A Posteriori Error Control of FBPs

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Abstract. A posteriori error estimators are computable quantities depending on the discrete solution(s) and data, which provide upper (and lower) bounds for the error; they are thus instrumental for adaptivity. This paper assesses the derivation of a posteriori error estimators in the context of free boundary problems (FBPs). The discussion is based on simple examples, from contact problems to curvature driven flows and crystal growth, and addresses both space and time discretization as well as both energy and maximum norm estimates (including interface error estimates).
Keywords: xx

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1. Residuals and A Posteriori Error Estimators

We consider estimating the error committed in approximating the PDE

$$u_t + \mathcal{F}(u) = f \tag{1}$$

`basic-pde`

solely relying on data and the computed solution U. This yields so-called *a posteriori* error estimates and is instrumental in modifying meshes and time steps (adaptivity). Adaptive error control is indeed a popular and exciting area of current research in science and engineering. The purpose of this paper is to survey recent results for (1) within the framework of *free boundary problems* (FBPs).

Error and Residual. Let U be the approximate solution, and let $\mathcal{R}$ be the *residual*

$$\mathcal{R} := -U_t - \mathcal{F}(U) + f, \tag{2}$$

`residual`

that is the amount by which U misses to be a solution of (1). If $e := u - U$ denotes the error, then it is satisfies the error equation

$$e_t + \mathcal{F}(u) - \mathcal{F}(U) = \mathcal{R} \tag{3}$$

`error`

Ideally, we would like to derive estimates of the form

$$C_1 \|\mathcal{R}\|_{\mathcal{Y}} \leq \|e\|_{\mathcal{X}} \leq C_1 \|\mathcal{R}\|_{\mathcal{Y}} \tag{4}$$

`equiv`

in suitable functional spaces $\mathcal{X}$ and $\mathcal{Y}$. The upper bound shows that the quantity $\|\mathcal{R}\|_{\mathcal{Y}}$ is reliable whereas the lower bound indicates it is efficient; we will focus on reliability in this paper. Key issues are to identify suitable pairs $(\mathcal{X}, \mathcal{Y})$ and evaluate the norm $\|\cdot\|_{\mathcal{Y}}$, which typically is a negative Sobolev norm.

Failure of Duality for FBPs. A popular technique from linear PDE theory to establish (4) is duality [10, 11, 13]. If $\mathcal{F}$ is Lipschitz, we can rewrite (3) as

$$e_t + \mathcal{A}e = \mathcal{R},$$

where

$$\mathcal{A}e := \int_0^1 \nabla\mathcal{F}(su + (1-s)U)\,ds.$$

If we formally multiply by $\varphi \in C^1(0,T)$ and integrate by parts over $(0,T)$ to get

$$\langle e(T), \varphi(T)\rangle = \langle e(0), \varphi(0)\rangle + \int_0^T \langle e, \varphi_t - \mathcal{A}^*\varphi\rangle + \int_0^T \langle \mathcal{R}, \varphi\rangle, \qquad (5)$$ err_intro

where $\mathcal{A}^*$ is the adjoint of $\mathcal{A}$. An error estimate follows by selecting φ in (5) as the solution of the *backward dual* problem

$$\varphi_t - \mathcal{A}^*\varphi = 0 \quad \text{in } (0,T), \qquad \varphi(T) = \rho, \qquad (6)$$ dual

and using *strong* stability properties of φ, such as a bound for φ_t in terms of ρ, for evaluating $\varphi(0)$ and $\langle \mathcal{R}, \varphi\rangle$. This program may fail to apply to the present low regularity setting because

- $\mathcal{F}$ may not be Lipschitz, and so $\mathcal{A}$ and $\mathcal{A}^*$ may be singular or not even defined;
- (6) may make no sense or φ' may be unbounded;
- φ is not computable because it depends on the unknown u;
- Replacing $\mathcal{A}$ by $\nabla\mathcal{F}(U)$ to determine φ, would lead to additional terms involving further derivatives of the possibly singular $\nabla\mathcal{F}$.

Therefore, except in special circumstances such as [5, 23], duality does not quite lead to rigorous error control for FBPs.

Plan of the Paper. We show below several novel techniques for error control applicable to FBPs. In §2 we present pointwise error estimates in space via contact problems and apply them for error control of free boundaries. In §3 we discuss error control for time discretizations using the implicit Euler method for (1) with $\mathcal{F}$ either subdifferential or angle-bounded operator (Hilbert theory), or accretive (Banach theory). We conclude in §4 with some extensions and applications.

S:space

2. Error Control in Space: Contact Problems

S:setting

2.1. Setting and Challenges

Let Ω be a bounded, polyhedral, not necessarily convex domain in $\mathbb{R}^d$ with $d \in \{1,2,3\}$. Let $f \in L^\infty(\Omega)$ be a load function, $\chi \in H^1(\Omega) \cap C^{0,\alpha}(\bar\Omega)$ be a lower obstacle, with $0 < \alpha \le 1$, which satisfies $\chi \le 0$ on $\partial\Omega$. Let $\mathcal{K}$ be the following non-empty, closed and convex subset of $\mathring{H}^1(\Omega)$:

$$\mathcal{K} := \{v \in \mathring{H}^1(\Omega) \mid v \ge \chi \text{ a.e. in } \Omega\}.$$

The variational formulation of the continuous *obstacle* problem reads as follows:

$$u \in \mathcal{K}: \qquad \langle \nabla u,\, \nabla(u - v)\rangle \le \langle f,\, u - v\rangle \qquad \text{for all } v \in \mathcal{K}. \qquad (7)$$ IE:P

Hereafter, $\langle \varphi, \psi \rangle$ denotes the scalar product in $L^2(\Omega)$ as well as the duality pairing between $\mathring{H}^1(\Omega)$ and $H^{-1}(\Omega) = \mathring{H}^1(\Omega)^*$; we refer to [12, 15, 27]. We are interested in the approximation of both the solution u in $\mathcal{X} := L^\infty(\Omega)$ and the *contact set*

$$\Lambda := \{u = \chi\} := \{x \in \Omega \mid u(x) = \chi(x)\},$$

or equivalently of the *free boundary* or *interface*

$$\mathcal{F} := \partial\{u > \chi\} \cap \Omega.$$

The location of Λ is encoded in the non-positive functional $\sigma \in H^{-1}(\Omega)$

$$\langle \sigma, \varphi \rangle := \langle f, \varphi \rangle - \langle \nabla u, \nabla \varphi \rangle \qquad \forall \varphi \in \mathring{H}^1(\Omega), \tag{8}$$ sigma

which plays the role of a *multiplier* for the unilateral constraint. In fact, we have $\sigma = f + \Delta\chi$ in the interior of the contact set $\Lambda = \{u = \chi\}$, where σ is typically < 0, and $\sigma = 0$ in the open *non-contact* set $\Omega \setminus \Lambda = \{u > \chi\}$.

Given a shape-regular partition $\mathcal{T}_h$ of Ω, the set of nodes of $\mathcal{T}_h$ is denoted by $\mathcal{N}_h$, and the subset of interior nodes by $\mathring{\mathcal{N}}_h$. Let $\mathbb{V}_h$ indicate the space of continuous piecewise affine finite element functions over $\mathcal{T}_h$ and $\mathring{\mathbb{V}}_h := \mathbb{V}_h \cap \mathring{H}^1(\Omega)$. The nodal basis functions of $\mathbb{V}_h$ are given by $(\phi_z)_{z \in \mathcal{N}_h}$, and they form a *partition of unity* of Ω, that is $\sum_{z \in \mathcal{N}_h} \phi_z = 1$. Let I_h be the Lagrange interpolation operator onto $\mathbb{V}_h$. Let $\chi_h := I_h \chi$ be the discrete obstacle. The discrete counterpart $\mathcal{K}_h$ of $\mathcal{K}$ is then

$$\mathcal{K}_h := \{v_h \in \mathring{\mathbb{V}}_h \mid v_h \geq \chi_h \text{ in } \Omega\}.$$

Note that it is sufficient to check the unilateral constraint of $\mathcal{K}_h$ only at the nodes. The set $\mathcal{K}_h$ is non-empty, convex, closed but in general not a subset of $\mathcal{K}$ (non-conforming approximation). The *discrete* obstacle problem reads as follows:

$$u_h \in \mathcal{K}_h : \quad \langle \nabla u_h, \nabla(u_h - v_h) \rangle \leq \langle f, u_h - v_h \rangle \qquad \forall v_h \in \mathcal{K}_h. \tag{9}$$ IE:Ph

Let $\omega_z = \operatorname{supp}(\phi_z)$ be the finite element star and γ_z be the union of all interior interelement boundaries (sides) in ω_z If J_h denotes the jump of the normal derivative of u_h across interior sides, we define the set of *full-contact nodes* to be

$$\mathcal{C}_h = \{z \in \mathcal{N}_h \mid u_h = \chi_h \text{ and } f \leq 0 \text{ in } \omega_z,\ J_h \leq 0 \text{ on } \gamma_z\}$$

and denote the discrete *full-contact set* and its complement by

$$\Omega_h^0 = \Big\{x \in \Omega \mid \sum_{z \in \mathcal{C}_h} \phi_z(x) = 1\Big\}, \qquad \Omega_h^+ = \Omega \backslash \Omega_h^0.$$

Furthermore we set $\Gamma_h^0 = \Gamma \cap \Omega_h^0$ and $\Gamma_h^+ = \Gamma \cap \Omega_h^+$, along with

$$\omega_z^+ = \omega_z \cap \Omega_h^+, \qquad \gamma_z^+ = \gamma_z \cap \Omega_h^+. \tag{10}$$ ^+

To shed some light on the inherent difficulties in estimating $\|e\|_{L^\infty(\Omega)}$ we consider the following 1d examples. The estimator should possess the properties:

- Be insensitive (apart from oscillations) to the forcing term f within Ω_h^0, which should not dictate mesh quality (*localization*). Figure 1 illustrates this property since the meshes are rather coarse in the contact sets.

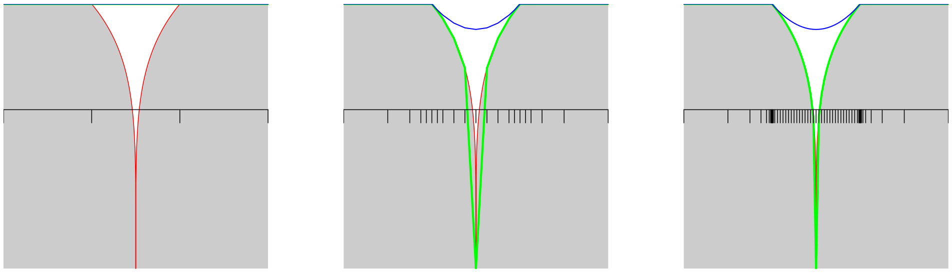

FIGURE 1. Localization for an obstacle with downward cusp

F:localization1

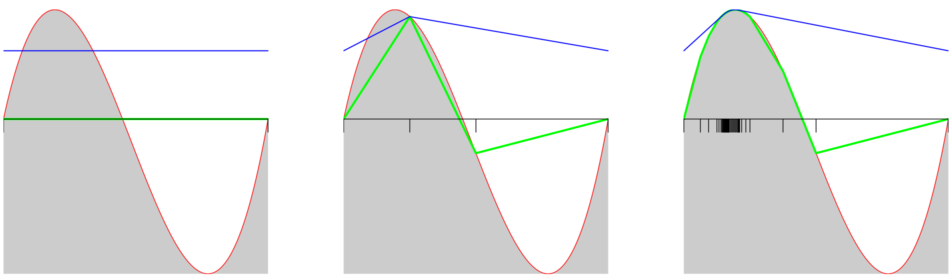

FIGURE 2. Localization for an obstacle not resolved on coarse grids

F:localization3

- Be insensitive to the obstacle within Ω_h^+ and thus reduce to the usual estimator for the (unconstrained) Laplacian. This effect is shown in Figure 1: the refinement is due to the curvature generated by $f = -1$ but not to the cusp of χ pointing downwards. Overall there is an excellent accuracy for u in the non-contact set even though the approximation of χ is rather rough.
- Be able to detect the non-conforming situation $\chi > u_h$, and refine accordingly. This is depicted in Figure 2, where the concave part of χ above u_h is detected early on and thereby the solution is lifted up.

Let $\Pi_h : L_1(\Omega) \to \mathring{\mathbb{V}}_h$ be the interpolation operator of [4]; see also [26]. Such a Π_h is both *positivity preserving* and *second order* accurate, and is crucial to define the discrete counterpart σ_h of σ: let $\sigma_h \in H^{-1}(\Omega)$ be $\langle \sigma_h, \varphi \rangle := \sum_{z \in \mathcal{N}_h} \langle \sigma_h, \varphi\, \phi_z \rangle$, where

$$\begin{aligned}\langle \sigma_h, \varphi\, \phi_z \rangle := \int_{\Omega_h^0} R_h\, \varphi\, \phi_z + \int_{\Gamma_h^0} J_h \varphi\, \phi_z \\ + \int_{\Omega_h^+} R_h\, (\Pi_h \varphi)(z)\, \phi_z + \int_{\Gamma_h^+} J_h\, (\Pi_h \varphi)(z)\, \phi_z,\end{aligned} \tag{11}$$

eq:sigmah

for all $z \in \mathcal{N}_h$ and $\varphi \in \mathring{H}^1(\Omega)$. Note that $\Pi_h \varphi$ is evaluated at the node z, and is thus a *constant* for each $z \in \mathcal{N}_h$. It turns out that

$$z \in \mathcal{N}_h \setminus \mathcal{C}_h \implies \langle \sigma_h, \varphi\,\phi_z \rangle = (\Pi_h \varphi)(z)\, s_z, \tag{12}$$

sigmaz_for_nfc

where s_z is a *nodal* multiplier:

$$s_z := \int_\Omega f\,\phi_z + \int_\Gamma J_h \phi_z, \qquad z \in \mathcal{N}_h. \tag{13}$$

eq:sigmaz

Moreover, s_z satisfies $s_z \le 0$ whenever $z \in \mathring{\mathcal{N}}_h \cup \mathcal{C}_h$ and $\sigma_h \le 0$. We finally let

$$\Lambda_h := \bigcup \{\omega_z : z \in \mathring{\mathcal{N}}_h \cup (\mathcal{C}_h \cap \partial\Omega) \text{ and } s_z < 0\} \tag{14}$$

contact-set

The discrete multiplier σ_h exhibits the following crucial properties:

- Cancellation with σ inside the discrete full contact set Ω_h^0;
- Localization to the non-contact set Ω_h^+;
- Non-positivity due to the use of Π_h in the discrete non-contact set Ω_h^+;
- Even though σ_h is non-computable, we only need the nodal multiplier s_z in (14) and Theorem 2.1 below.

:point-apost

2.2. Pointwise A Posteriori Error Estimates for Solutions

Let η_z be the star-based residual indicator

$$\eta_z := h_z^2 \|(f - \hat{f}_z)\,\phi_z\|_{0,\infty;\omega_z^+} + h_z\,\|J_h\,\phi_z\|_{0,\infty;\gamma_z^+}, \tag{15}$$

star_z

where ω_z^+, γ_z^+ are defined in (10) and $\hat{f}_z$ is any constant provided $\int_{\Omega_h^+} f\,\phi_z + \int_{\Gamma_h^+} J_h\,\phi_z = 0$ and 0 otherwise. The interior residual reduces to *oscillation* of f.

T:upper

Theorem 2.1 (Reliability). *Let u be the continuous solution satisfying* (7) *and let u_h be the discrete solution satisfying* (9)*, respectively. Then the following global a posteriori upper bound holds:*

$$\|u - u_h\|_{0,\infty;\Omega} \le \mathcal{E}_h, \tag{16}$$

estimator

where the error estimator $\mathcal{E}_h$ is given by

$$\begin{aligned} \mathcal{E}_h &:= C_* |\log h_{\min}|^2 \ \max\nolimits_{z\in\mathcal{N}_h} \eta_z && \textit{localized residual} \\ &\quad + \|(\chi - u_h)^+\|_{0,\infty;\Omega} + \|(u_h - \chi)^+\|_{0,\infty;\Lambda_h} && \textit{localized obstacle approx.} \end{aligned}$$

C_* is a constant solely depending on mesh regularity, and Λ_h is defined in (14)*.*

The derivation of this optimal bound is done as follows. We first note that both σ and σ_h are designed to restore the equality in (7) and (9). We then form the so-called *Galerkin functional* $\mathcal{G}_h \in H^{-1}(\Omega)$:

$$\langle \mathcal{G}_h, \varphi \rangle = \langle \nabla(u - u_h), \nabla\varphi \rangle + \langle \sigma - \sigma_h, \varphi \rangle = -\langle \nabla u_h, \nabla\varphi \rangle + \langle f - \sigma_h, \varphi \rangle\,.$$

This concept, introduced in [31], plays the role of residual in the linear setting. A simple manipulation reveals the localization effect built in (11), namely,

$$\langle \mathcal{G}_h, \varphi \rangle = \int_{\Omega_h^+} f[\varphi - \Pi_h \varphi] + \int_{\Gamma_h^+} J_h\,[\varphi - \Pi_h \varphi]. \tag{17}$$

Gh-local

We next let $w \in \mathring{H}^1(\Omega)$ be the the Riesz representation of $\mathcal{G}_h$, namely $-\Delta w = \mathcal{G}_h$, and use (17) to derive the pointwise estimate

$$\|w\|_{0,\infty;\Omega} \leq C|\log h_{\min}|^2 \max_{z\in\mathcal{N}_h} \eta_z.$$

Such w is employed to correct u_h and thereby construct barrier functions for (7), which are of the form $u_h + w \pm \|w\|_{0,\infty;\Omega}$ plus additional terms involving $u_h - \chi$. The *continuous* maximum principle allows us to compare these barriers with u and derive (16). A full proof is given in [25]. We also refer to [24, 25] for lower bounds.

Example: Lipschitz Obstacle. Let $\Omega := \{x \in \mathbb{R}^2 : |x|_1 < 1\}$, $f := -5$, and the obstacle be $\chi(x) := \mathrm{dist}(x, \partial\Omega) - \frac{1}{5}$. The corresponding multiplier σ is a measure singular with respect to the Lebesgue measure since it has a mass supported along the edges of the pyramid within the contact set.

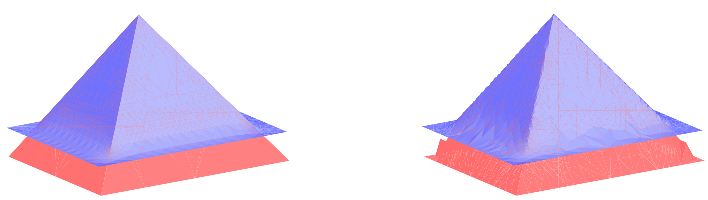

FIGURE 3. Discrete solution and obstacle on grids aligned with the edges of the obstacle (left) and non-aligned (right).

F:pw-linear

Figure 3 displays u_h and χ_h over two meshes, one aligned and the other non-aligned with the edges of χ: in the latter the representation χ_h of χ is rather crude. In contrast, the aligned meshes provide excellent approximability of χ, and the full localization property of $\mathcal{E}_h$ is clearly reflected in the meshes on the left of Figure 4): the refinement along the diagonals is avoided. This is a distintive improvement of the estimator of [25] with respect to the partially localized estimator of [24]. The refinement for the non-aligned meshes is instead due to lack of resolution of χ and thus of u (see right of Figure 4). Note that the non-aligned grids do not satisfy the discrete maximum principle.

:barrier-set

2.3. A Posteriori Error Estimates for Interfaces: Barrier Sets

The fact that the estimator $\mathcal{E}_h$ controls the pointwise error $\|u - u_h\|_{0,\infty;\Omega}$ allows in certain situations for more accurate *a posteriori* information on Λ and also on the exact free boundary (or interface) $\mathcal{F}$. We consider the nondegenerate situation when one knows $\lambda > 0$ such that

$$\langle f, \varphi\rangle - \langle \nabla\chi, \nabla\varphi\rangle \;\leq\; -\lambda \int_\Omega \varphi, \qquad \forall\varphi \in \mathring{H}^1(\Omega), \varphi \geq 0. \tag{18}$$

stable

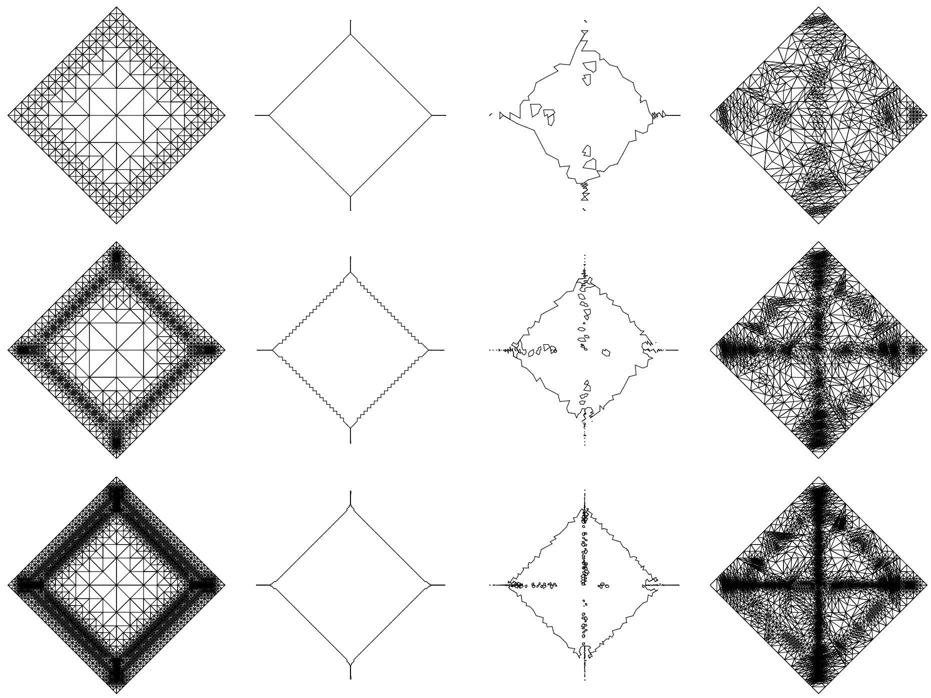

FIGURE 4. Grids and $\partial\{u_h = \chi_h\}$ on grids aligned to the edges of the obstacle (left) and non-aligned (right) for adaptive iterations $j = 1, 7, 15$. The benefits of full localization are apparent since the refinement on the diagonals in contact is avoided (left).

F:grid-inter

Condition (18) guarantees *stability* of the exact free boundary $\mathcal{F}$ and is due to CAFFARELLI [2]; see also [12, §2.10]. This condition has been crucial in the a priori error analysis of free boundaries [1, 19] as well. If

$$r_h^2 := \frac{2d}{\lambda}\Big(2\mathcal{E}_h + \|(\chi_h - \chi)^+\|_{0,\infty;\{u_h \le \chi_h + \mathcal{E}_h\}}\Big). \qquad (19) \quad \boxed{\texttt{rh}}$$

we then define $K := \{\text{dist}(\cdot, \partial\Omega) \ge r_h\}$ and the *barrier sets*

$$\Lambda^* := \{u_h \le \chi + \mathcal{E}_h\}, \qquad \Lambda_* := \Big\{\text{dist}\big(\cdot, \{u_h \ge \chi_h + \mathcal{E}_h\}\big) \ge r_h\Big\}. \qquad (20) \quad \boxed{\texttt{sets}}$$

The following result, based on Theorem 2.1, locates the exact contact set Λ and the free boundary $\mathcal{F}$ a posteriori.

T:Interface **Theorem 2.2** (A posteriori control of contact set and interface). *The set Λ^* is an upper barrier set for the exact contact set $\Lambda = \{u = \chi\}$, i.e. $\Lambda \subset \Lambda^*$.*

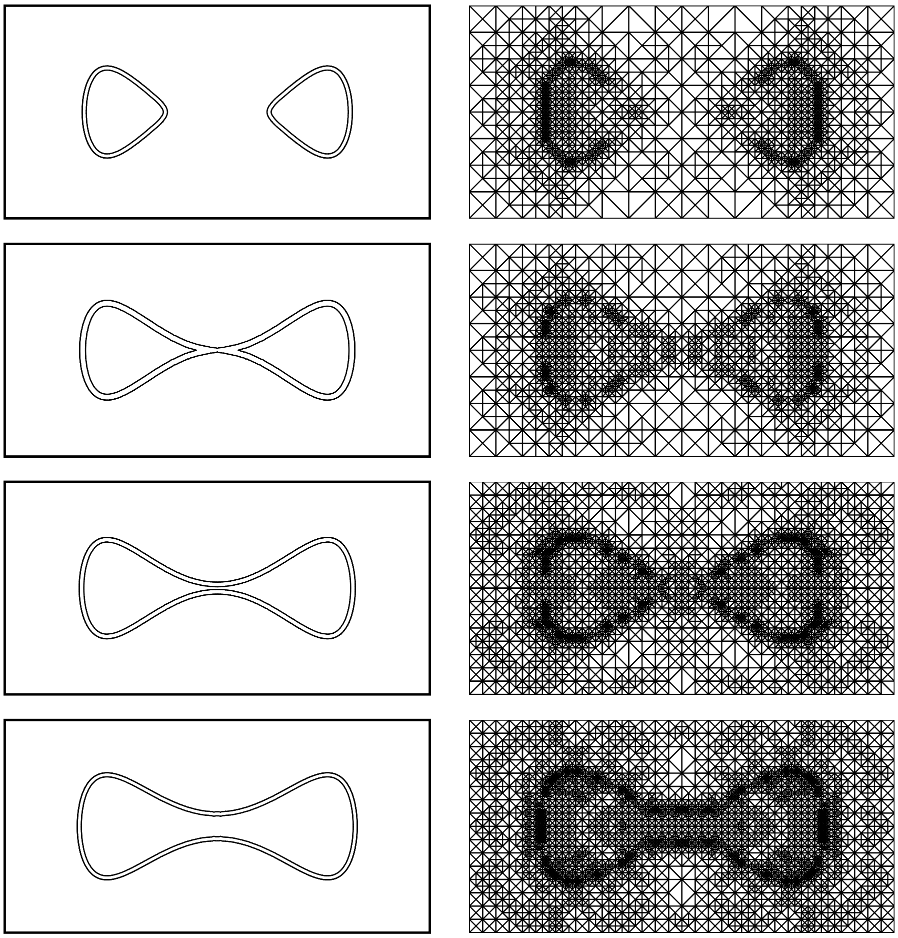

FIGURE 5. From balls to bones: Interface barriers for tolerance ≈ 0.01 (left) and adaptive grids for tolerance ≈ 0.15 (right) in 2d for forcing term $f = 0, -5.9, -8.1, -15$ (from top to bottom). The distance of the barriers is ≈ 0.05 for all four forces.

F:topo-change-2d

Moreover, if the stability condition (18) *holds, then the set* Λ_* *is a lower barrier set for* Λ *in the sense that* $\Lambda_* \cap K \subset \Lambda \cap K$, *whence*

$$\mathcal{F} \cap K \subset \big(\Lambda^* \cap K\big) \setminus \operatorname{int}\big(\Lambda_* \cap K\big).$$

A proof is given in [25]. Note that λ dictates the thickness of the strips $\Omega \setminus K$ and $\big(\Lambda^* \cap K\big) \setminus \operatorname{int}\big(\Lambda_* \cap K\big)$, and thus acts as a condition number for the free boundary. Also, if $\chi \in H^2(\Omega)$, one can adaptively compute the condition number λ by $\lambda = -\sup_{\{u_h \le \chi_h + \mathcal{E}_h\}}(f + \Delta\chi)$. This is used in the following example.

Example: From Balls to Bones. Let $\Omega = (-2,2) \times (-1,1)$ and the obstacle be $\chi(x) = 10 - 6(x_1^2 - 1)^2 - 20(|x|^2 - x_1^2)$, which consists of two hills connected by a saddle. The left column in Figure 5 illustrates the interface barriers for four constant loads $f = 0, -5.9, -8.1, -15$ for about the same tolerance $\tau \approx 0.01$; the exterior curves correspond to $\partial\Lambda^*$ whereas the interior curves display $\partial\Lambda_*$. For $f = 0$, the contact set does not contain the saddle, whereas, for $f = -15$, it does. This happens because the solution, being pushed down by f, adheres longer to the obstacle. During the transition between these two extreme cases, the free boundary has a singular point, namely a "double-cusp" at the origin, for some critical value f_{crit}. The barrier sets Λ_*, Λ^* give a reliable range for f_{crit}; see [25]. Although $\mathcal{F}$ develops a singularity, it is worth noticing that $u \in W^2_\infty(\Omega)$ and thus no special refinement is needed to approximate u Moreover, $f + \Delta\chi \leq -16$ in Ω for the 4 loads, which shows that the double-cusp is not due to lack of stability. The interface estimate of Theorem 2.2 thus applies and provides a posteriori error control of the entire free boundary including the double-cusp.

3. Error Control in Time

S:time

Given the abstract PDE in either Hilbert or Banach space

$$u_t + \mathcal{F}(u) = 0, \tag{21}$$

ode

we now derive error estimates without regularity assumptions on $\mathcal{F}$ for

$$\frac{1}{\tau_n}\big(U_n - U_{n-1}\big) + \mathcal{F}(U_n) = 0. \tag{22}$$

euler

Let $U(t)$ be the piecewise linear interpolant of $\{U_n\}_{n=0}^N$ and $e := u - U$.

3.1. Hilbert Theory: Subdifferential Operators

S:hilbert

Let $\mathcal{H}$ be a Hilbert space, with scalar product $\langle\cdot,\cdot\rangle$ and norm $|\cdot|$, and let $\phi : \mathcal{H} \to \mathbb{R} \cup \{\infty\}$ be a proper lower semicontinuous convex function, with domain $D(\phi)$. Let $\mathcal{F} = \partial\phi : \mathcal{H} \to 2^{\mathcal{H}}$ be the *subdifferential* of ϕ, with domain $D(\mathcal{F}) \subset D(\phi)$. Then (21) is equivalent to

$$\langle u_t, u - v\rangle + \phi(u) - \phi(v) \leq 0 \qquad \forall v \in D(\phi), \tag{23}$$

vi-c

and satisfies the energy identity

$$|u_t(t)|^2 + \tfrac{d}{dt}\phi(u(t)) = 0 \quad \text{a.e. } t \in (0,T), \tag{24}$$

energy_ODE

Energy Dissipation Estimator. On the other hand, (22) is equivalent to

$$\frac{1}{\tau_n}\langle U_n - U_{n-1}, U_n - v\rangle + \phi(U_n) - \phi(v) \leq 0, \qquad \forall v \in D(\phi), \tag{25}$$

vi-d

which, upon taking $v = U_{n-1}$, yields the discrete energy inequality

$$-\mathcal{E}_n := \left|\frac{U_n - U_{n-1}}{\tau_n}\right|^2 + \frac{\phi(U_n) - \phi(U_{n-1})}{\tau_n} \leq 0 \quad \forall\, 1 \leq n \leq N. \tag{26}$$

energy_DODE

The discrete quantity $\mathcal{E}_n \geq 0$ in (26) is thus a measure of the deviation of $\{U_n\}_{n=0}^N$ from satisfaction of the conservation form (24).

T:apost-1 **Theorem 3.1.** *If* $U_0 \in D(\phi)$, *then* $\max_{t\in[0,T]} |e(t)|^2 \leq |e(0)|^2 + \sum_{n=1}^N \tau_n^2 \mathcal{E}_n$.

Proof. We first write a *continuous* evolution variational inequality for U

$$\langle U_t(t), U(t) - v\rangle + \phi(U(t)) - \phi(v) \leq \mathcal{R}(t), \quad \forall v \in D(\phi), \tag{27}$$ cont_DEVI

where $\mathcal{R}(t)$ is a residual term, independent of the test function v, given by

$$\mathcal{R}(t) := \langle U'(t), U(t) - U_n\rangle + \phi(U(t)) - \phi(U_n), \quad \forall t \in (t_{n-1}, t_n).$$

We next estimate $\mathcal{R}(t)$. In view of the elementary identity

$$U(t) - U_n = \frac{t - t_n}{\tau_n}(U_n - U_{n-1}) = (t - t_n)U'(t),$$

and the convexity of ϕ

$$\phi(U(t)) \leq \frac{t_n - t}{\tau_n}\,\phi(U_{n-1}) + \frac{t - t_{n-1}}{\tau_n}\,\phi(U_n),$$

(26) implies $\mathcal{R}(t) \leq (t_n - t)\mathcal{E}_n$. Finally, choosing $v = U(t)$ in (23), $v = u(t)$ in (27), and adding the two inequalities, we see that the terms involving ϕ cancel out and we end up with the error inequality

$$\tfrac{1}{2}\tfrac{d}{dt}|e(t)|^2 \leq (t_n - t)\mathcal{E}_n \quad \text{a.e. } t \in (t_{n-1}, t_n).$$

Upon integration in time, this upper bound readily implies the assertion. □

Monotone Residual Estimator. The discrete counterpart of the dissipation energy inequality $\frac{d}{dt}|u'(t)|^2 \leq 0$, namely,

$$\tau_n^{-2}\left|U_n - U_{n-1}\right|^2 \leq \tau_{n-1}^{-2}\left|U_{n-1} - U_{n-2}\right|^2 \quad \forall\, 1 \leq n \leq N, \tag{28}$$ disres

can be derived as follows. Taking $v = U_n$ in (25) at the time-step $n-1$, with $U_{-1} := U_0 - \tau_0 \mathcal{F}(U_0)$, we find

$$\tau_{n-1}^{-1}\langle U_{n-1} - U_{n-2}, U_{n-1} - U_n\rangle + \phi(U_{n-1}) - \phi(U_n) \leq 0. \tag{29}$$ disres1

Dividing (29) by τ_n and replacing it into (26), (28) follows from the elementary inequality $2\langle v - w, v\rangle \geq |v|^2 - |w|^2$ for $v, w \in \mathcal{H}$. Recalling (22), we also deduce a crucial bound of $\mathcal{E}_n$ in terms of a monotone residual estimator $\mathcal{D}_n$:

$$\mathcal{E}_n \leq \tau_n^{-1}\langle \mathcal{F}(U_n) - \mathcal{F}(U_{n-1}), U_n - U_{n-1}\rangle =: \mathcal{D}_n. \tag{30}$$ res

Combining (30) with Theorem 3.1 yields the following error estimate.

T:apost-2 **Theorem 3.2.** $\max_{t\in[0,T]} |e(t)|^2 \leq |e(0)|^2 + \sum_{n=1}^N \tau_n^2 \mathcal{D}_n$.

Rate of Convergence. We now prove that the estimates in Theorems 3.1 and 3.2 give rise to upper bounds of the error with respect to the largest time-step τ (*a priori* bounds). A simple first result is directly suggested by (26), which implies

$$0 \leq \tau_n \mathcal{E}_n \leq \phi(U_{n-1}) - \phi(U_n).$$

Therefore, we end up with a telescopic sum

$$\sum_{n=1}^{N} \tau_n^2 \mathcal{E}_n \le \tau \sum_{n=1}^{N} \big(\phi(U_{n-1}) - \phi(U_n)\big) = \tau\big(\phi(U_0) - \phi(U_N)\big).$$

Without loss of generality we may assume $\phi \ge 0$, for otherwise we may add an affine function. We then obtain a rate of convergence of order $O(\sqrt{\tau})$

T:apost-3 **Theorem 3.3.** *If* $U_0 \in D(\phi)$, *then* $\max_{t\in[0,T]} |e(t)|^2 \le |e(0)|^2 + \phi(U_0)\,\tau$.

On the other hand, making use of (25), in conjunction with (30), we can rewrite the monotone residual estimator $\mathcal{D}_n$ as follows:

$$\mathcal{D}_n = \langle \mathcal{F}(U_{n-1}) - \mathcal{F}(U_n), \mathcal{F}(U_n)\rangle.$$

By virtue of property $\mathcal{D}_n \ge 0$ and inequality $2\langle v-w, v\rangle \ge |v|^2 - |w|^2$, we then see that $\sum_{n=1}^{N} \mathcal{D}_n$ telescopes

$$2\sum_{n=1}^{N} \tau_n^2 \mathcal{D}_n \le \tau^2 \sum_{n=1}^{N} \big(|\mathcal{F}(U_{n-1})|^2 - |\mathcal{F}(U_n)|^2\big) \le \tau^2 |\mathcal{F}(U_0)|^2.$$

We then obtain the following *linear* rate of convergence.

T:apost-4 **Theorem 3.4.** *If* $U_0 \in D(\mathcal{F})$, *then* $\max_{t\in[0,T]} |e(t)|^2 \le |e(0)|^2 + \frac{1}{2}|\mathcal{F}(U_0)|^2\tau^2$.

We point out that no regularity of ϕ or $\mathcal{F}$ has been used as well as no constraints between consecutive time-steps. We stress that the *a priori* rate of convergence depends on the regularity of u_0, which dictates the size of $|e(0)|$. We also note that a linear rate of convergence cannot be expected in general for monotone operators without further structure [28]. We finally refer to [29] for extensions to the Wasserstein metric.

Examples. We consider two prototype parabolic FBPs for which duality does not give optimal results. The first one is the *parabolic obstacle problem* in $\mathcal{H} = L_2(\Omega)$:

$$u \ge \chi: \quad \langle u_t, u - v\rangle + \langle \nabla u, \nabla(u-v)\rangle. \quad \forall\, v \ge \chi.$$

If we denote $Z_n := \Delta U_n - \frac{1}{\tau_n}(U_n - U_{n-1})$ the discrete multiplier corresponding to the unilateral constraint, then

$$\mathcal{D}_n = \frac{1}{\tau_n}\|\nabla(U_n - U_{n-1})\|^2_{L^2(\Omega)} + \frac{1}{\tau_n}\langle Z_n - Z_{n-1}, U_n - U_{n-1}\rangle.$$

The second example is *degenerate parabolic problems* in $\mathcal{H} = H^{-1}(\Omega)$, which for β non-decreasing read

$$u_t - \Delta\beta(u) = 0.$$

Then

$$\mathcal{D}_n = \frac{1}{\tau_n}\langle \beta(U_n) - \beta(U_{n-1}), U_n - U_{n-1}\rangle.$$

ngle-bounded

3.2. Hilbert Theory: Angle-Bounded Operators

Angled-bounded operators form a class of monotone operators larger than subdifferential for which optimal error control is possible. They satisfy for $\gamma > 0$

$$\langle \mathcal{F}(v) - \mathcal{F}(w),\, w - z\rangle \le \gamma \,\langle \mathcal{F}(v) - \mathcal{F}(z),\, v - z\rangle \quad \forall v, w, z \in D(\mathcal{F}).$$

T:apost-5

Theorem 3.5. *The results of Theorems 3.2 and 3.4 are valid for $\mathcal{F}$ angle-bounded.*

Example. We consider the convection-diffusion equation in $\mathcal{H} = L^2(\Omega)$:

$$\mathcal{F}(v) = -\nu^2 \Delta v + b \cdot \nabla v + cv$$

If $|b(x)| \le b_0$ and $d(x) = -\frac{1}{2}\mathrm{div} b(x) + c(x) \ge d_0^2$, then we prove in [22] that

$$\gamma^2 = \frac{1}{4}\Big(1 + \frac{b_0^2}{\nu^2(d_0^2 + \nu^2 p_0^2)}\Big),$$

where p_0 is the Poincaré constant for zero Dirichlet boundary values, along with the optimal a posteriori error estimate

$$\|u - U\|^2_{L_\infty(0,T;L_2(\Omega))},\ \nu^2\|\nabla(u - U)\|^2_{L_2(0,T;L_2(\Omega))} \le \|u_0 - U_0\|^2_{L_2(\Omega)}$$
$$+ 2\gamma^2 \sum_{n=1}^N \tau_n^2 \Big(\int_\Omega \nu^2 \|\nabla(U_n - U_{n-1}\|^2_{L_2(\Omega)} + d(x)\|U_n - U_{n-1}\|^2_{L_2(\Omega)}\Big).$$

3.3. Banach Theory: Accretive Operators

We consider now a Banach space $\mathcal{B}$ with norm $\|\cdot\|$ and dual $\mathcal{B}^*$. Let $\langle\cdot,\cdot\rangle$ be the duality pairing between $\mathcal{B}$ and $\mathcal{B}^*$, and let $J : \mathcal{B} \to 2^{\mathcal{B}^*}$ be the subdifferential of the norm, which satisfies $\|v\| = \langle v, J(v)\rangle$ for all $v \in \mathcal{B}$. Let $\mathcal{F} : \mathcal{B} \to 2^{\mathcal{B}}$ be a (multivalued) *accretive* operator, namely,

$$\big\langle \mathcal{F}(u) - \mathcal{F}(v), J(u - v)\big\rangle \ge 0 \quad \forall\, u, v \in D(\mathcal{F}). \tag{31}$$ j-accretivity

If $\bar U(t) = U_n$ for $t_{n-1} \le t < t_n$ is a piecewise constant interpolant of $\{U_n\}_{n=0}^N$, then (22) also reads

$$U_t(t) + \mathcal{F}(\bar U(t)) = 0 \quad \text{a.e. in } (0,T). \tag{32}$$ easy-DODE

If, to derive an error bound, we naively take the difference of (21) and (32), and multiply it by $J(u(t) - \bar U(t))$ to exploit (31), we realize that $\langle u_t - U_t, J(u - \bar U)\rangle$ is no longer the derivative of $\|u - U\|$. The difficulty of dealing with two strong nonlinearities, $\mathcal{F}$ and J, arises and prevents us from deriving error bounds. We are thus forced to deal with the continuous and the discrete equations separately; below are the crucial steps of our argument. We refer to [20] for details.

Evolution Equation for the Continuous Solution. Since J is the subdifferential of the norm, (21) is in fact equivalent of the evolution equation

$$\frac{d}{dt}\|u(t) - v\| = -\big\langle \mathcal{F}(u(t)), J(u(t) - v)\big\rangle \quad \forall\, v \in D(\mathcal{F}), \tag{33}$$ eq:126

which we will try to reproduce in the discrete setting, starting from (32).

Evolution Inequalities for the Discrete Solutions. The map $s \mapsto \|U(s) - V\|$ is convex in each interval $(t_{n-1}, t_n]$ and therefore its derivative is not decreasing and it is bounded by its value at $s = t_n$. Then, for all $V \in \mathcal{B}$ and a.e. $t \in (0, T)$

$$\frac{d}{ds}\|U(s) - V\| = \langle U_s(s), J(U(s) - V)\rangle \le \langle U_s(s), J(\bar{U}(s) - V)\rangle.$$

Combining (32) with (**??**), for all $V \in \mathcal{B}$ and a.e. $t \in (0, T)$, we obtain

$$\frac{d}{ds}\|U(s) - V\| \le -\langle \mathcal{F}(\bar{U}(s)), J(\bar{U}(s) - V)\rangle. \tag{34}$$

eq:127

Doubling Variables. To combine (33) with (34) via (31), we would like to choose $v := U$ and $V := u$ and add the equations. However, it is *impossible* to write (33), (34) at the same time "$t = s$", since we derived the equations with respect to *time-independent* test "elements" v, V. Therefore we keep two distinct "time" variables t, s and choose $v := \bar{U}(s),\ V := u(t)$ obtaining, by (31),

$$\frac{\partial}{\partial s}\|U(s) - u(t)\| + \frac{\partial}{\partial t}\|\bar{U}(s) - u(t)\| \le 0. \tag{35}$$

eq:128

Penalization. To prevent t and s from getting too far apart, we penalize their distance with a parameter $\varepsilon \in (0, T)$, and thus integrate (35) in the 2d strip

$$S^{\varepsilon}_{0,T} := \big\{(s,t) \in \mathbb{R}^2 : 0 \le t \le T, \quad t - \varepsilon \le s \le t\big\}. \tag{36}$$

eq:stripQe0T

In order to deal with negative values of s, we extend $U, \bar{U}$ in $(-\varepsilon, 0)$ by

$$\bar{U}(s) := U_0, \quad U(s) := U_0 - s\mathcal{F}(U_0) \tag{37}$$

eq:129

so that (32) still holds. Applying the Gauss-Green formula in $S^{\varepsilon}_{0,T}$ gives

$$\begin{aligned}\int_{T-\varepsilon}^{T} \|\bar{U}(s) - u(T)\|\, ds &\le \varepsilon\|u_0 - U_0\| \\ &+ \int_0^T \Big(\|\bar{U}(t) - u(t)\| - \|U(t) - u(t)\|\Big)\, dt \\ &+ \int_0^T \Big(\|U(t-\varepsilon) - u(t)\| - \|\bar{U}(t-\varepsilon) - u(t)\|\Big)\, dt.\end{aligned} \tag{38}$$

eq:130

Stability. We take the difference between two consecutive equations (22), and multiply by $J(U_n - U_{n-1})$, to arrive at

$$\begin{aligned}\frac{1}{\tau_n}\big\langle U_n - U_{n-1}, J(U_n - U_{n-1})\big\rangle + \big\langle \mathcal{F}(U_n) - \mathcal{F}(U_{n-1}), J(U_n - U_{n-1})\big\rangle \\ = \frac{1}{\tau_{n-1}}\big\langle U_{n-1} - U_{n-2}, J(U_n - U_{n-1})\big\rangle.\end{aligned}$$

Making use of (31), together with property $\langle v, j(w)\rangle \le \|v\|$ for all $v \in \mathcal{B}$ with equality for $w = v$, we get

$$\frac{1}{\tau_n}\|U_n - U_{n-1}\| \le \frac{1}{\tau_{n-1}}\|U_{n-1} - U_{n-2}\|, \quad \forall\ 1 \le n \le N.$$

If we now choose $U_{-1} = U_0 - \tau_0 \mathcal{F}(U_0)$ with $\tau_0 \le \varepsilon$, which is consistent with (37), recursion yields the following discrete stability estimate:

$$\sup_{t\in(0,T)} \|U_t(t)\| = \sup_{1\le n\le N} \frac{1}{\tau_n} \|U_n - U_{n-1}\| \le \|\mathcal{F}(U_0)\|. \qquad (39)$$ eq:131

A Posteriori Error Estimate. Since

$$\|\bar U(t) - u(t)\| - \|U(t) - u(t)\| \le \|\bar U(t) - U(t)\|,$$
$$\|U(t-\varepsilon) - u(t)\| - \|\bar U(t-\varepsilon) - u(t)\| \le \|\bar U(t-\varepsilon) - U(t-\varepsilon)\|,$$

and $\int_{-\varepsilon}^0 \|\bar U(t) - U(t)\| dt = \frac{\varepsilon}{2}\|\mathcal{F}(U_0)\|$, a simple manipulation of (38) implies

$$\frac{1}{\varepsilon}\int_{T-\varepsilon}^T \|U(s) - u(T)\|\, ds \le \frac{1}{\varepsilon}\int_{T-\varepsilon}^T \big(\|\bar U(s) - u(T)\| + \|\bar U(s) - U(s)\|\big) ds$$
$$\le \|u_0 - U_0\| + \frac{\varepsilon}{2}\|\mathcal{F}(U_0)\| + \frac{2}{\varepsilon}\int_0^T \|\bar U(t) - U(t)\|\, dt$$

Since

$$\int_0^T \|U(t) - \bar U(t)\|\, dt = \frac{1}{2}\sum_{n=1}^N \tau_n \|U_n - U_{n-1}\|,$$

and (39) leads to

$$\frac{1}{\varepsilon}\int_{T-\varepsilon}^T \|U(s) - U(T)\|\, ds \le \frac{\varepsilon}{2}\|\mathcal{F}(U_0)\|, \qquad (40)$$ eq:132

we readily infer that

$$\|u(T) - U(T)\| \le \|u_0 - U_0\| + \varepsilon\|\mathcal{F}(U_0)\| + \frac{1}{\varepsilon}\sum_{n=1}^N \tau_n \|U_n - U_{n-1}\|.$$

Upon *optimizing* ε, we conclude the desired a posteriori error bound.

T:apost-6 **Theorem 3.6.** *If* $U_0 \in D(\mathcal{F})$, *then*

$$\|e(T)\| \le \|e(0)\| + 2\|\mathcal{F}(U_0)\|^{1/2}\Big(\sum_{n=1}^N \tau_n \|U_n - U_{n-1}\|\Big)^{1/2}.$$

The idea of doubling the variables and penalizing goes back to Kružkov for first order conservation laws [16].

A Priori Error Estimate. To show that the above error bound exhibits the correct asymptotic order of convergence, we resort to (39) to deduce

$$\sum_{n=1}^N \tau_n \|U_n - U_{n-1}\| \le \tau T \|\mathcal{F}(U_0)\|.$$

This yields the following celebrated a priori estimate of Crandall and Liggett [7], originally derived for constant time steps:

$$\|e(T)\| \le \|e(0)\| + 2\|\mathcal{F}(U_0)\|\sqrt{\tau T}. \qquad (41)$$ c-1

S:extensions

4. Extensions

We finally discuss briefly two extensions. We refer to [17, 18] for details.

S:mcf

4.1. Mean Curvature Flow of Graphs

Let a surface $\Gamma(t)$ be described by the graph $u : \Omega \times [0,T] \to \mathbb{R}$. Let

$$Qu := \big(1 + |\nabla u|^2\big)^{1/2}, \quad Nu := (\nabla u, -1)/Qu, \quad Vu := \partial_t u/Qu,$$

be the elementary area, the unit normal vector and the scalar normal velocity. We assume that $\Gamma(t)$ according to the geometric law

$$\frac{\partial_t u}{Qu} - \operatorname{div}\Big(\frac{\nabla u}{Qu}\Big) = f(x,t).$$

Note the presence of Qu in the first term, which makes the study of this equation harder than (21). Let $U : [0,T] \to \mathbb{V}_h$ denote the semidiscrete finite element approximation

$$U(t) \in \mathbb{V}_h : \quad \int_\Omega \frac{\partial_t U}{QU} V + \frac{\nabla U \nabla V}{QU} = \int_\Omega fV \quad \forall V \in \mathbb{V}_h.$$

A key step in the analysis is to identify the correct geometric quantities to estimate. This was done by Deckelnick and Dziuk for the a priori analysis [8], and boilds down to examining

$$E(t) := \int_\Omega |Nu - NU|^2 Qu + \int_0^t \int_\Omega |Vu - VU|^2 Qu.$$

T:mcf **Theorem 4.1** (Conditional Estimate). *There exist two computable estimators $\mathcal{E}_\infty(t)$ and $\mathcal{E}_2(t)$, and a constant C_0 such that if $\mathcal{E}_\infty(t) \le \frac{1}{8}$ then $E(t) \le C_0 \mathcal{E}_2(t)$.*

S:allen-cahn

4.2. Allen-Cahn Equation: Circumventing Gronwall's Inequality

We finally consider the singularly perturbed parabolic equation

$$\varepsilon \langle \partial_t u, v\rangle + \varepsilon \langle \nabla u, \nabla v\rangle + \frac{1}{\varepsilon} \langle f(u), v\rangle = 0,$$

where $f(u) := u(u^2 - 1)$, and its finite element discretization: find $U_n \in \mathbb{V}_n$

$$\frac{\varepsilon}{\tau_n} \langle U_n - I_n U_{n-1}, V\rangle + \varepsilon \langle \nabla U_n, \nabla V\rangle + \frac{1}{\varepsilon} \langle f(I_n U_{n-1}), V\rangle + \frac{1}{\varepsilon} \langle f'(I_n U_{n-1})(U_n - I_n U_{n-1}), V\rangle = 0 \quad \forall\, V \in \mathbb{V}_n.$$

Let $U(t)$ be the piecewise linear interpolant of $\{U_n\}_{n=0}^N$ and $\mathcal{R}(t)$ be the residual

$$\langle \mathcal{R}(t), v\rangle := \varepsilon \langle \partial_t U, v\rangle + \varepsilon \langle \nabla U, \nabla v\rangle + \frac{1}{\varepsilon} \langle f(U), v\rangle$$

We assume that the initial condition u_0 is such that interfaces are already developed. Then we have the following *spectral estimate* [3, 9]:

$$\varepsilon \|\nabla v\|^2_{L_2(\Omega)} + \frac{1}{\varepsilon} \langle f'(u)v, v\rangle \ge -\lambda_0 \varepsilon \|v\|^2_{L_2(\Omega)}, \quad \forall\, v \in H^1(\Omega). \tag{42}$$ spectral

T:ac **Theorem 4.2** (Polynomial Error Control). *Let $\theta > 0$ be a tolerance, and let $\mathcal{E}_0, \mathcal{E}_1$ be parabolic error estimators. If* (42) *is valid, there exist constants $(\Lambda_i)_{i=0}^4$, depending exponential on $\lambda_0 T$ but independent of ε, such that if*

$$\theta \leq \Lambda_0 \varepsilon^4, \quad \|e(0)\|_{L_2(\Omega)} \leq \Lambda_1 \theta, \quad \mathcal{E}_0 \leq \Lambda_2 \varepsilon \theta, \quad \mathcal{E}_1 \leq \lambda_2 \varepsilon^2 \theta,$$

then

$$\|e\|_{L_\infty(0,T;L_2(\Omega))} \leq \theta.$$

We observe that the dependence on ε^{-1} is polynomial and not exponential, as could be expected from a naive application of Gronwall's inequality. This result is inspired in the a priori analysis of Feng and Prohl [14].

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