplifies inequality (30) while keeping δ independent of θ. In fact we now have

$$L_{f'}C_{\mathrm{S}}\frac{\theta}{\varepsilon^2} + \delta \le \frac{\mathrm{e}^{-4\lambda_0 T}}{4L_f\alpha T}\varepsilon^2. \tag{34}$$

Combining the latter with (30) and (28), we infer that for all t in I_θ,

$$\begin{aligned} \|e\|^2_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))} \le\ & \|e_0\|^2_{\mathrm{L}^2(\Omega)}\mathrm{e}^{4\lambda_0 T} \\ & + \frac{\mathrm{e}^{4\lambda_0 T}}{2\lambda_0}\left(\frac{\eta_0}{\varepsilon}\right)^2 \\ & + \frac{1}{8L_f\alpha}\varepsilon^2\theta^2 \\ & + \frac{1}{4L_f\alpha T}\varepsilon^2\|e_0\|^2_{\mathrm{L}^2(\Omega)} \\ & + \frac{\theta^2}{\alpha} \\ & + \frac{1}{8L_f^2\alpha T}\varepsilon^2\eta_0^2 \\ & + \frac{1}{4L_f\alpha T}\eta_1^2 \\ & + 8L_f\alpha T\mathrm{e}^{8\lambda_0 T}\frac{\eta_1^2}{\varepsilon^4}. \end{aligned} \tag{35}$$

To have a sufficient condition to conclude the argument, we want the first, second, fifth and last terms of the the right-hand side of the above inequality to be lower than $\theta^2/8$, and the remaining terms to be lower than

$\theta^2/16$. This can be achieved by setting $\alpha = 8$ and then fulfilling the following seven conditions:

$$\|e_0\|_{\mathrm{L}^2(\Omega)} \le \frac{\mathrm{e}^{-2\lambda_0 T}}{2\sqrt{2}}\theta \equiv \Lambda_1\theta, \tag{36}$$

$$\frac{\eta_0}{\varepsilon} \le \frac{\sqrt{\lambda_0}\mathrm{e}^{-2\lambda_0 T}}{2}\theta \equiv \Lambda_2\theta, \tag{37}$$

$$\varepsilon \le 2\sqrt{L_f}, \tag{38}$$

$$\varepsilon\|e_0\|_{\mathrm{L}^2(\Omega)} \le \sqrt{2L_f T}\theta, \tag{39}$$

$$\varepsilon\eta_0 \le 2L_f\sqrt{T}\theta, \tag{40}$$

$$\eta_1 \le \sqrt{2L_f T}\theta, \tag{41}$$

$$\frac{\eta_1}{\varepsilon^2} \le \frac{\mathrm{e}^{-4\lambda_0 T}}{16\sqrt{2L_f T}}\theta \equiv \Lambda_3\theta. \tag{42}$$

Notice that for sufficiently small ε, condition (38) is trivial and conditions (39)–(41) are consequences of the remaining conditions. Therefore, if inequalities (31, 36, 37) and (42) are satisfied, then $\|e(t)\|_{\mathrm{L}^2(\Omega)} \le 3\theta/4$ for all t in I_θ, and the interval I_θ is open. We can then close the continuation argument and conclude that under these conditions, $I_\theta = [0, T]$. This is summarized in the following Theorem.

Theorem 3.1 (Error control)**.** *Let u be a solution of the Allen–Cahn problem with interface width ε, with an initial condition u_0 that corresponds to developed interfaces, in the sense that the spectral estimate* (3) *is valid. Let U be a conforming approximation of u, whose residual can be controlled by a posteriori estimators η_0 and η_1 according to* (8)*. Let the ε-independent constants $\Lambda_0, \ldots, \Lambda_3$ be defined as follows:*

$$\Lambda_0 = \frac{\mathrm{e}^{-4\lambda_0 T}}{8L_f L_{f'} C_{\mathrm{S}}\alpha T}, \tag{43}$$

$$\Lambda_1 = \frac{\mathrm{e}^{-2\lambda_0 T}}{2\sqrt{2}}, \tag{44}$$

$$\Lambda_2 = \frac{\sqrt{\lambda_0}\mathrm{e}^{-2\lambda_0 T}}{2}, \tag{45}$$

$$\Lambda_3 = \frac{\mathrm{e}^{-4\lambda_0 T}}{16\sqrt{2L_f T}}. \tag{46}$$

For ε sufficiently small, if a tolerance θ is given subject to the constraint

$$\theta \le \Lambda_0\varepsilon^4, \tag{47}$$

and the initial error e_0 and residual estimators η_0 and η_1 satisfy the conditions

$$\|e_0\|_{\mathrm{L}^2(\Omega)} \le \Lambda_1\theta, \tag{48}$$

$$\eta_0 \le \Lambda_2\varepsilon\theta, \tag{49}$$

$$\eta_1 \le \Lambda_3\varepsilon^2\theta, \tag{50}$$

then

$$\|e\|_{\mathrm{L}^\infty(0,T;\mathrm{L}^2(\Omega))} \le \theta. \tag{51}$$

Remark 3.2 (Comparison between coarse and fine estimates)**.** A consequence of Theorem 3.1 is that if a tolerance θ is given under constraint (47), then

$$\Lambda_1^{-1} \|e_0\|_{\mathrm{L}^2(\Omega)} + \Lambda_2^{-1} \frac{\eta_0}{\varepsilon} + \Lambda_3^{-1} \frac{\eta_1}{\varepsilon^2} \le \theta \quad \Longrightarrow \quad \|e\|_{\mathrm{L}^\infty(0,T;\mathrm{L}^2(\Omega))} \le \theta. \tag{52}$$

Correspondingly, a consequence of the coarse estimate (14) was that for any given tolerance θ,

$$\left(\|e_0\|_{\mathrm{L}^2(\Omega)} + (2L_f)^{-1/2}\eta_0 + \frac{\eta_1}{\varepsilon}\right) \exp\left(\frac{2L_f}{\varepsilon^2}T\right) \le \theta \quad \Longrightarrow \quad \|e\|_{\mathrm{L}^\infty(0,T;\mathrm{L}^2(\Omega))} \le \theta. \tag{53}$$

Therefore we can see that, subject to constraint (47), we have been able to remove an exponential dependence on ε^{-2}, and replace it by low degree polynomial dependence on ε^{-1}.

3.6. **Conclusion**

Given a tolerance θ, we can guarantee that the error of a solution of the Numerical Scheme 2.5 with respect to the solution of the Allen–Cahn Problem 2.2 is below this tolerance in the $\|.\|_{\mathrm{L}^\infty(0,t;\mathrm{L}^2(\Omega))}$ norm if conditions (47–50) are fulfilled. These conditions rely only on *a posteriori* quantities. There is no exponential dependence on ε. In this section, we assumed that *a posteriori* residual estimators η_0 and η_1 could be computed for a conforming discretization of (1). In the next section, we actually show a way to do this in the case of the adaptive finite element method (4).

4. Residual estimators

In this section we want to derive an *a posteriori* estimation of the residual r defined in equation (7), when the discrete problem is defined by (4) and (5). If $t \in (t_{n-1}, t_n)$, then for all $v \in \mathbb{V}$,

$$\langle r|v \rangle = \varepsilon \left(\left(\frac{1}{\tau_n} + \frac{f'(I_n U_{n-1})}{\varepsilon^2} \right) (U_n - I_n U_{n-1}), v \right) + \varepsilon (\nabla U_n, \nabla v) + \frac{1}{\varepsilon} (f(I_n U_{n-1}), v) \tag{54}$$

$$+\varepsilon (\nabla (U - U_n), \nabla v) + \frac{1}{\varepsilon} (f(U) - f(U_n), v) \tag{55}$$

$$+\frac{\varepsilon}{\tau_n} (I_n U_{n-1} - U_{n-1}, v) \tag{56}$$

$$+\frac{1}{\varepsilon} (f(U_n) - f(I_n U_{n-1}) - f'(I_n U_{n-1}) (U_n - I_n U_{n-1}), v). \tag{57}$$

In this way we have clearly split the residual in three distinct contributions: a *space discretization residual* r^h in (54), a *time discretization residual* r^t in (55), and a *coarsening residual* r^c in (56). The *linearization residual* r^l in (57) is a higher order term that will eventually be neglected. We will now proceed to estimate each of them separately.

4.1. **Space discretization residual**

This contribution to the residual is actually described by the operator of the discrete problem extended to apply to the whole space $\mathbb{V}$. So in particular, in view of (4), it is clear that for $t \in (t_{n-1}, t_n)$,

$$\langle r^h|V \rangle = 0, \quad \forall V \in \mathbb{V}_n. \tag{58}$$

This so-called Galerkin orthogonality is true in particular for $V = \pi_n v$, the Clément interpolant of an arbitrary element v of $\mathbb{V}$. Therefore, from the definition of r^h and (58), it follows that in $t \in (t_{n-1}, t_n)$, for all v in $\mathbb{V}$,

$$\langle r^h | v \rangle = \varepsilon \left(\left(\frac{1}{\tau_n} + \frac{f'(I_n U_{n-1})}{\varepsilon^2} \right) (U_n - I_n U_{n-1}), v - \pi_n v \right) + \varepsilon \left(\nabla U_n, \nabla (v - \pi_n v) \right) + \frac{1}{\varepsilon} \left(f(I_n U_{n-1}), v - \pi_n v \right). \quad (59)$$

To estimate this contribution to the residual, we proceed as for a standard *elliptic* residual: we split the integrals in (59) over the elements of the triangulation, and integrate by part on each element, where the finite element functions are polynomials and therefore infinitely differentiable. Thus, for $t \in (t_{n-1}, t_n)$,

$$\langle r^h | v \rangle = \sum_{S \in \mathcal{T}_n} (R_n, v - \pi_n v)_{\mathrm{L}^2(S)} + \sum_{\gamma \in \Gamma_n} (J_n, v - \pi_n v)_{\mathrm{L}^2(\gamma)}, \quad \forall v \in \mathbb{V}, \quad (60)$$

where Γ_n is the set of all interior edges of the triangulation $\mathcal{T}_n$, and the element residual R_n and the jump residual J_n are defined respectively by

$$R_n|_S = \left(\frac{1}{\tau_n} + \frac{f'(I_n U_{n-1})}{\varepsilon^2} \right) (U_n - I_n U_{n-1}) - \varepsilon (\triangle U_n)|_S + \frac{1}{\varepsilon} f(I_n U_{n-1}), \quad \forall S \in \mathcal{T}_n, \quad (61)$$

and

$$J_n|_\gamma = \left[\frac{\partial U_n}{\partial \nu} \right]_\gamma, \quad \forall \gamma \in \Gamma_n. \quad (62)$$

Using the standard error estimates for Clément interpolation [5], we can therefore conclude that for $t \in (t_{n-1}, t_n)$

$$\langle r^h | v \rangle \le C_{Cl} \left(\| h R_n \|_{\mathrm{L}^2(\Omega)} + \left\| h^{1/2} J_n \right\|_{\mathrm{L}^2(\mathcal{T}_n)} \right) \| \nabla v \|_{\mathrm{L}^2(\Omega)}, \quad \forall v \in \mathbb{V}, \quad (63)$$

where C_{Cl} is a constant from the interpolation estimate depending only on the maximum number of neighbours a simplex can have in $\mathcal{T}_n$. This constant is independent of the mesh size h in the case of shape-regular meshes, *e.g.* adaptive meshes obtained by a bisection algorithm as in the finite element package ALBERT [12].

Remark 4.1. We stress that the mesh-dependent weights in (63) correspond to the correct scaling for the gradient ∇e of the error and *not* for e! Since ∇e does not appear explicitly in (51), we conclude that (63) is suboptimal. For linear parabolic problems, it is possible to restore the expected order *via* elliptic reconstruction [10]. The situation is much more subtle for nonlinear parabolic problems, and even more extreme if they are singularly perturbed. We refer to Section 5, where this statement is corroborated by simulations.

4.2. Time discretization residual

It is straightforward that for $t \in (t_{n-1}, t_n)$,

$$\langle r^t | v \rangle \le \varepsilon \| \nabla (U_n - U_{n-1}) \|_{\mathrm{L}^2(\Omega)} \| \nabla v \|_{\mathrm{L}^2(\Omega)} + \frac{L_f}{\varepsilon} \| U_n - U_{n-1} \|_{\mathrm{L}^2(\Omega)} \| v \|_{\mathrm{L}^2(\Omega)}, \quad \forall v \in \mathbb{V}. \quad (64)$$

4.3. Coarsening residual

It is also straightforward that for $t \in (t_{n-1}, t_n)$,

$$\langle r^c | v \rangle = (r^c, v) \le \frac{\varepsilon}{\tau_n} \| U_{n-1} - I_n U_{n-1} \|_{\mathrm{L}^2(\Omega)} \| v \|_{\mathrm{L}^2(\Omega)}, \quad \forall v \in \mathbb{V}. \quad (65)$$

4.4. **Linearization residual**

By Taylor's expansion,

$$\left|f(U_n) - f(I_nU_{n-1}) - f'(I_nU_{n-1})\,(U_n - I_nU_{n-1})\right| \leq \frac{L_{f'}}{2}\left|U_n - I_nU_{n-1}\right|^2, \tag{66}$$

so

$$\left|f(U_n) - f(I_nU_{n-1}) - f'(I_nU_{n-1})\,(U_n - I_nU_{n-1})\right| \leq L_{f'}\left|U_n - U_{n-1}\right|^2 + L_{f'}\left|U_{n-1} - I_nU_{n-1}\right|^2. \tag{67}$$

When the time-steps are small enough, these higher order terms are much smaller than the corresponding lower-order terms already present in the time residual r^t and coarsening residual r^c. We can therefore neglect them, and the linearization residual r^l will not be taken into account.

4.5. **Residual estimators**

Putting all estimators together, we conclude that for *a.e.* $t \in (0,T)$, inequality (8) holds, with $\eta_0 = \eta_0^t + \eta_0^c$ and $\eta_1 = \eta_1^h + \eta_1^t$, where

$$\eta_1^h = C_{Cl}\left(\sum_{n=1}^{N}\tau_n\left(\sum_{S\in\mathcal{T}_n}\|hR_n\|^2_{\mathrm{L}^2(S)} + \sum_{\gamma\in\Gamma_n}\left\|h^{1/2}J_n\right\|^2_{\mathrm{L}^2(\gamma)}\right)\right)^{1/2} \tag{68}$$

$$\eta_1^t = \varepsilon\left(\sum_{n=1}^{N}\tau_n\left\|\nabla\left(U_n - U_{n-1}\right)\right\|^2_{\mathrm{L}^2(\Omega)}\right)^{1/2} \tag{69}$$

$$\eta_0^t = \frac{L_f}{\varepsilon}\left(\sum_{n=1}^{N}\tau_n\left\|U_n - U_{n-1}\right\|^2_{\mathrm{L}^2(\Omega)}\right)^{1/2} \tag{70}$$

$$\eta_0^c = \varepsilon\left(\sum_{n=1}^{N}\tau_n^{-1}\left\|U_{n-1} - I_nU_{n-1}\right\|^2_{\mathrm{L}^2(\Omega)}\right)^{1/2}. \tag{71}$$

According to Theorem 3.1, control of these residual estimators via (49) and (50), for sufficiently low tolerance θ and initial error e_0, will ensure that the $\mathrm{L}^2(\Omega)$ error of the adaptive finite element approximation remains below the tolerance θ throughout the simulation.

5. Numerical experiments

We have implemented numerical simulations of the Allen–Cahn problem using the adaptive finite element package ALBERT [12]. In ALBERT, an initial simplicial macro-mesh is refined by successive bisections of its elements. It can later also be coarsened, by operations of junction of two elements which initially constituted a single element. The refining and coarsening algorithms ensure that the mesh remains conforming at every computation of each timestep of the solution. We have chosen ALBERT's error equidistribution strategy for mesh adaptation, *i.e.* both refinement and coarsening of the successive meshes based on residual estimators (68) and (71). For the following tests, we have however kept fixed time steps, since we are inclined to believe (and the tests have verified) that for the Allen–Cahn problem, fixed time-step computations lead to errors of the same order of magnitude at each time step (whereas a fixed mesh clearly does not yield the same order of magnitude of error for each element).

To perform numerical error convergence tests, we have imposed as an exact solution a propagating front, with which to compare the numerical solution by adding an extra artificial source term to the right hand side

TABLE 1. $\varepsilon = 0.08$.

i	θ	$\#DOFs$	$\max_t \min_x h$	N_τ	e	OC
0	4.00e+01	19	3.12e-02	250	1.30e-01	—
1	2.00e+01	33	1.56e-02	500	5.30e-02	1.30
2	1.00e+01	60	7.81e-03	1000	1.33e-02	2.00
3	5.00e+00	108	3.91e-03	2000	3.38e-03	1.97
4	2.50e+00	209	1.95e-03	4000	9.68e-04	1.80
5	1.25e+00	269	1.95e-03	8000	1.96e-04	2.30
6	6.25e-01	530	9.77e-04	16000	4.80e-05	2.03

of the Allen–Cahn equation: we have imposed the solution

$$\hat{u}(x,t) = \tanh\left(\frac{x_1 - 0.6t - 0.2}{\varepsilon\sqrt{2}}\right),$$

thus requiring the extra source term

$$\hat{g}(x,t) = \frac{0.6}{\varepsilon\sqrt{2}}\left(\hat{u}^2(x,t) - 1\right),$$

which is just a convenient way of writing $\partial\hat{u}/\partial t$. The imposed solution $\hat{u}$ verifies exactly the *stationary* Allen–Cahn equation for all t, which is an indication that it satisfies the "profile across the interface" required by Lemma 2.4.

Before presenting numerical results, let us mention that our earlier numerical tests have shown us that an explicit time discretization for the nonlinearity f leads to largely dominant error from time discretization. It seems that the speed of the front is not captured well. To reach a similar error as from space discretization, millions of time steps are needed even for relatively large values of ε. In contrast, the linearization approach that we later adopted (see (4)) leads to much better resolution of the interface speed and thus a much smaller time discretization error, making the use of reasonable time step sizes possible, as demonstrated in the numerical examples. Notice that the theory is essentially the same with or without linearization, or even with a fully implicit scheme. It is the numerical experiments that convinced us that the linearized implicit approach gives us the best of two worlds: *reasonable time discretization error and linear discrete equation.*

We now present a table of numerical results for the $\mathrm{L}^\infty(0,T;\mathrm{L}^2(\Omega))$ error between the numerical solution U of numerical scheme (4) with added source term $\hat{g}$ and the exact solution $\hat{u}$, for different values of ε and space dimension $d = 1$. We have decreased the space error tolerance θ linearly with the timestep τ, with ratios experimentally chosen for each value of ε in order to get efficient convergence results. We denote by N_τ the number of timesteps in the time interval $[0,T]$. Important characteristics of the adaptively refined mesh are the average number of degrees of freedom throughout a computation ($\#DOFs$), as well as the maximum in time of the minimal mesh element size ($\max_t \min_x h$), which is a characteristic of the resolution of the transition zone. The solution itself is characterized by its error $e = \|U - \hat{u}\|_{\mathrm{L}^\infty(0,T;\mathrm{L}^2(\Omega))}$. Finally, the quantity we are most interested in is the experimental order of convergence

$$OC = \frac{\ln e_i - \ln e_{i-1}}{\ln\theta_i - \ln\theta_{i-1}},$$

where i is an index for the successive tests; see Tables 1–3.

We also summarize the numerical results with graphics of the error as a function of the tolerance in log-log scale. In Figure 1, we can observe that the error does not decrease linearly with the tolerance, as would be expected if our error control was optimal, but quadratically. This can be explained by the fact that the space residual estimator we use is linear in the local mesh size h, whereas it is *a priori* expected that the L^2 error should decrease in fact as h^2. Therefore, our numerical experiments show that the theoretical results of this

TABLE 2. $\varepsilon = 0.04$.

i	θ	$\#DOFs$	$\max_t \min_x h$	N_τ	e	OC
0	4.00e+01	38	7.81e-03	1000	4.90e-02	—
1	2.00e+01	68	3.91e-03	2000	1.96e-02	1.32
2	1.00e+01	130	3.91e-03	4000	4.74e-03	2.05
3	5.00e+00	253	1.95e-03	8000	1.34e-03	1.83
4	2.50e+00	499	1.95e-03	16000	3.26e-04	2.04
5	1.25e+00	990	9.77e-04	32000	7.90e-05	2.05
6	6.25e-01	1972	9.77e-04	64000	1.86e-05	2.08

TABLE 3. $\varepsilon = 0.02$

i	θ	$\#DOFs$	$\max_t \min_x h$	N_τ	e	OC
0	4.00e+01	114	3.91e-03	4000	4.93e-02	—
1	2.00e+01	146	1.95e-03	8000	6.46e-03	2.93
2	1.00e+01	285	1.95e-03	16000	1.53e-03	2.08
3	5.00e+00	561	9.77e-04	32000	4.29e-04	1.83
4	2.50e+00	1114	9.77e-04	64000	1.04e-04	2.04
5	1.25e+00	2219	4.88e-04	128000	2.58e-05	2.01

paper are not optimal with respect to the numerical parameters; this is consistent with Remark 4.1, and is due to the energy argument. We conjecture that an optimal space residual estimator could be obtained using a duality technique, but nonstandard though if one seeks to remain rigorous throughout the derivation of the result [8].

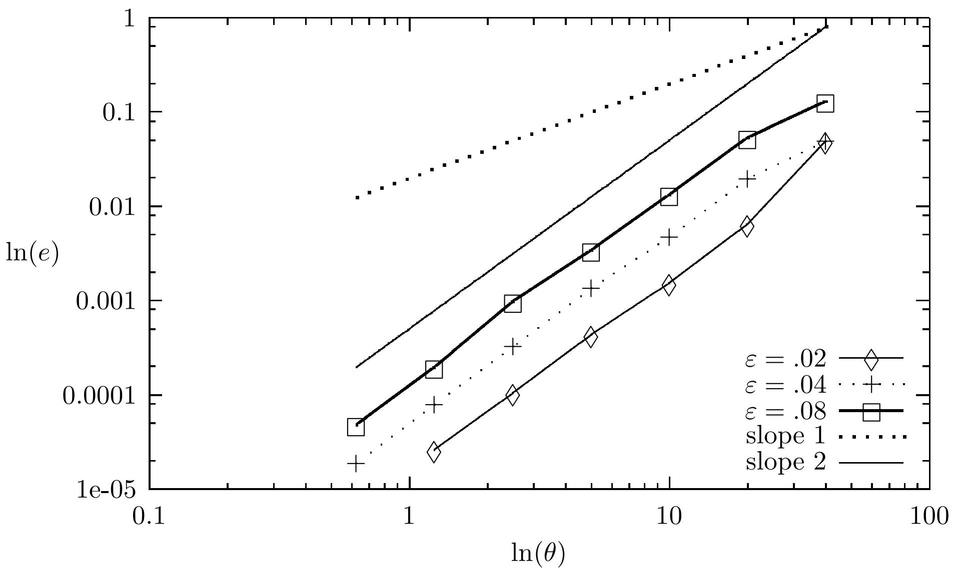

FIGURE 1. Error reduction.

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