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GOAL-ORIENTED ERROR ESTIMATION AND ADAPTIVITY FOR FREE-BOUNDARY PROBLEMS: THE DOMAIN-MAP LINEARIZATION APPROACH*

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Abstract. In free-boundary problems, the accuracy of a goal quantity of interest depends on both the accuracy of the approximate solution and the accuracy of the domain approximation. We develop duality-based a posteriori error estimates for functional outputs of solutions of free-boundary problems that include both sources of error. The derivation of an appropriate dual problem (linearized adjoint) is, however, nonobvious for free-boundary problems. To derive an appropriate dual problem, we present the domain-map linearization approach. In this approach, the free-boundary problem is first transformed into an equivalent problem on a fixed reference domain after which the dual problem is obtained by linearization with respect to the domain map. We show for a Bernoulli-type free-boundary problem that this dual problem corresponds to a Poisson problem with a nonlocal Robin-type boundary condition. Furthermore, we present numerical experiments that demonstrate the effectivity of the dual-based error estimate and its usefulness in goal-oriented adaptive mesh refinement.

Key words. goal-oriented error estimation, a posteriori error estimation, Bernoulli free-boundary problem, domain-map linearization, linearized adjoint, adaptive mesh refinement

AMS subject classifications. 35R35, 49M29, 65N15, 65N50

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1. Introduction.

Free-boundary problems arise in various applications such as free-surface flow, fluid-structure interaction, and Stefan problems; see [15,18]. The numerical simulation of free-boundary problems is a challenging endeavor, as it requires the simultaneous solution of both the unknown function and its domain of definition and these two solution components can display distinct length (and/or time) scales. In many free-boundary problems, practical interest is restricted to a prescribed response quantity in the form of a goal functional of the solution rather than full norm resolution. However, the accuracy of the goal quantity depends on both the accuracy of the approximate solution and the accuracy of the domain approximation. In general, this dependence is nonobvious, and heuristic approaches, such as a priori mesh refinement in the vicinity of the free boundary [14, 42], lead to inefficient approximations of the goal quantity.

Finite-element techniques employing *goal-oriented adaptive* strategies can offer a significant efficiency improvement in such simulations. Starting with a coarse discretization, only those refinements are made which benefit substantially to the accuracy of the goal functional, in contrast to global norm-oriented adaptive strategies which make refinements which benefit the accuracy of the solution in the full

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norm [1, 50]. Such goal-oriented adaptive-refinement strategies result in optimal discretizations of both the unknown function and its domain of definition for the goal functional under consideration, each with appropriate resolution.

Goal-oriented adaptive strategies rely on local error indicators obtained from duality-based a posteriori error estimates for the functional of interest. These so-called *goal-oriented error estimates* require the solution of a dual problem, which is essentially a *linearized adjoint* problem. Pioneering work on a posteriori estimation of errors in goal functionals has been performed by Becker and Rannacher and Prudhomme and Oden; see their comprehensive overviews [3, 36, respectively] and also [16, 41]. The error estimation procedure was coined *goal-oriented error estimation* in 1999 by Prudhomme and Oden [35].

The goal-oriented error estimation framework is in principle immediately applicable to all (non)linear problems that can be cast in canonical variational form. Goal-oriented adaptive methods have recently been applied to a large variety of problems, although the convergence of several specific goal-oriented adaptive methods has only recently been established theoretically; see [31, 32].[1] Examples of goal-oriented adaptivity applied to problems with elliptic operators can be found in [28, 30, 38]. Examples with hyperbolic operators can be found in [19, 20, 23, 24]. Applications to multiphysics problems can be found in [10, 27, 48].

Free-boundary problems elude the standard goal-oriented error estimation framework on account of the fact that their typical variational form is noncanonical: The trial and test spaces in the variational formulation are domain dependent, but the domain itself constitutes an unknown. This impedes the direct derivation of an appropriate linearized adjoint.

In this work we consider the application of goal-oriented error estimation to free-boundary problems and, in particular, the formulation of appropriate linearized adjoints for this class of problems. As a model problem, we consider a Bernoulli-type free-boundary problem. By means of a domain map, which provides an isomorphism between the unknown domain of the free-boundary problem and a fixed reference domain, the free-boundary problem can be transformed into an equivalent problem on the fixed domain. The variational formulation of the transformed problem is in canonical form, although it contains intricate terms involving the domain map. The linearized adjoint is obtained by linearizing the transformed problem with respect to the domain map. We refer to this linearization technique as *domain-map linearization.* We show that the dual solution obtained by the domain-map linearization approach is essentially independent of the selected reference domain, in that the dual solutions corresponding to two distinct reference domains are related by the obvious map between the reference domains. Furthermore, we give an interpretation of the dual problem by showing that it corresponds to a Poisson problem with a nonlocal Robin-type boundary condition.

The present article is one of a pair of papers on goal-oriented error estimation for free-boundary problems. In the companion paper [49] we consider an alternative type of domain linearization based on shape derivatives [8, 34, 37]. It is noteworthy that these two linearization approaches have recently been investigated for Newton-type iterative solution algorithms for free-boundary problems. The domain-map linearization has been used in the context of fluid-structure-interaction problems;

[1]The convergence of adaptive finite-element methods is not only nontrivial for goal-oriented adaptive strategies but also for conventional energy norm–based adaptive methods [33, 39].

see [2,13]. The shape-linearization approach has been investigated for Bernoulli-type free-boundary problems in [14,25].

The content of this paper is arranged as follows: Section 2 introduces the free-boundary model problem and specifies some relevant goal functionals for this problem. In section 3 we review the basic theory of goal-oriented error estimation for canonical variational forms. In section 4 we consider the domain-map linearization approach and apply the canonical framework to the free-boundary model problem. Section 5 presents an analysis of the associated dual problem. Numerical experiments are presented in section 6. Finally, section 7 contains concluding remarks. We present a comparison of the domain-map linearization approach and the shape-linearization approach in the companion paper [49].

2. Problem statement.

In this work, we shall focus on a Bernoulli-type free-boundary problem; see [11,14], for instance. In particular, we consider the Laplace operator on a variable domain, with Dirichlet boundary conditions along the entire boundary and Neumann boundary conditions along the part corresponding to the free boundary. We present a weak formulation for this problem based on a parametrization of the domain. In addition, we present several relevant goal functionals.

2.1. Bernoulli-type free-boundary problem.

Let u denote an unknown scalar function from an a priori unknown bounded open domain $\Omega \subset \mathbb{R}^N$ into $\mathbb{R}$. The boundary $\partial\Omega$ of Ω consists of two complementary parts, viz., a fixed part, $\Gamma_{\mathcal{D}}$, on which Dirichlet boundary conditions are imposed and a variable part, Γ, referred to as the free boundary, on which both Dirichlet and Neumann boundary conditions are imposed; see Figure 1. Within this setting, we formulate the following Bernoulli-type free-boundary problem: Find the domain Ω (or equivalently, its free boundary Γ) and a function $u : \Omega \to \mathbb{R}$ such that

$$-\Delta u = f \quad \text{in } \Omega\,, \tag{2.1a}$$

$$\partial_n u = g \quad \text{on } \Gamma\,, \tag{2.1b}$$

$$u = h\big|_{\Gamma} = 1 \quad \text{on } \Gamma\,, \tag{2.1c}$$

$$u = h\big|_{\Gamma_{\mathcal{D}}} \quad \text{on } \Gamma_{\mathcal{D}}\,, \tag{2.1d}$$

where we assume $f \in C^{0,1}(\mathbb{R}^N)$, $g \in C^{1,1}(\mathbb{R}^N)$, together with a lower bound $g \geq g_0 > 0$, and $h \in C^{1,1}(\mathbb{R}^N)$, with $C^{p,q}$ the (p,q) Hölder space. Note that, in accordance with (2.1c), $h|_\Gamma = 1$ is required for all admissible free boundaries. In the following, we assume that the data is such that there exists a (possibly nonunique) Lipschitz domain Ω and a corresponding solution $u \in H^1(\Omega)$ which solve (2.1).[2]

Let us remark that for $f = 0$ and $\overline{\Gamma} \cap \overline{\Gamma_{\mathcal{D}}} = \emptyset$ (typically, annular domains), this problem corresponds to the interior or exterior Bernoulli free-boundary problem. A concise review of existence and regularity results as well as numerical solution algorithms for this case can be found in Flucher and Rumpf [14]. Other numerical approaches can be found in, for instance, [5,11,21,26,44,51].

To enable an interpretation of (2.1), we note that in two dimensions, the function u can be thought of as the stream function of a steady free-surface potential-flow problem. The constant Dirichlet condition at the free boundary expresses flow tangency, and the Neumann boundary condition corresponds with a simplified version of Bernoulli's equation (no surface tension); see, for instance [25,29].

[2]Note that for certain trivial data, such as $f = 0$, $g = g_0 > 0$, and $h = 1$ on $\Gamma_{\mathcal{D}}$, one can show that there does not exist any solution to (2.1). We exclude such trivial data.

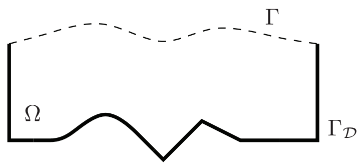

FIG. 1. *Geometric setup of the free-boundary problem: domain* Ω*, fixed boundary* $\Gamma_{\mathcal{D}}$*, and free boundary* Γ*.*

2.2. Parametrization of the unknown domain. To avoid the complications of searching for an unknown domain in some set of subsets of $\mathbb{R}^N$, one often resorts to finding a parametrization of the variable domain in a vector space. We construct variable domains as transformations of a reference domain Ω_0 by perturbations of the identity map $Id : \mathbb{R}^N \to \mathbb{R}^N$; see, for instance, [7, 8]. Let us note that, alternatively, the domains could have been constructed by means of the velocity method; see [7, 37]. The boundary $\partial\Omega_0 = \overline{\Gamma_0} \cup \overline{\Gamma_{\mathcal{D}}}$ consists of the fixed parts $\Gamma_{\mathcal{D}}$ and Γ_0, where Γ_0 corresponds to the free boundary in the reference configuration.

Let us denote by $\Theta_{\text{Lip}} := \Theta_{\text{Lip}}(\Omega_0)$ the space of Lipschitz perturbation-vector fields which vanish at $\Gamma_{\mathcal{D}}$, i.e.,

$$\Theta_{\text{Lip}}(\Omega_0) := \left\{ \theta \in C^{0,1}(\overline{\Omega_0}; \mathbb{R}^N) \,\middle|\, \theta = 0 \text{ on } \Gamma_{\mathcal{D}} \right\} .$$

To each $\theta \in \Theta_{\text{Lip}}$ we associate a transformation map $T_\theta := Id + \theta$ on $\overline{\Omega_0}$. This transformation leads to the perturbed domain Ω_θ and the corresponding free boundary Γ_θ:

$$\begin{aligned} \Omega_\theta &:= T_\theta(\Omega_0) = \left\{ x \in \mathbb{R}^N \,\middle|\, x = T_\theta(x_0)\ \forall x_0 \in \Omega_0 \right\} , \\ \Gamma_\theta &:= T_\theta(\Gamma_0) = \left\{ x \in \mathbb{R}^N \,\middle|\, x = T_\theta(x_0)\ \forall x_0 \in \Gamma_0 \right\} ; \end{aligned}$$

see Figure 2. Note that the free boundary is fixed at possible intersections with the fixed part of the boundary. For Lipschitz domains and Lipschitz perturbation fields, the transformation T_θ is invertible and both T_θ and T_θ^{-1} are Lipschitz continuous, provided that θ is not too large. Moreover, T_θ maps interior (resp., boundary) points of Ω_0 onto interior (resp. boundary) points of Ω_θ [7, 8]. In practice, this means that the reference domain should be sufficiently close to the actual domain.

Obviously, many perturbation fields in Θ_{Lip} vanish at the free boundary Γ_0 and, accordingly, do not yield perturbed domains. Furthermore, a particular perturbed domain has nonunique parametrizations in Θ_{Lip}; i.e., there exist distinct perturbation fields that give the same domain. To have a unique association between the domains and their parametrization, we need to consider a subspace $\Theta \subset \Theta_{\text{Lip}}$ of suitable perturbation fields. These perturbation fields are Lipschitz continuous extensions of functions that are only defined on the free boundary Γ_0. Examples of such

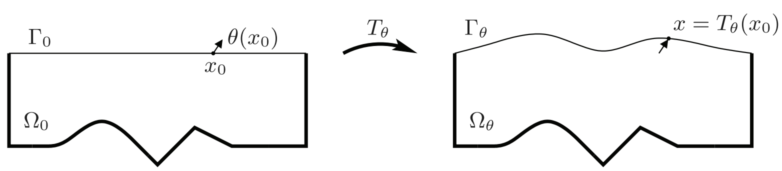

FIG. 2. *Illustration of the transformation* T_θ*, mapping the reference domain* Ω_0 *onto* Ω_θ*.*

extensions are the classical normal extension [34], smoothed-normal extensions [43], and extensions of hypograph perturbations [8, 22].

2.3. Weak form of the free-boundary problem. For admissible $\theta \in \Theta$ and corresponding domain Ω_θ, we denote by $H^1_{0,\gamma}(\Omega_\theta)$ the space of H^1-functions with a zero trace on $\gamma \subseteq \partial\Omega_\theta$, i.e.,

$$H^1_{0,\gamma}(\Omega_\theta) := \left\{ v \in H^1(\Omega_\theta) : \ v = 0 \text{ on } \gamma \right\} .$$

To deal with nonzero traces, we define the (affine) space incorporating h as

$$H^1_h(\Omega_\theta) := h|_{\Omega_\theta} + H^1_{0,\partial\Omega_\theta}(\Omega_\theta) .$$

A weak formulation of (2.1) is obtained by multiplying (2.1a) with $v \in H^1_{0,\Gamma_\mathcal{D}}(\Omega_\theta)$, integrating over $\Omega = \Omega_\theta$, and integrating by parts the Laplacian. As v is nonzero on Γ_θ, we invoke (2.1b) to incorporate the Neumann boundary condition weakly. Furthermore, the Dirichlet boundary conditions (2.1c) and (2.1d) can be imposed strongly. We then arrive at the variational formulation:[3]

(2.2)
$$\boxed{\begin{array}{l}\text{Find } \theta \in \Theta \text{ and } u \in H^1_h(\Omega_\theta) : \\ \displaystyle\int_{\Omega_\theta} \nabla u \cdot \nabla v = \int_{\Omega_\theta} f\, v + \int_{\Gamma_\theta} g\, v \qquad \forall v \in H^1_{0,\Gamma_\mathcal{D}}(\Omega_\theta) .\end{array}}$$

Because the solution of (2.2) consists of both θ and u, the variational problem is of mixed type. Moreover, it is nonlinear in θ. Standard variational arguments show that smooth solutions of (2.2) satisfy (2.1).

Last but not least, it is important to observe that the variational statement (2.2) is noncanonical in the sense that u and v reside in function spaces that depend on the solution component θ. We will return to this issue in section 4.

2.4. Goal functionals and approximation errors. Our interest is restricted to specific qoal quantities of the solution (θ, u) of (2.2), i.e., quantities of interest $\mathcal{Q}(\theta, u) \in \mathbb{R}$. This implies that approximations to the solution are only viewed as a means to produce approximate goal quantities. An example goal quantity is the weighted *average* of u defined by[4]

$$\mathcal{Q}^{\text{ave}}(\theta; u) := \int_{\Omega_\theta} q^{\text{ave}}\, u,$$

where the weight $q^{\text{ave}} \in H^1(\mathbb{R}^N)$ is a given function. Another example of relevance in free-surface flows is the weighted *elevation* of the free boundary:

$$\mathcal{Q}^{\text{elev}}(\theta) := \int_{\Gamma_0} q^{\text{elev}}\, \alpha_\theta .$$

Here, the weight $q^{\text{elev}} \in L^2(\Gamma_0)$ is given, and the elevation $\alpha_\theta := \alpha(\Omega_\theta) : \Gamma_0 \to \mathbb{R}$ is a scalar function which associates to a specific domain Ω_θ the vertical deviation of the free boundary with respect to the rest position, Γ_0.

[3]For notational convenience, we often neglect the integration measure in integrals. Domain and boundary integrals are to be integrated with respect to the usual volume and surface measures. For example, we write $\int_{\Gamma_\theta} f$ instead of $\int_{\Gamma_\theta} f \,\mathrm{d}\Gamma_\theta$.

[4]For semilinear functionals, we use the convention that the functional is linear with respect to the arguments after the semicolon ";".

Let $\theta^{\mathsf{h}} \in \Theta$ and $u^{\mathsf{h}} \in H_h^1(\Omega_{\theta^{\mathsf{h}}})$ be approximations obtained by applying, for example, the Galerkin method to (2.2) with suitable finite-dimensional subspaces. For later reference, we note that the approximation u^{h} thus satisfies the Dirichlet boundary condition, $u^{\mathsf{h}} = 1$, on the approximate free boundary $\Gamma_{\theta^{\mathsf{h}}}$. The corresponding approximate value of the goal functional is $\mathcal{Q}(\theta^{\mathsf{h}}, u^{\mathsf{h}})$. It is our objective to derive a dual-based estimate of the goal error,

$$\mathcal{E}_{\mathcal{Q}} := \mathcal{Q}(\theta, u) - \mathcal{Q}(\theta^{\mathsf{h}}, u^{\mathsf{h}}) \,,$$

and to employ this estimate to control the goal error using goal-oriented adaptive strategies. In the next section we review relevant theory on goal-oriented error estimation for canonical variational forms, and following this, in section 4 we show how to apply this theory to our model free-boundary problem.

3. Goal-oriented error estimation for canonical variational forms. A general paradigm for a posteriori error estimation of quantities of interest has been established for canonical variational formulations (canonical in the sense that it fits the form in (3.1) below); see in particular [1,3,16,36,50]. In this paradigm, a computable error estimate is obtained by evaluating the residual at the solution of a suitable dual problem. This section gives a brief summary of the theory established in the literature.

3.1. Canonical setting. Let U and V denote Banach spaces. Consider the canonical variational problem, referred to as the primal problem:

$$\boxed{\begin{array}{l}\text{Find } \mu \in U : \\ \qquad \mathcal{N}(\mu;\nu) = \ell(\nu) \qquad \forall \nu \in V \,,\end{array}} \tag{3.1}$$

where $\mathcal{N} : U \times V \to \mathbb{R}$ is a semilinear form (nonlinear in the first entry) and $\ell(\cdot)$ is a linear functional on V. The quantity of interest is the value of the (possibly nonlinear) goal functional $\mathcal{Q} : U \to \mathbb{R}$ for the solution μ of (3.1). Given any approximation $\mu^{\mathsf{h}} \in U$, the purpose of a posteriori error estimation is to obtain an estimate of the error $\mathcal{E}_{\mathcal{Q}} := \mathcal{Q}(\mu) - \mathcal{Q}(\mu^{\mathsf{h}})$.

3.2. Dual-based error representation. In a dual-based approach, one solves the dual (or linearized adjoint) problem:

$$\boxed{\begin{array}{l}\text{Find } \zeta \in V : \\ \qquad \mathcal{N}'(\mu^{\mathsf{h}};\zeta)(\delta\mu) = \mathcal{Q}'(\mu^{\mathsf{h}})(\delta\mu) \qquad \forall \delta\mu \in U \,,\end{array}} \tag{3.2}$$

where the prime indicates the Gâteaux differentiation with respect to the nonlinear arguments. That is, $\mathcal{N}'(\mu^{\mathsf{h}};\zeta)$ and $\mathcal{Q}'(\mu^{\mathsf{h}})$ are linear functionals on U such that

$$\begin{aligned}\mathcal{N}'(\mu^{\mathsf{h}};\zeta)(\delta\mu) &= \lim_{t\to 0} \frac{\mathcal{N}(\mu^{\mathsf{h}} + t\,\delta\mu;\zeta) - \mathcal{N}(\mu^{\mathsf{h}};\zeta)}{t} \,, \\ \mathcal{Q}'(\mu^{\mathsf{h}})(\delta\mu) &= \lim_{t\to 0} \frac{\mathcal{Q}(\mu^{\mathsf{h}} + t\,\delta\mu) - \mathcal{Q}(\mu^{\mathsf{h}})}{t}\end{aligned}$$

$\forall\, \delta\mu \in U$. Note that the dual problem (3.2) is a linear problem obtained by linearization of $\mathcal{N}$ and $\mathcal{Q}$ at the approximate solution μ^{h}. Compared with the primal problem, the test and trial spaces have reversed roles. The dual solution ζ is the key element in relating the error in the quantity of interest to the residual at μ^{h}:

$$\mathcal{R}(\mu^{\mathsf{h}};\cdot) := \ell(\cdot) - \mathcal{N}(\mu^{\mathsf{h}};\cdot) \ .$$

THEOREM 3.1 (error representation). *Given any approximation $\mu^{\mathsf{h}} \in U$ of the solution μ of* (3.1), *let $\zeta \in V$ be the solution of the dual problem* (3.2). *It holds that*

$$\boxed{\mathcal{E}_{\mathcal{Q}} := \mathcal{Q}(u) - \mathcal{Q}(\mu^{\mathsf{h}}) = \mathcal{R}(\mu^{\mathsf{h}};\zeta) + R \ ,} \tag{3.3}$$

with quadratic remainder $R := R_{\mathcal{Q}} - R_{\mathcal{N}}$, where

$$\begin{aligned} R_{\mathcal{Q}} &:= \int_0^1 \mathcal{Q}''(\mu^{\mathsf{h}} + t\, e)(e)(e)\,(1-t)\ \mathrm{d}t \ , \\ R_{\mathcal{N}} &:= \int_0^1 \mathcal{N}''(\mu^{\mathsf{h}} + t\, e;\zeta)(e)(e)\,(1-t)\ \mathrm{d}t \ , \end{aligned}$$

and $e := \mu - \mu^{\mathsf{h}}$ is the error.

Proof. The proof makes use of the following standard Taylor series formulae:

$$\begin{aligned} \mathcal{Q}(\mu) &= \mathcal{Q}(\mu^{\mathsf{h}}) + \mathcal{Q}'(\mu^{\mathsf{h}})(e) + R_{\mathcal{Q}} \ , \\ \mathcal{N}(\mu;\zeta) &= \mathcal{N}(\mu^{\mathsf{h}};\zeta) + \mathcal{N}'(\mu^{\mathsf{h}};\zeta)(e) + R_{\mathcal{N}} \ , \end{aligned}$$

which are valid for any $\zeta \in V$. Consider the goal error $\mathcal{E}_{\mathcal{Q}} = \mathcal{Q}(\mu) - \mathcal{Q}(u^{\mathsf{h}})$. Using the first Taylor series formula gives

$$\mathcal{E}_{\mathcal{Q}} = \mathcal{Q}'(\mu^{\mathsf{h}})(e) + R_{\mathcal{Q}} = \mathcal{N}'(\mu^{\mathsf{h}};\zeta)(e) + R_{\mathcal{Q}} \ ,$$

where we used the dual problem (3.2) in the second step. It follows from the second Taylor series formula that

$$\mathcal{E}_{\mathcal{Q}} = \mathcal{N}(\mu;\zeta) - \mathcal{N}(\mu^{\mathsf{h}};\zeta) + R_{\mathcal{Q}} - R_{\mathcal{N}} \ .$$

Finally, we obtain the proof by noting that $\mathcal{N}(\mu;\zeta) = \ell(\zeta)$ according to the primal problem (3.1) and by definition of $\mathcal{R}$. ∎

Note that the remainder term R in (3.3) is quadratic in the error e. Hence, the residual evaluated at the dual solution, $\mathcal{R}(\mu^{\mathsf{h}};\zeta)$, provides an error estimate which is second-order accurate. This estimate is exact if $\mathcal{N}(\cdot;\cdot)$ and $\mathcal{Q}(\cdot)$ are linear functionals.

By employing a dual problem obtained by linearizing in between μ and μ^{h}, it is possible to obtain an error representation formula with zero remainder for nonlinear problems and quantities of interest. However, this dual variant cannot be used directly in practice for error estimation, since it involves the unknown solution μ. Instead, it is used to study the effect of the nonlinearity in error estimators; see [3] for more details.

3.3. Approximate dual solution. The dual problem (3.2) cannot in general be solved exactly, and we will have to deal with approximations instead. Let $\zeta^{\mathsf{h}} \in V$ be an approximation to the solution ζ of (3.2). Furthermore, setting $e_\zeta := \zeta - \zeta^{\mathsf{h}}$, we have the representation formula

$$\mathcal{E}_{\mathcal{Q}} = \mathcal{R}(\mu^{\mathsf{h}};\zeta^{\mathsf{h}}) + \mathcal{R}(\mu^{\mathsf{h}};e_\zeta) + R \ . \tag{3.4}$$

Accordingly, we can estimate the goal error by using the residual evaluated at the approximate dual solution, giving the dual-based error estimate

$$\mathrm{Est}_{\mathcal{Q}} := \mathcal{R}(\mu^{\mathsf{h}}; \zeta^{\mathsf{h}}) \ .$$

This estimate is first-order accurate with respect to the dual error e_ζ and second-order accurate with respect to the primal error e.

If one uses a test space $\hat{V} \subset V$ for the approximation of the primal problem and a trial space $\bar{V} \subset V$ for the approximation of the dual problem, then $\mathcal{R}(\mu^{\mathsf{h}}; \zeta^{\mathsf{h}}) = 0$ if $\bar{V} \subseteq \hat{V}$ on account of the Galerkin orthogonality. The estimate is then useless, of course. Therefore, in practice, the dual problem is either solved using a larger space, $\bar{V} \supset\supset \hat{V}$, or it is solved on a dedicated dual-problem space such that $\hat{V} \not\subseteq \bar{V} \not\subseteq \hat{V}$. For such choices of the dual trial space, moreover, the dual error e_ζ is relatively small so that the second term in the right member of (3.4) can indeed be ignored; see also [3].

4. Goal-oriented error estimation by domain-map linearization. We now turn our attention to goal-oriented error estimation for the free-boundary problem (2.2). For convenience, we rewrite (2.2) in abstract form as:

$$\boxed{\begin{aligned}&\text{Find } \theta \in \Theta \text{ and } u \in H^1_h(\Omega_\theta) : \\ &\qquad \mathcal{N}\big((\theta, u); v\big) = 0 \qquad \forall v \in H^1_{0,\Gamma_{\mathcal{D}}}(\Omega_\theta) \ ,\end{aligned}} \tag{4.1}$$

where

$$\mathcal{N}\big((\theta, u); v\big) := \mathcal{A}\big(\theta; u, v\big) - \mathcal{F}\big(\theta; v\big) - \mathcal{G}\big(\theta; v\big) \tag{4.2}$$

and the semilinear forms are defined as

$$\mathcal{A}\big(\theta; u, v\big) := \int_{\Omega_\theta} \nabla u \cdot \nabla v \ , \qquad \mathcal{F}\big(\theta; v\big) := \int_{\Omega_\theta} f\, v \ , \qquad \mathcal{G}\big(\theta; v\big) := \int_{\Gamma_\theta} g\, v \ .$$

Furthermore, we recall our interest in the goal functional $\mathcal{Q}(\theta, u)$. The variational problem (4.1) eludes the general error estimation paradigm of section 3 because it is in noncanonical form: The functions u and v reside in spaces that depend on θ, which is itself an unknown in the problem.

To elucidate this complication, let us consider a central element of the proof of Theorem 3.1, viz., the Taylor series formula

$$\mathcal{Q}(\theta, u) - \mathcal{Q}(\theta^{\mathsf{h}}, u^{\mathsf{h}}) = \mathcal{Q}'(\theta^{\mathsf{h}}, u^{\mathsf{h}})(e_\theta, e_u) + \text{higher-order terms},$$

where $e_\theta := \theta - \theta^{\mathsf{h}} \in \Theta$. However, at this point it is not clear how e_u should be defined. Simply setting $e_u := u - u^{\mathsf{h}}$ is meaningless, since $u \in H^1_h(\Omega_\theta)$ and $u^{\mathsf{h}} \in H^1_h(\Omega_{\theta^{\mathsf{h}}})$. The essential issue is that we are comparing functions on different domains; see the illustration in Figure 3.

To cast (4.1) into canonical form, we introduce a domain map, which provides an isomorphism between the θ-dependent domain and a fixed reference domain, and apply this map to remove the θ-dependence of the test and trial spaces from the variational formulation. In section 4.1 we consider the transformation to the most obvious reference domain, Ω_0. In section 4.2 we consider the transformation to the approximate domain, $\Omega_{\theta^{\mathsf{h}}}$, which yields a more natural dual formulation. Finally, it is shown in section 4.3 that the dual problems corresponding to the two transformations are equivalent.

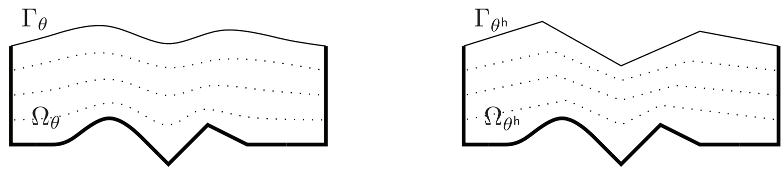

FIG. 3. *Comparing functions on different domains. The solution $u \in H^1_h(\Omega_\theta)$ lives on Ω_θ (left), and the approximation $u^h \in H^1_h(\Omega_{\theta^h})$ lives on Ω_{θ^h} (right).*

4.1. Domain-map linearization at reference domain. Recall from section 2.2 the transformation $T_\theta = Id + \theta$ from the reference domain Ω_0 to Ω_θ. For all admissible $\theta \in \Theta$, T_θ constitutes a $C^{0,1}$-diffeomorphism, and the function transportation map

$$H^1(\Omega_0) \ni v_0 \mapsto v_0 \circ T_\theta^{-1} \in H^1(\Omega_\theta)$$

is a linear bijection; see [17, p. 21] or [8, p. 406]. In essence, this transportation of domain-dependent functions allows a reformulation of the free-boundary problem on a fixed domain. As $\Gamma_\mathcal{D}$ is invariant under T_θ, we have the equality of spaces

$$H^1_{0,\Gamma_\mathcal{D}}(\Omega_\theta) = \left\{ v = v_0 \circ T_\theta^{-1} : v_0 \in H^1_{0,\Gamma_\mathcal{D}}(\Omega_0) \right\} . \tag{4.3}$$

4.1.1. Transformed free-boundary problem. Let us introduce the semilinear form $\mathcal{N}_0 : (\Theta \times H^1(\Omega_0)) \times H^1(\Omega_0) \to \mathbb{R}$ defined as:

$$\mathcal{N}_0\big((\theta, w_0); v_0\big) := \mathcal{N}\big((\theta, w_0 \circ T_\theta^{-1}); v_0 \circ T_\theta^{-1}\big) \qquad \forall v_0, w_0 \in H^1(\Omega_0) . \tag{4.4}$$

This is essentially the transformed form of $\mathcal{N}$ taking functions on Ω_0. Furthermore, if we denote by

$$u_0 := u \circ T_\theta \in H^1_h(\Omega_0) \tag{4.5}$$

the solution of (4.1) transformed to Ω_0, then by using (4.3), we can easily verify that the solution (θ, u_0) satisfies

$$\mathcal{N}_0\big((\theta, u_0); v_0\big) = 0 \qquad \forall v_0 \in H^1_{0,\Gamma_\mathcal{D}}(\Omega_0) .$$

To specify this abstract variational statement, let us denote by

$$\mathrm{D}T_\theta := \partial T_\theta(x_1, \dots, x_N)/\partial(x_1, \dots, x_N) \quad \text{and} \quad J_\theta := \det \mathrm{D}T_\theta$$

the Jacobian matrix and the Jacobian determinant, respectively, of the transformation map T_θ. Furthermore, let

$$\omega_\theta := J_\theta \, |\mathrm{D}T_\theta^{-\mathsf{T}} n|$$

denote the tangential Jacobian on Γ_0, which is of use in transforming surface integrals. The variational statement is explicitly given in the following.

PROPOSITION 4.1. *The transformed free-boundary problem solution $(\theta, u_0) \in \Theta \times H^1_h(\Omega_0)$ satisfies*

$$\boxed{\int_{\Omega_0} (A_\theta \nabla u_0) \cdot \nabla v_0 - \int_{\Omega_0} f_\theta \, v_0 - \int_{\Gamma_0} g_\theta \, v_0 = 0 \qquad \forall v_0 \in H^1_{0,\Gamma_\mathcal{D}}(\Omega_0) ,} \tag{4.6}$$

where

$$A_\theta := J_\theta\, \mathrm{D}T_\theta^{-1}\, \mathrm{D}T_\theta^{-\mathsf{T}}\,, \qquad f_\theta := J_\theta\,(f \circ T_\theta)\,, \qquad g_\theta := \omega_\theta\,(g \circ T_\theta)\,.$$

Basically, this proposition follows by transforming the integrals in (4.1) to Ω_0. We first recall the following basic results; see, for example, [8, 37].

LEMMA 4.2. *Let* $\phi \in L^2(\Omega_\theta)$ *and* $\psi \in L^2(\Gamma_\theta)$*. Then*

$$\int_{\Omega_\theta} \phi = \int_{\Omega_0} (\phi \circ T_\theta)\, J_\theta\,, \tag{4.7a}$$

$$\int_{\Gamma_\theta} \psi = \int_{\Gamma_0} (\psi \circ T_\theta)\, \omega_\theta\,, \tag{4.7b}$$

with $\phi \circ T_\theta \in L^2(\Omega_0)$ *and* $\psi \circ T_\theta \in L^2(\Gamma_0)$.

Proof of Proposition 4.1. Consider any $v \in H^1_{0,\Gamma_{\mathcal{D}}}(\Omega_\theta)$. To transform $\mathcal{A}(\theta; u, v)$ in (4.2), we use (4.7a) and the identity

$$(\nabla w) \circ T_\theta = \mathrm{D}T_\theta^{-\mathsf{T}} \nabla (w \circ T_\theta) \qquad \forall w \in H^1(\Omega_\theta)\,,$$

to obtain

$$\mathcal{A}\big((\theta, u); v\big) = \int_{\Omega_0} \Big(\mathrm{D}T_\theta^{-\mathsf{T}} \nabla(u \circ T_\theta)\Big) \cdot \Big(\mathrm{D}T_\theta^{-\mathsf{T}} \nabla(v \circ T_\theta)\Big)\, J_\theta\,.$$

Replacing $u \circ T_\theta$ with u_0 in accordance with (4.5) and setting $v \circ T_\theta =: v_0 \in H^1_{0,\Gamma_{\mathcal{D}}}(\Omega_0)$, we obtain the first term in (4.6). The other two terms follow from Lemma 4.2 by replacing $v \circ T_\theta$ with v_0. ∎

The goal functional $\mathcal{Q}$ can be expressed in terms of u_0 as

$$\mathcal{Q}(\theta, u) = \mathcal{Q}(\theta, u_0 \circ T_\theta^{-1}) =: \mathcal{Q}_0(\theta, u_0)\,.$$

Note that $\mathcal{Q}_0$ is defined on $\Theta \times H^1(\Omega_0)$. For the weighted average functional, we obtain, in particular,

$$\mathcal{Q}_0^{\mathrm{ave}}(\theta; u_0) = \int_{\Omega_0} q_\theta^{\mathrm{ave}}\, u_0\,,$$

where

$$q_\theta^{\mathrm{ave}} := J_\theta\,(q^{\mathrm{ave}} \circ T_\theta)\,.$$

As the other goal functional, the weighted elevation functional, is independent of u, we simply have $\mathcal{Q}_0^{\mathrm{elev}} = \mathcal{Q}^{\mathrm{elev}}$.

4.1.2. Dual-based error representation. Because $\mathcal{N}_0$ and $\mathcal{Q}_0$ act on fixed spaces, we can essentially follow the standard framework of section 3 hereafter. First, we denote by

$$u_0^{\mathsf{h}} := u^{\mathsf{h}} \circ T_{\theta^{\mathsf{h}}} \in H_h^1(\Omega_0) \tag{4.8}$$

the approximation u^{h} transported to Ω_0. Accordingly, we define the dual problem by linearizing $\mathcal{N}_0$ and $\mathcal{Q}_0$ about $(\theta^{\mathsf{h}}, u_0^{\mathsf{h}})$.

(4.9)

Find $z_0 \in H^1_{0,\Gamma_{\mathcal{D}}}(\Omega_0)$: $\mathcal{N}_0'\big((\theta^{\mathsf{h}}, u_0^{\mathsf{h}}); z_0\big)(\delta\theta, \delta u_0) = \mathcal{Q}_0'\big(\theta^{\mathsf{h}}, u_0^{\mathsf{h}}\big)(\delta\theta, \delta u_0) \quad \forall(\delta\theta, \delta u_0) \in \Theta_{\Gamma_0} \times H^1_{0,\partial\Omega}(\Omega_0)$.

We refrain here from a precise specification of the derivatives in (4.9). In section 4.3 it will be shown that (4.9) can be equivalently expressed on the approximate domain $\Omega_{\theta^{\mathsf{h}}}$, and this equivalent formulation will be considered in more detail in section 5. Proceeding under the assumption that there exists a unique dual solution z_0 to (4.9), this z_0 is indeed appropriate for linking the error in the goal with the residual of the primal problem (4.1),

$$\mathcal{R}\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); \cdot\big) := -\mathcal{N}\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); \cdot\big) \, . \tag{4.10}$$

This is expressed by the following theorem.

THEOREM 4.3 (error representation based on z_0). *Given any approximation $(\theta^{\mathsf{h}}, u^{\mathsf{h}}) \in \Theta \times H^1_h(\Omega_{\theta^{\mathsf{h}}})$ of the solution $(\theta, u) \in \Theta \times H^1_h(\Omega_\theta)$ of the free-boundary problem (4.1), let $z_0 \in H^1_{0,\Gamma_{\mathcal{D}}}(\Omega_0)$ be the solution of dual problem (4.9). It holds that*

$$\boxed{\mathcal{E}_{\mathcal{Q}} := \mathcal{Q}(\theta, u) - \mathcal{Q}(\theta^{\mathsf{h}}, u^{\mathsf{h}}) = \mathcal{R}\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); z_0 \circ T^{-1}_{\theta^{\mathsf{h}}}\big) + R \, ,} \tag{4.11}$$

with quadratic remainder $R = R_{\mathcal{Q}_0} - R_{\mathcal{N}_0}$, where

$$R_{\mathcal{Q}_0} := \int_0^1 \mathcal{Q}_0''\big(\theta^{\mathsf{h}} + t\, e^\theta, u_0^{\mathsf{h}} + t\, e_0^u\big)(e^\theta, e_0^u)(e^\theta, e_0^u)\,(1-t)\,\mathrm{d}t \, ,$$
$$R_{\mathcal{N}_0} := \int_0^1 \mathcal{N}_0''\big((\theta^{\mathsf{h}} + t\, e^\theta, u_0^{\mathsf{h}} + t\, e_0^u); z_0\big)(e^\theta, e_0^u)(e^\theta, e_0^u)\,(1-t)\,\mathrm{d}t \, ,$$

and the errors are defined as $e^\theta := \theta - \theta^{\mathsf{h}}$ and

$$\boxed{e_0^u := u \circ T_\theta - u^{\mathsf{h}} \circ T_{\theta^{\mathsf{h}}} \, .}$$

This error representation formula for free-boundary problems is the analogue of the canonical formula (3.3). It shows how the dual solution z_0 in the reference domain is employed in the residual evaluation for obtaining the error estimate. That is, before evaluation in the residual, z_0 is transported back to the approximate domain $\Omega_{\theta^{\mathsf{h}}}$.

Theorem 4.3 also provides an interpretation of the error terms in the quadratic remainder R. With respect to the exact $u \in H^1(\Omega_\theta)$ and approximate $u^{\mathsf{h}} \in H^1(\Omega_{\theta^{\mathsf{h}}})$, which reside on different domains, the remainder forms a quadratic term in their difference on the reference domain, that is, $e_0^u \in H^1_0(\Omega_0)$. Moreover, trivially, R is a quadratic term in the error $e^\theta = \theta - \theta^{\mathsf{h}} \in \Theta$.

We end this section with a proof of Theorem 4.3. An essential element of the proof is provided by Taylor series formulae of the functionals $\mathcal{Q}$ and $\mathcal{N}$.

LEMMA 4.4. *The following Taylor series formulae hold:*

$$\mathcal{Q}(\theta, u) = \mathcal{Q}(\theta^{\mathsf{h}}, u^{\mathsf{h}}) + \mathcal{Q}_0'\big(\theta^{\mathsf{h}}, u_0^{\mathsf{h}}\big)(e^\theta, e_0^u) + R_{\mathcal{Q}_0} \, , \tag{4.12a}$$

$$\mathcal{N}\big((\theta, u); z_0 \circ T_\theta^{-1}\big) = \mathcal{N}\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); z_0 \circ T^{-1}_{\theta^{\mathsf{h}}}\big) + \mathcal{N}_0'\big((\theta^{\mathsf{h}}, u_0^{\mathsf{h}}); z_0\big)(e^\theta, e_0^u) + R_{\mathcal{N}_0} \tag{4.12b}$$

for any $z_0 \in H^1_{0,\Gamma_{\mathcal{D}}}(\Omega_0)$, with remainders $R_{\mathcal{Q}_0}$ and $R_{\mathcal{N}_0}$ as defined in Theorem 4.3.

It is to be noted that these formulae relate the values of the functionals on different domains and for different functions by a linear functional on the reference domain (up to higher-order terms).

Proof. By the definitions of $\mathcal{N}_0$, u_0, and u_0^{h} in (4.4), (4.5), and (4.8), respectively, we have the identity

$$\mathcal{N}\big((\theta, u); z_0 \circ T_\theta^{-1}\big) - \mathcal{N}\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); z_0 \circ T^{-1}_{\theta^{\mathsf{h}}}\big) = \mathcal{N}_0\big((\theta, u_0); z_0\big) - \mathcal{N}_0\big((\theta^{\mathsf{h}}, u_0^{\mathsf{h}}); z_0\big).$$

The first two entries of $\mathcal{N}_0\big((\cdot,\cdot);z_0\big)$ are elements of the fixed spaces Θ and $H^1_h(\Omega_0)$. Therefore, we can apply a standard Taylor series formula to the right-hand side, yielding (4.12b). Equation (4.12a) can be established analogously. $\square$

Proof of Theorem 4.3. Consider the goal error $\mathcal{E}_\mathcal{Q} = \mathcal{Q}(\theta,u) - \mathcal{Q}(\theta^\mathsf{h},u^\mathsf{h})$. Using (4.12a), and subsequently invoking the dual problem (4.9), we obtain

$$\mathcal{E}_\mathcal{Q} = \mathcal{Q}_0'(\theta^\mathsf{h},u_0^\mathsf{h})(e^\theta,e_0^u) + R_{\mathcal{Q}_0} = \mathcal{N}_0'\big((\theta^\mathsf{h},u_0^\mathsf{h});z_0\big)(e^\theta,e_0^u) + R_{\mathcal{Q}_0} \;.$$

Next, applying (4.12b), it follows that

$$\mathcal{E}_\mathcal{Q} = \mathcal{N}\big((\theta,u);z_0\circ T_\theta^{-1}\big) - \mathcal{N}\big((\theta^\mathsf{h},u^\mathsf{h});z_0\circ T_{\theta^\mathsf{h}}^{-1}\big) + R_{\mathcal{Q}_0} - R_{\mathcal{N}_0} \;.$$

Notice that $\mathcal{N}\big((\theta,u);z_0\circ T_\theta^{-1}\big) = 0$ in accordance with our primal problem (4.1). Finally, we obtain the proof by substituting the residual $\mathcal{R} = -\mathcal{N}$ according to (4.10). $\square$

4.2. Domain-map linearization at approximate domain. A more natural dual formulation is obtained by transforming the free-boundary problem to the approximate domain corresponding to θ^h. For convenience of notation, we introduce the notations

$$\hat\Omega := \Omega_{\theta^\mathsf{h}} \qquad \text{and} \qquad \hat\Gamma := \Gamma_{\theta^\mathsf{h}} \;.$$

We now require a bijective transformation which maps $\hat\Omega$ onto admissible domains Ω_θ. We denote this map by

$$\hat T_\theta : \hat\Omega \to \Omega_\theta \;.$$

It is convenient (but not necessary) to define $\hat T_\theta$ via the transformation $T_{(\cdot)}$ introduced in section 2.2:

$$\hat T_\theta := T_\theta \circ T_{\theta^\mathsf{h}}^{-1} = Id + (\theta - \theta^\mathsf{h}) \circ T_{\theta^\mathsf{h}}^{-1} \qquad \forall\theta\in\Theta \;; \tag{4.13}$$

see Figure 4 for a graphical illustration. Note that $\hat T_\theta$ constitutes a perturbation of the identity with perturbation-vector field $(\theta-\theta^\mathsf{h})\circ T_{\theta^\mathsf{h}}^{-1}$. The corresponding function transportation map leads to the following equality of spaces:

$$H^1_{0,\Gamma_\mathcal{D}}(\Omega_\theta) = \Big\{ v = \hat v \circ \hat T_\theta^{-1} \,:\, \hat v \in H^1_{0,\Gamma_\mathcal{D}}(\hat\Omega) \Big\} \;. \tag{4.14}$$

4.2.1. Transformed free-boundary problem. Proceeding as in section 4.1.1, let us now introduce the transformed functional $\hat{\mathcal{N}} : \big(\Theta \times H^1(\hat\Omega)\big) \times H^1(\hat\Omega) \to \mathbb{R}$:

$$\hat{\mathcal{N}}\big((\theta,\hat w);\hat v\big) := \mathcal{N}\big((\theta,\hat w\circ\hat T_\theta^{-1});\hat v\circ\hat T_\theta^{-1}\big) \qquad \forall\hat v,\hat w\in H^1(\hat\Omega) \;. \tag{4.15}$$

Next, let us denote the u-solution of (4.1) transformed to $\hat\Omega$ by

$$\hat u := u \circ \hat T_\theta \in H^1_h(\hat\Omega) \;. \tag{4.16}$$

By invoking (4.14), it follows that

$$\hat{\mathcal{N}}\big((\theta,\hat u);\hat v\big) = 0 \qquad \forall\hat v\in H^1_{0,\Gamma_\mathcal{D}}(\hat\Omega) \;.$$

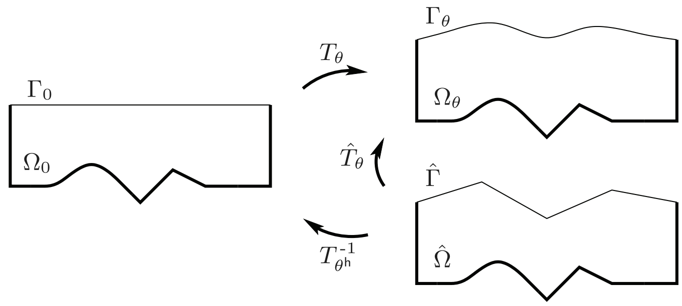

FIG. 4. *Defining the map* $\hat{T}_\theta : \hat{\Omega} \to \Omega_\theta$ *via the reference domain, i.e.,* $\hat{T}_\theta : \hat{\Omega} \xrightarrow{T^{-1}_{\theta^h}} \Omega_0 \xrightarrow{T_\theta} \Omega_\theta$.

The precise specification of this abstract variational statement can be derived by applying Proposition 4.1 to this situation with the necessary modifications. First, we define the Jacobian and tangential Jacobian associated with $\hat{T}$ by

$$\hat{J}_\theta := \det \mathrm{D}\hat{T}_\theta \qquad \text{and} \qquad \hat{\omega}_\theta := \hat{J}_\theta \, |\mathrm{D}\hat{T}_\theta^{-\mathsf{T}} \, n| \; . \tag{4.17}$$

PROPOSITION 4.5. *The transformed free-boundary problem solution* $(\theta, \hat{u}) \in \Theta \times H^1_h(\hat{\Omega})$ *satisfies*

$$\boxed{\int_{\hat{\Omega}} (A_\theta \nabla \hat{u}) \cdot \nabla \hat{v} - \int_{\hat{\Omega}} f_\theta \, \hat{v} - \int_{\hat{\Omega}} g_\theta \, \hat{v} = 0 \qquad \forall \hat{v} \in H^1_{0,\Gamma_{\mathcal{D}}}(\hat{\Omega}) \; ,}$$

where[5]

$$A_\theta := \hat{J}_\theta \, \mathrm{D}\hat{T}_\theta^{-1} \, \mathrm{D}\hat{T}_\theta^{-\mathsf{T}} \; , \qquad f_\theta := \hat{J}_\theta \, (f \circ \hat{T}_\theta) \; , \qquad g_\theta := \hat{\omega}_\theta \, (g \circ \hat{T}_\theta) \; .$$

The corresponding transformation of $\mathcal{Q}$ is given by

$$\hat{\mathcal{Q}}(\theta, \hat{u}) := \mathcal{Q}(\theta, \hat{u} \circ \hat{T}_\theta^{-1}) = \mathcal{Q}(\theta, u) \; .$$

4.2.2. Dual-based error representation. In this case, contrary to linearization at Ω_0, it is not necessary to transport the approximation u^{h}, as it is already defined on $\hat{\Omega}$. Hence, we can immediately proceed to the following definition of the dual problem at $(\theta^{\mathsf{h}}, u^{\mathsf{h}})$:

$$\boxed{\begin{aligned} &\text{Find } \hat{z} \in H^1_{0,\Gamma_{\mathcal{D}}}(\hat{\Omega}) : \\ &\qquad \hat{\mathcal{N}}'\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); \hat{z}\big)(\delta\theta, \delta\hat{u}) = \hat{\mathcal{Q}}'\big(\theta^{\mathsf{h}}, u^{\mathsf{h}}\big)(\delta\theta, \delta\hat{u}) \\ &\qquad\qquad\qquad\qquad\qquad\qquad \forall (\delta\theta, \delta\hat{u}) \in \Theta \times H^1_{0,\partial\Omega}(\hat{\Omega}) \; . \end{aligned}} \tag{4.18}$$

We provide a specification of the functionals in (4.18) in section 5.1. Continuing under the assumption that (4.18) has a unique solution $\hat{z}$, we provide the error representation formula based on $\hat{z}$:

[5]To avoid the proliferation of "ˆ" symbols, we allow ambiguous notations here. The precise connotation of A_θ, f_θ, or g_θ will be clear from the context.

THEOREM 4.6 (error representation based on $\hat{z}$). *Given any approximation $(\theta^{\mathsf{h}}, u^{\mathsf{h}}) \in \Theta \times H^1_h(\hat{\Omega})$ of the solution $(\theta, u) \in \Theta \times H^1_h(\Omega_\theta)$ of the free-boundary problem* (4.1)*, let $\hat{z} \in H^1_{0,\Gamma_{\mathcal{D}}}(\hat{\Omega})$ be the solution of dual problem* (4.18)*. It holds that*

$$\boxed{\mathcal{E}_{\mathcal{Q}} := \mathcal{Q}(\theta, u) - \mathcal{Q}(\theta^{\mathsf{h}}, u^{\mathsf{h}}) = \mathcal{R}\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); \hat{z}\big) + R\,,} \tag{4.19}$$

with quadratic remainder $R = R_{\hat{\mathcal{Q}}} - R_{\hat{\mathcal{N}}}$, where

$$R_{\hat{\mathcal{Q}}} := \int_0^1 \hat{\mathcal{Q}}''\big(\theta^{\mathsf{h}} + t\, e^\theta, u^{\mathsf{h}} + t\, \hat{e}^u\big)(e^\theta, \hat{e}^u)(e^\theta, \hat{e}^u)\,(1-t)\;\mathrm{d}t\,,$$
$$R_{\hat{\mathcal{N}}} := \int_0^1 \hat{\mathcal{N}}''\big((\theta^{\mathsf{h}} + t\, e^\theta, u^{\mathsf{h}} + t\, \hat{e}^u); \hat{z}\big)(e^\theta, \hat{e}^u)(e^\theta, \hat{e}^u)\,(1-t)\;\mathrm{d}t\,,$$

and where $e^\theta := \theta - \theta^{\mathsf{h}}$ and

$$\boxed{\hat{e}^u := u \circ \hat{T}_\theta - u^{\mathsf{h}}\,.}$$

Note that the remainder now forms a quadratic term in the difference on the approximate domain, that is, $\hat{e}^u \in H^1_0(\hat{\Omega})$.

Proof. The proof proceeds analogously as the proof of Theorem 4.3. ∎

4.3. Equivalence of dual problems. The essential difference between mapping to Ω_0 and $\hat{\Omega}$ occurs in the corresponding dual problems (4.9) and (4.18). The corresponding dual solutions z_0 on Ω_0 and $\hat{z}$ on $\hat{\Omega}$ are, however, equivalent in the following sense.

PROPOSITION 4.7. *Given the transformation $\hat{T}_\theta$ according to* (4.13)*, the solution z_0 of dual problem* (4.9) *transported to the approximate domain $\hat{\Omega}$ is equal to the solution $\hat{z}$ of dual problem* (4.18)*, that is,*

$$z_0 \circ T^{-1}_{\theta^{\mathsf{h}}} = \hat{z} \in H^1_{0,\Gamma_{\mathcal{D}}}(\hat{\Omega})\,.$$

Note that this implies that the residuals and the remainders in the error representations corresponding to Ω_0 and $\hat{\Omega}$, in (4.11) and (4.19), respectively, coincide. In fact, it does not matter which domain is taken as a reference: The dual solutions corresponding to two distinct reference domains are related by the map between the domains.

Proof of Proposition 4.7. The proof is obtained by showing that $z_0 \circ T^{-1}_{0,\theta^{\mathsf{h}}}$ satisfies dual problem (4.18). Consider $v_0 \in H_{0,\Gamma_{\mathcal{D}}}(\Omega_0)$ and $w_0 \in H^1_h(\Omega_0)$. By the definitions of $\mathcal{N}_0$ and $\hat{\mathcal{N}}$, in (4.4) and (4.15), respectively, we have the key identity

$$\begin{aligned}\mathcal{N}_0\big((\theta, w_0); v_0\big) &= \mathcal{N}\big((\theta, w_0 \circ T^{-1}_\theta); v_0 \circ T^{-1}_\theta\big)\\ &= \hat{\mathcal{N}}\big((\theta, w_0 \circ T^{-1}_\theta \circ \hat{T}_\theta); v_0 \circ T^{-1}_\theta \circ \hat{T}_\theta\big)\\ &= \hat{\mathcal{N}}\big((\theta, w_0 \circ T^{-1}_{\theta^{\mathsf{h}}}); v_0 \circ T^{-1}_{\theta^{\mathsf{h}}}\big)\,,\end{aligned}$$

where we used (4.13) in the last step. Taking the derivative at the approximation $(\theta^{\mathsf{h}}, u_0^{\mathsf{h}})$ yields the following relation between $\mathcal{N}_0'$ and $\hat{\mathcal{N}}'$:

$$\begin{aligned}&\mathcal{N}_0'\big((\theta^{\mathsf{h}}, u_0^{\mathsf{h}}); v_0\big)(\delta\theta, \delta u_0)\\ &\quad= \lim_{t\to 0} \frac{1}{t}\Big(\mathcal{N}_0\big((\theta^{\mathsf{h}} + t\,\delta\theta, u_0^{\mathsf{h}} + t\,\delta u_0); v_0\big) - \mathcal{N}_0\big((\theta^{\mathsf{h}}, u_0^{\mathsf{h}}); v_0\big)\Big)\\ &\quad= \lim_{t\to 0} \frac{1}{t}\Big(\hat{\mathcal{N}}\big((\theta^{\mathsf{h}} + t\,\delta\theta, u^{\mathsf{h}} + t\,\delta u_0 \circ T^{-1}_{\theta^{\mathsf{h}}}); v_0 \circ T^{-1}_{\theta^{\mathsf{h}}}\big) - \hat{\mathcal{N}}\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); v_0 \circ T^{-1}_{\theta^{\mathsf{h}}}\big)\Big)\\ &\quad= \hat{\mathcal{N}}'\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); v_0 \circ T^{-1}_{\theta^{\mathsf{h}}}\big)(\delta\theta, \delta u_0 \circ T^{-1}_{\theta^{\mathsf{h}}})\,.\end{aligned}$$

Notice that we used $u_0^{\mathsf{h}} = u^{\mathsf{h}} \circ T_{\theta^{\mathsf{h}}}$ in the second step; see (4.8). Similarly, we have

$$\mathcal{Q}_0'\big(\theta^{\mathsf{h}}, u_0^{\mathsf{h}}\big)(\delta\theta, \delta u_0) = \hat{\mathcal{Q}}'\big(\theta^{\mathsf{h}}, u^{\mathsf{h}}\big)(\delta\theta, \delta u_0 \circ T_{\theta^{\mathsf{h}}}^{-1}) \, .$$

Hence, substituting the above identities in the Ω_0-dual problem (4.9), it follows that z_0 satisfies

$$\hat{\mathcal{N}}'\big((\theta, u^{\mathsf{h}}); z_0 \circ T_{\theta^{\mathsf{h}}}^{-1}\big)\big)(\delta\theta, \delta u_0 \circ T_{\theta^{\mathsf{h}}}^{-1}) = \hat{\mathcal{Q}}'\big(\theta, u^{\mathsf{h}}\big)(\delta\theta, \delta u_0 \circ T_{\theta^{\mathsf{h}}}^{-1})$$

$\forall\,(\delta\theta, \delta u_0) \in \Theta \times H^1_{0,\partial\Omega_0}(\Omega_0)$. Finally, recall that the function transportation map, $\delta u_0 \mapsto \delta u_0 \circ T_{\theta^{\mathsf{h}}}^{-1}$, is a linear bijection (cf. (4.3)), implying the equality of spaces

$$H^1_{0,\partial\hat{\Omega}}(\hat{\Omega}) = \Big\{\delta\hat{u} = \delta u_0 \circ T_{\theta^{\mathsf{h}}}^{-1} \, : \, \delta u_0 \in H^1_{0,\partial\Omega_0}(\Omega_0)\Big\} \, .$$

Hence, we have

$$\hat{\mathcal{N}}'\big((\theta, u^{\mathsf{h}}); z_0 \circ T_{\theta^{\mathsf{h}}}^{-1}\big)\big)(\delta\theta, \delta\hat{u}) = \hat{\mathcal{Q}}'\big(\theta, u^{\mathsf{h}}\big)(\delta\theta, \delta\hat{u})$$

$\forall\,(\delta\theta, \delta\hat{u}) \in \Theta \times H^1_{0,\partial\hat{\Omega}}(\hat{\Omega})$, which concludes the proof. □

5. Analysis of the dual problem.

In this section, we analyze the $\hat{\Omega}$-dual problem (4.18). First, we specify the derivatives in (4.18). Then, we interpret the dual problem by extracting the corresponding partial differential equation and boundary conditions.

Recall the $\hat{\Omega}$-dual problem (4.18):

$$\begin{aligned} &\text{Find } z \in H^1_{0,\Gamma_{\mathcal{D}}}(\hat{\Omega}) : \\ &\hat{\mathcal{N}}'\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); z\big)(\delta\theta, \delta u) = \hat{\mathcal{Q}}'\big(\theta^{\mathsf{h}}, u^{\mathsf{h}}\big)(\delta\theta, \delta u) \\ &\qquad\qquad\qquad\qquad \forall(\delta\theta, \delta\hat{u}) \in \Theta \times H^1_{0,\partial\Omega}(\hat{\Omega}) \, . \end{aligned} \tag{5.1}$$

The semilinear form $\hat{\mathcal{N}}$ is given by

$$\begin{aligned} \hat{\mathcal{N}}\big((\theta, w); v\big) &= \int_{\hat{\Omega}} (A_\theta \nabla w) \cdot \nabla v - \int_{\hat{\Omega}} f_\theta \, v - \int_{\hat{\Gamma}} g_\theta \, v \\ &= \hat{\mathcal{A}}\big(\theta; w, v\big) - \hat{\mathcal{F}}\big(\theta; v\big) - \hat{\mathcal{G}}\big(\theta; v\big) \, , \end{aligned}$$

where, for convenience, we have introduced transformed functionals of $\mathcal{A}$, $\mathcal{F}$, and $\mathcal{G}$:

$$\begin{aligned} \hat{\mathcal{A}}\big(\theta; w, v\big) &= \mathcal{A}\big(\theta; w \circ \hat{T}_\theta^{-1}, v \circ \hat{T}_\theta^{-1}\big) \, , \\ \hat{\mathcal{F}}\big(\theta; v\big) &= \mathcal{F}\big(\theta; v \circ \hat{T}_\theta^{-1}\big) \, , \\ \hat{\mathcal{G}}\big(\theta; v\big) &= \mathcal{G}\big(\theta; v \circ \hat{T}_\theta^{-1}\big) \end{aligned}$$

$\forall\, v, w \in H^1(\hat{\Omega})$. We consider the dual problem for a goal functional consisting of the sum of the average and elevation functional. When transformed to $\hat{\Omega}$, the goal functional is given by

$$\hat{\mathcal{Q}}(\theta, \hat{u}) = \hat{\mathcal{Q}}^{\text{ave}}(\theta; \hat{u}) + \hat{\mathcal{Q}}^{\text{elev}}(\theta) = \int_{\hat{\Omega}} q_\theta^{\text{ave}} \, \hat{u} + \int_{\Gamma_0} q^{\text{elev}} \, \alpha_\theta \, ,$$

with

$$q_\theta^{\text{ave}} := \hat{J}_\theta \, (q_\theta^{\text{ave}} \circ \hat{T}_\theta) \, . \tag{5.2}$$

5.1. Specification of the dual problem. The variational statement (5.1) can be logically separated into two equations corresponding to δu and $\delta\theta$. Since only $\hat{\mathcal{A}}$ and $\hat{\mathcal{Q}}^{\text{ave}}$ depend on u and, moreover, the dependence is linear, the δu-equation is simply

$$\hat{\mathcal{A}}\big(\theta^h;\delta u,z\big)=\hat{\mathcal{Q}}^{\text{ave}}\big(\theta^h;\delta u\big)\qquad\forall\delta u\in H^1_{0,\partial\hat\Omega}(\hat\Omega)\ .$$

Furthermore, in view of $\hat{T}_{\theta^{\mathsf{h}}}=Id$, we have $\hat{\mathcal{A}}\big(\theta^{\mathsf{h}};\cdot,\cdot\big)=\mathcal{A}\big(\theta^{\mathsf{h}};\cdot,\cdot\big)$ and $\hat{\mathcal{Q}}^{\text{ave}}\big(\theta^{\mathsf{h}};\cdot\big)=\mathcal{Q}^{\text{ave}}\big(\theta^{\mathsf{h}};\cdot\big)$. Hence, the above expression corresponds to

$$\boxed{\int_{\hat\Omega}\nabla\delta u\cdot\nabla z=\int_{\hat\Omega}q^{\text{ave}}\,\delta u\qquad\forall\delta u\in H^1_{0,\partial\hat\Omega}(\hat\Omega)\ .}\tag{5.3a}$$

The $\delta\theta$-equation, on the other hand, is given by

$$\begin{aligned}\hat{\mathcal{A}}'\big(\theta^{\mathsf{h}};u^{\mathsf{h}},z\big)(\delta\theta)-\hat{\mathcal{F}}'\big(\theta^{\mathsf{h}};z\big)(\delta\theta)-\hat{\mathcal{G}}'\big(\theta^{\mathsf{h}};z\big)(\delta\theta)&\\ =\hat{\mathcal{Q}}^{\text{ave}\prime}(\theta^{\mathsf{h}};u^{\mathsf{h}})(\delta\theta)+\hat{\mathcal{Q}}^{\text{elev}\prime}(\theta^{\mathsf{h}})(\delta\theta)&\qquad\forall\delta\theta\in\Theta\ .\end{aligned}$$

For a specification of this equation, we require the derivatives of A_θ, f_θ, g_θ, q^{ave}_θ, and α_θ. Let us first state some elementary derivatives. Generally, such derivatives are given for a linearization at $\theta=0$, that is, at the unperturbed configuration; see [8,37], for example. However, linearizations about nonzero θ can simply be obtained by translation. In particular, note that $\hat{T}_\theta$ can be written as a perturbation of the identity starting from θ^{h}:

$$\hat{T}_{\theta^{\mathsf{h}}+t\,\delta\theta}=Id+t\,(\delta\theta\circ T^{-1}_{\theta^{\mathsf{h}}})=Id+t\,\hat{\delta\theta}\ ,$$

where

$$\hat{\delta\theta}:=\delta\theta\circ T^{-1}_{\theta^h}\in\hat\Theta:=\big\{\hat{\delta\theta}=\delta\theta\circ T^{-1}_{\theta^{\mathsf{h}}}\ \forall\delta\theta\in\Theta\big\}\ ;$$

see (4.13). A proof of the following lemmata then follows from standard results in [8,37], for example.

LEMMA 5.1. *For $\hat{T}_\theta$, $\hat{J}$, and $\hat\omega$ defined in* (4.13) *and* (4.17)*, we have*

$$\begin{aligned}\big\langle\partial_\theta\mathrm{D}\hat{T}_{\theta^{\mathsf{h}}},\delta\theta\big\rangle&=\mathrm{D}\hat{\delta\theta}\ ,&\qquad\big\langle\partial_\theta\hat{J}_{\theta^{\mathsf{h}}},\delta\theta\big\rangle&=\operatorname{div}\hat{\delta\theta}\ ,\\ \big\langle\partial_\theta\mathrm{D}\hat{T}^{-1}_{\theta^{\mathsf{h}}},\delta\theta\big\rangle&=-\mathrm{D}\hat{\delta\theta}\ ,&\qquad\big\langle\partial_\theta\hat\omega_{\theta^{\mathsf{h}}},\delta\theta\big\rangle&=\operatorname{div}_\Gamma\hat{\delta\theta}\end{aligned}$$

$\forall\,\hat{\delta\theta}\in\hat\Theta$.

The tangential (or surface) divergence in Lemma 5.1 is defined as [9]:

$$\operatorname{div}_\Gamma(\cdot):=\operatorname{div}(\cdot)\big|_\Gamma-\partial_n(\cdot)\cdot n\ .$$

LEMMA 5.2. *Let $\phi\in H^1(\mathbb{R}^N)$. Then the map $\theta\mapsto\phi\circ\hat{T}_\theta$ is differentiable at $\theta^h\in\Theta$ in $L^2(\hat\Omega)$. The derivative is given by*

$$\big\langle\partial_\theta(\phi\circ\hat{T}_\theta)\big|_{\theta^h},\delta\theta\big\rangle=\nabla\phi\cdot\hat{\delta\theta}$$

$\forall\,\hat{\delta\theta}\in\hat\Theta$.

Using these results, we can easily derive the derivatives of $A_\theta, f_\theta, g_\theta$, and q_θ^{ave} from their definitions in Proposition 4.5 and (5.2):

$$\left\langle \partial_\theta A_{\theta^h}, \delta\theta \right\rangle = (\operatorname{div} \hat{\delta\theta})\, I - \mathrm{D}\hat{\delta\theta} - \mathrm{D}\hat{\delta\theta}^{\mathsf{T}} \,, \qquad \left\langle \partial_\theta f_{\theta^h}, \delta\theta \right\rangle = \operatorname{div}(f\, \hat{\delta\theta}) \,,$$
$$\left\langle \partial_\theta g_{\theta^h}, \delta\theta \right\rangle = g\, \operatorname{div}_\Gamma \hat{\delta\theta} + \nabla g \cdot \hat{\delta\theta} \,, \qquad \left\langle \partial_\theta q_{\theta^h}^{\mathrm{ave}}, \delta\theta \right\rangle = \operatorname{div}(q^{\mathrm{ave}}\, \hat{\delta\theta}) \,,$$

with I the identity matrix. The derivative of α_θ required for the linearization of $\hat{\mathcal{Q}}^{\mathrm{elev}}$ is a bit more involved. Therefore, it is derived in Appendix A for the two-dimensional case. Its final result is the linearization

$$\hat{\mathcal{Q}}^{\mathrm{elev}\prime}(\theta^h)(\delta\theta) = \int_{\hat{\Gamma}} q^{\mathrm{elev}}\, \delta\theta \cdot n \,,$$

where since q^{elev} is only defined on Γ_0, it should be interpreted with the aid of a projection along the x_N-axis, that is,

$$q^{\mathrm{elev}}(x_1, \ldots, x_N) = q^{\mathrm{elev}}(x_1, \ldots, x_{N-1}, x_N^{\Gamma_0}),$$

with $x_N^{\Gamma_0}$ being the x_N-coordinate of Γ_0.

The above results lead to the following specification of the $\delta\theta$-equation.

PROPOSITION 5.3. *Given an approximation $\theta^{\mathsf{h}} \in \Theta$ with corresponding domain $\hat{\Omega} = \Omega_{\theta^{\mathsf{h}}}$ and an approximation $u^{\mathsf{h}} \in H_h^1(\hat{\Omega})$, the $\delta\theta$-equation in dual problem* (5.1) *is given by*

$$\boxed{\begin{aligned} &\int_{\hat{\Omega}} \Big(\big[\operatorname{div} \delta\theta\, I - \mathrm{D}\delta\theta - \mathrm{D}\delta\theta^{\mathsf{T}} \big] \nabla u^h \Big) \cdot \nabla z \\ &\quad - \int_{\hat{\Omega}} \operatorname{div}(f\, \delta\theta)\, z - \int_{\hat{\Gamma}} \big(g\, \operatorname{div}_\Gamma \delta\theta + \nabla g \cdot \delta\theta \big)\, z \\ &\qquad = \int_{\hat{\Omega}} \operatorname{div}(q^{\mathrm{ave}}\, \delta\theta)\, u^h + \int_{\hat{\Gamma}} q^{\mathrm{elev}}\, \delta\theta \cdot n \qquad \forall \delta\theta \in \hat{\Theta} \,. \end{aligned}} \tag{5.3b}$$

For a given approximate domain $\hat{\Omega}$ and approximation u^{h}, the complete dual problem for $z \in H^1_{0,\Gamma_{\mathcal{D}}}(\hat{\Omega})$ is specified by (5.3a) and (5.3b). Note that the dual problem is independent of the particular parametrization in Θ_{Lip} that gives $\hat{\Omega}$. The dual problem is, however, dependent on the extension into $\hat{\Omega}$ of the perturbations $\delta\theta \in \hat{\Theta}$; cf. the final remark in section 2.2.

5.2. Interpretation of the dual problem. At this point, we are ready to interpret the dual problem. A priori we know that the dual solution z is in $H^1_{0,\Gamma_{\mathcal{D}}}(\hat{\Omega})$. Hence, z satisfies the boundary condition

$$z = 0 \qquad \text{on } \Gamma_{\mathcal{D}} \,.$$

To extract the partial differential equation in $\hat{\Omega}$ and the boundary condition on $\hat{\Gamma}$, we assume that $z \in H^1_{0,\Gamma_{\mathcal{D}}}(\hat{\Omega}) \cap H^2(\hat{\Omega})$ and, furthermore, that $\hat{\Gamma}$ is smooth enough; for example, $\hat{\Gamma}$ is $C^{1,1}$. By integration by parts and standard variational arguments, the δu-equation (5.3a) yields a Poisson equation driven by our interest in the following average goal:

$$-\Delta z = q^{\mathrm{ave}} \qquad \text{in } \hat{\Omega} \,.$$

The $\delta\theta$-equation in principle specifies a boundary condition on $\hat{\Gamma}$, which completes the boundary value problem for z. However, it does not generally correspond to an ordinary local boundary condition. In particular, the $\delta\theta$-equation enforces a boundary condition involving a nonlocal operator associated with the residual. This is evidenced by the following proposition, whose proof we delay until the end of this section.

PROPOSITION 5.4. *If* $\hat{\Gamma}$ *is* $C^{1,1}$ *and* $z \in H^1_{0,\Gamma_{\mathcal{D}}}(\hat{\Omega}) \cap H^2(\hat{\Omega})$, *then the* $\delta\theta$*-equation* (5.3b) *can be written as*

$$\mathcal{R}\big((\theta^h, u^h); \nabla z \cdot \delta\theta\big) - \int_{\hat{\Gamma}} \Big(g\,\partial_n z + \big(f + \partial_n g + \kappa\, g\big)\, z + q^{\text{ave}} + q^{\text{elev}}\Big)\,\delta\theta \cdot n = 0$$

$\forall\, \delta\theta \in \hat{\Theta}$, *where* $\kappa := \operatorname{div}_\Gamma n$ *coincides with the additive curvature (sum of* $N-1$ *curvatures) of* $\hat{\Gamma}$.

To establish that the above condition indeed corresponds to a nonlocal boundary condition, we recall from the final remark in section 2.2 that $\hat{\Theta}$ consists of perturbation fields that are extensions of functions on $\hat{\Gamma}$ and that yield unique perturbed domains. For a $C^{1,1}$ free boundary, this implies that $\delta\theta \cdot n \neq 0\ \forall\, \delta\theta \in \hat{\Theta} \setminus \{0\}$ and, moreover, $\delta\theta_1 \cdot n \neq \delta\theta_2 \cdot n$ for distinct $\delta\theta_1, \delta\theta_2 \in \hat{\Theta}$. Accordingly, we can identify the residual term with a local free-boundary term by means of the $L^2(\hat{\Gamma})$ Riesz representant $r^h(z)$:

$$\int_{\hat{\Gamma}} r^h(z)\,\delta\theta \cdot n = \mathcal{R}\big((\theta^h, u^h); \nabla z \cdot \delta\theta\big) \qquad \forall \delta\theta \in \hat{\Theta}\,.$$

Note that $r^h(z)$ is dependent on the particular extension into $\hat{\Omega}$ of perturbations $\delta\theta \in \hat{\Theta}$. With the $L^2(\hat{\Gamma})$ identification, we can summarize the dual problem for z as:

$$\boxed{\begin{aligned} -\Delta z &= q^{\text{ave}} && \text{in } \hat{\Omega}\,,\\ z &= 0 && \text{on } \Gamma_{\mathcal{D}}\,,\\ r^h(z) - g\,\partial_n z - \big(f + \partial_n g + \kappa\, g\big)\, z &= q^{\text{ave}} + q^{\text{elev}} && \text{on } \hat{\Gamma}\,. \end{aligned}}$$

At the solution (θ, u) the residual vanishes, and accordingly, the nonlocal boundary term $r^h(z)$ vanishes too. The boundary condition on $\hat{\Gamma}$ then reduces to an ordinary Robin boundary condition, and its dependency on the particular extension into $\hat{\Omega}$ of the perturbations $\delta\theta \in \hat{\Theta}$ disappears.

Similar Robin problems are also encountered in the shape-linearized Bernoulli free-boundary problem (cf. [14,25]) and in its shape-linearized adjoint which is considered in our companion work [49]. A standard sufficiency condition for well posedness of the dual problem at the solution (for which $r^h(z) = 0$) is $(f + \partial_n g)/g + \kappa \geq 0$ on $\hat{\Gamma}$. Such conditions on the data also appear in [11, 12].

Proof of Proposition 5.4. We will rewrite the terms in (5.3b) one after another. To rewrite the first term, we need the gradient of an inner product. That is, let ξ and η denote two H^1 vector functions. Then $\nabla(\xi \cdot \eta) = \mathrm{D}\xi^{\mathsf{T}}\,\eta + \mathrm{D}\eta^{\mathsf{T}}\,\xi$. We can then verify

$$\begin{aligned} &\int_{\hat{\Omega}} \Big(\big[-\mathrm{D}\delta\theta - \mathrm{D}\delta\theta^{\mathsf{T}}\big]\nabla u^{\mathsf{h}}\Big) \cdot \nabla z \\ &= \int_{\hat{\Omega}} \Big(\delta\theta \cdot \nabla(\nabla u^{\mathsf{h}} \cdot \nabla z) - \nabla u^{\mathsf{h}} \cdot \nabla(\nabla z \cdot \delta\theta) - \nabla z \cdot \nabla(\nabla u^{\mathsf{h}} \cdot \delta\theta)\Big) \\ &= \int_{\hat{\Omega}} \Big(\delta\theta \cdot \nabla(\nabla u^{\mathsf{h}} \cdot \nabla z) - \nabla u^{\mathsf{h}} \cdot \nabla(\nabla z \cdot \delta\theta) + \Delta z\,(\nabla u^{\mathsf{h}} \cdot \delta\theta)\Big) - \int_{\hat{\Gamma}} \partial_n u^{\mathsf{h}}\,\partial_n z\,\delta\theta \cdot n\,, \end{aligned}$$

where in the last step, we performed an integration by parts on the third term. Furthermore, we invoked $\delta\theta = 0$ on $\Gamma_{\mathcal{D}}$ and the fact that u^{h} is constant (=1) on $\hat{\Gamma}$ so that $\nabla u^{\mathsf{h}} = \partial_n u^{\mathsf{h}}\, n$ on $\hat{\Gamma}$. Substituting the above result in the first term of (5.3b) gives

$$\int_{\hat{\Omega}} \big([\operatorname{div}\delta\theta\, I - \mathrm{D}\delta\theta - \mathrm{D}\delta\theta^{\mathsf{T}}]\nabla u^h\big)\cdot\nabla z$$
$$= \int_{\hat{\Omega}} \Big(\operatorname{div}\big(\delta\theta\,(\nabla u^{\mathsf{h}}\cdot\nabla z)\big) - \nabla u^{\mathsf{h}}\cdot\nabla(\nabla z\cdot\delta\theta) + \Delta z\,(\nabla u^{\mathsf{h}}\cdot\delta\theta)\Big)$$
$$- \int_{\hat{\Gamma}} \partial_n u^{\mathsf{h}}\,\partial_n z\,\delta\theta\cdot n$$
$$= \int_{\hat{\Omega}} \Big(-\nabla u^{\mathsf{h}}\cdot\nabla(\nabla z\cdot\delta\theta) + \Delta z\,(\nabla u^{\mathsf{h}}\cdot\delta\theta)\Big)\,, \tag{5.4a}$$

where in the last step we used the divergence theorem on the first term and invoked the same arguments as before on $\delta\theta$ and u^{h} to cancel the $\hat{\Gamma}$-term. Next, we continue with the terms involving f, q^{ave}, and q^{elev} in (5.3b). By integration by parts, we simply obtain

$$-\int_{\hat{\Omega}} \operatorname{div}(f\,\delta\theta)\,z = \int_{\hat{\Omega}} f\,\nabla z\cdot\delta\theta - \int_{\hat{\Gamma}} f\,z\,\delta\theta\cdot n\,, \tag{5.4b}$$

(5.4c)
$$\int_{\hat{\Omega}} \operatorname{div}(q^{\mathrm{ave}}\,\delta\theta)\,u^{\mathsf{h}} + \int_{\hat{\Gamma}} q^{\mathrm{elev}}\,\delta\theta\cdot n = -\int_{\hat{\Omega}} q^{\mathrm{ave}}\,(\nabla u^h\cdot\delta\theta) + \int_{\hat{\Gamma}} \big(q^{\mathrm{ave}} + q^{\mathrm{elev}}\big)\,\delta\theta\cdot n\,.$$

Finally, we take up the term involving g in (5.3b). For this, we require additional tangential calculus; see, for instance, [8, 9]. At $\hat{\Gamma}$, a gradient splits into a tangential gradient and a normal component: $\nabla(\cdot) = \nabla_\Gamma(\cdot) + \partial_n(\cdot)\,n$. Hence,

$$\nabla g\cdot\delta\theta = \nabla_\Gamma g\cdot\delta\theta + \partial_n g\,\delta\theta\cdot n\,.$$

We can combine the tangential divergence and tangential gradient and apply a tangential Green's identity as follows:

$$\int_{\hat{\Gamma}} \big(g\,\operatorname{div}_\Gamma\delta\theta + \nabla_\Gamma g\cdot\delta\theta\big)\,z = \int_{\hat{\Gamma}} \operatorname{div}_\Gamma(g\,\delta\theta)\,z = \int_{\hat{\Gamma}} \kappa\,g\,z\,\delta\theta\cdot n - \int_{\hat{\Gamma}} g\,\delta\theta\cdot\nabla_\Gamma z\,.$$

It then follows that the term involving g in (5.3b) can be written as

(5.4d)
$$-\int_{\hat{\Gamma}} \big(g\,\operatorname{div}_\Gamma\delta\theta + \nabla g\cdot\delta\theta\big)\,z = \int_{\hat{\Gamma}} \Big(g\,\nabla z\cdot\delta\theta - \big((\partial_n g + \kappa\,g)\,z + g\,\partial_n z\big)\,\delta\theta\cdot n\Big)\,.$$

We finish by gathering the contributions in (5.4a)–(5.4d). Basically, we can distinguish three different groups: domain contributions involving $\nabla u^{\mathsf{h}}\cdot\delta\theta$ and $\nabla z\cdot\delta\theta$ and free-boundary contributions involving $\delta\theta\cdot n$. The first group cancels since $-\Delta z = q^{\mathrm{ave}}$. The second group adds up to the residual term $\mathcal{R}\big((\theta^{\mathsf{h}}, u^{\mathsf{h}}); \nabla z\cdot\delta\theta\big)$. The last group forms the free-boundary integral as stated in the proposition. ∎

6. Numerical experiments. In this section, we present numerical experiments. First, to exemplify essential attributes, we consider in section 6.1 the free-boundary problem in one dimension. Similar one-dimensional free-boundary problems have been considered in [6, 14, 47]. One-dimensional free-boundary problems are attractive for a number of reasons. The first is that the free boundary has no geometry; i.e., it is merely a point. Also, it is rather effortless to obtain exact expressions for dual solutions. Therefore, error estimates are inexact only due to nonlinearity.

In section 6.2 we take up the free-boundary problem in two dimensions. Approximations to the free-boundary problem are obtained by using linear finite elements. Here, we focus on the effectivity of the error estimate on uniform meshes. In addition, we show an example of goal-oriented adaptive mesh refinement.

6.1. One-dimensional application. In the one-dimensional setting, we characterize the variable domain as $\Omega_\vartheta = (0,\vartheta) \subset \mathbb{R}$. The Dirichlet boundary and free boundary correspond to single points, $\Gamma_{\mathcal{D}} = \{0\}$ and $\Gamma_\vartheta = \{\vartheta\}$, respectively. The semilinear form $\mathcal{N}$ $(= -\,\mathcal{R})$ and the goal functionals are given by

$$\begin{aligned}\mathcal{N}\big((\vartheta,u);v\big) &= \int_{\Omega_\vartheta} \big(u_x\, v_x - f\, v\big)\,\mathrm{d}x - g(\vartheta)\, v(\vartheta)\ ,\\ \mathcal{Q}^{\mathrm{ave}}(\vartheta;u) &= \int_{\Omega_\vartheta} q^{\mathrm{ave}}\, u\,\mathrm{d}x\ ,\\ \mathcal{Q}^{\mathrm{elev}}(\vartheta) &= q^{\mathrm{elev}}\,\vartheta\ ,\end{aligned}$$

where $(\cdot)_x = \mathrm{d}(\cdot)/\mathrm{d}x$ and $q^{\mathrm{elev}} \in \mathbb{R}$. To a free-boundary approximation $\vartheta^{\mathsf{h}} > 0$, we associate a domain transformation from $\hat\Omega = \Omega_{\vartheta^{\mathsf{h}}}$ to Ω_ϑ by the linear map

$$x = \hat T_\vartheta(\hat x) = \frac{\vartheta}{\vartheta^{\mathsf{h}}}\hat x = \hat x + \frac{\vartheta - \vartheta^{\mathsf{h}}}{\vartheta^{\mathsf{h}}}\hat x\ .$$

Let, furthermore, $u^{\mathsf{h}} \in H^1_h(\hat\Omega)$ be given. It can be verified that the $\hat\Omega$-dual problem (4.18) reduces in this setting to the following: Find $z \in H^1_{0,\Gamma_{\mathcal{D}}}(\hat\Omega)$:

$$\begin{aligned}\int_{\hat\Omega} \delta u_x\, z_x\,\mathrm{d}x &= \int_{\hat\Omega} q^{\mathrm{ave}}\,\delta u\,\mathrm{d}x\ ,\\ -\frac{\delta\vartheta}{\vartheta^{\mathsf{h}}}\int_{\hat\Omega}\big(u^{\mathsf{h}}_x\, z_x + (f\,x)_x\, z\big)\,\mathrm{d}x - g_x(\vartheta^{\mathsf{h}})\, z(\vartheta^{\mathsf{h}})\,\delta\vartheta &= \frac{\delta\vartheta}{\vartheta^{\mathsf{h}}}\int_{\hat\Omega}(q^{\mathrm{ave}}\,x)_x\, u^{\mathsf{h}}\,\mathrm{d}x + q^{\mathrm{elev}}\,\delta\vartheta\end{aligned}$$

$\forall\,(\delta\vartheta,\delta u) \in \mathbb{R}\times H^1_{0,\partial\hat\Omega}(\hat\Omega)$. The dual problem translates into the boundary value problem:

$$\begin{aligned}-z_{xx}(x) &= q^{\mathrm{ave}}(x) \qquad \forall x \in \hat\Omega\ ,\\ z(0) &= 0\ ,\\ \mathcal{R}\big((\vartheta^{\mathsf{h}},u^{\mathsf{h}}); z_x\, x/\vartheta^{\mathsf{h}}\big) - \big(g\, z_x + (f+g_x)\, z\big)(\vartheta^{\mathsf{h}}) &= q^{\mathrm{ave}}(\vartheta^{\mathsf{h}}) + q^{\mathrm{elev}}\ .\end{aligned}$$

6.1.1. Typical error estimate. In the following numerical example, we consider the data and goal functionals as indicated in Table 1. Table 1 also contains the

TABLE 1
Specification of the data for the one-dimensional example.

$f(x)$	$g(x)$	$q^{\mathrm{ave}}(x)$	q^{elev}	ϑ	$u(x)$	$\mathcal{Q}^{\mathrm{ave}}(\vartheta;u)$	$\mathcal{Q}^{\mathrm{elev}}(\vartheta)$
$-\frac{1}{2}$	$x-1$	1	1	2	$\frac{1}{4}x^2$	$\frac{2}{3}$	2

corresponding exact solution. Consider the following approximation of the solution and the corresponding goal values:

$$\big(\vartheta^{\mathsf{h}}, u^{\mathsf{h}}(x)\big) = \left(\frac{3}{2}, \frac{2}{3}x\right) , \qquad \mathcal{Q}^{\mathrm{ave}}\big(\vartheta^{\mathsf{h}}; u^{\mathsf{h}}\big) = \frac{3}{4} , \qquad \mathcal{Q}^{\mathrm{elev}}\big(\vartheta^{\mathsf{h}}\big) = \frac{3}{2} .$$

Figure 5 (left) shows a graphical illustration of the exact and approximate solutions. Furthermore, Figure 5 (right) shows the dual solutions for $\mathcal{Q}^{\mathrm{ave}}$ and $\mathcal{Q}^{\mathrm{elev}}$:

$$z^{\mathrm{ave}}(x) = \frac{45}{86}x - \frac{1}{2}x^2 , \qquad z^{\mathrm{elev}}(x) = -\frac{24}{43}x, \text{ respectively.}$$

The corresponding dual-based error estimate, $\mathrm{Est}_{\mathcal{Q}} := \mathcal{R}\big((\vartheta^{\mathsf{h}}, u^{\mathsf{h}}); z\big)$, and the true goal-error, $\mathcal{E}_{\mathcal{Q}}$, are as follows:

$$\begin{aligned} \mathrm{Est}_{\mathcal{Q}^{\mathrm{ave}}} &= \frac{15}{344} , & \mathrm{Est}_{\mathcal{Q}^{\mathrm{elev}}} &= \frac{39}{86} , \\ \mathcal{E}_{\mathcal{Q}^{\mathrm{ave}}} &= -\frac{1}{12} , & \mathcal{E}_{\mathcal{Q}^{\mathrm{elev}}} &= \frac{1}{2} . \end{aligned}$$

Note that the difference in the error estimate and the true error is caused by linearization, which is rather large for $\mathcal{Q}^{\mathrm{ave}}$ due to the crude approximation ϑ^{h}. The only source of nonlinearity is the domain dependence, and one can easily verify that the estimates are exact if $\vartheta^{\mathsf{h}} = \vartheta$.

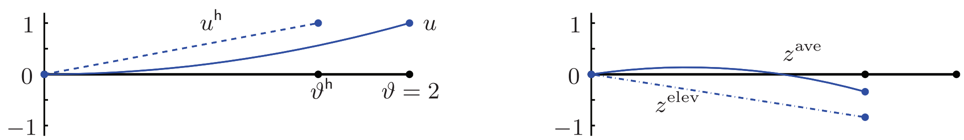

FIG. 5. *Exact solution (ϑ, u) and approximation $(\vartheta^{\mathsf{h}}, u^{\mathsf{h}})$ (left). Dual solutions z^{ave} and z^{elev} corresponding to goal functionals $\mathcal{Q}^{\mathrm{ave}}$ and $\mathcal{Q}^{\mathrm{elev}}$, respectively (right).*

6.1.2. Convergence of error estimates. In this example, the data is again specified as in Table 1. To investigate the convergence of the dual-based error estimate, we consider the following $\Delta\vartheta$-family of approximate solutions:

$$\big(\vartheta^{\mathsf{h}}, u^{\mathsf{h}}\big) = \big(\vartheta - \Delta\vartheta \ , \ u \circ \hat{T}_{\vartheta}\big) . \tag{6.1}$$

This family converges to the exact solution as $\Delta\vartheta \to 0$. Note that for each $\Delta\vartheta$, u^{h} is simply a scaling of u along the x-axis. This also implies that $\hat{e}^u = u \circ \hat{T}_{\vartheta} - u^{\mathsf{h}} = 0$. Hence, from the perspective of the error representation (see Theorem 4.6), the only relevant error is $e^{\vartheta} = \Delta\vartheta$.

For the goal functional $\mathcal{Q}^{\mathrm{ave}}$, Figure 6 (left) plots the true value $\mathcal{E}_{\mathcal{Q}^{\mathrm{ave}}}$ and the dual-based estimate $\mathrm{Est}_{\mathcal{Q}^{\mathrm{ave}}}$ with respect to $\Delta\vartheta$. It can be seen that the estimate approaches the exact error as $\Delta\vartheta \to 0$. Moreover, the slopes of the two curves are identical at $\Delta\vartheta = 0$. To further elucidate the convergence behavior, Figure 6 (right) presents a log-log plot of the error in the estimate $|\mathcal{E}_{\mathcal{Q}^{\mathrm{ave}}} - \mathrm{Est}_{\mathcal{Q}^{\mathrm{ave}}}|$ versus the norm of the error:

$$\big\|(e^{\vartheta}, \hat{e}^u)\big\|^2 = |\vartheta - \vartheta^{\mathsf{h}}|^2 + \big|u \circ \hat{T}_{\vartheta} - u^{\mathsf{h}}\big|^2_{H^1(\hat{\Omega})} = |\Delta\vartheta|^2 .$$

Both figures confirm that the estimate converges as $\mathcal{O}(\|(e^{\vartheta}, \hat{e}^u)\|^2)$.

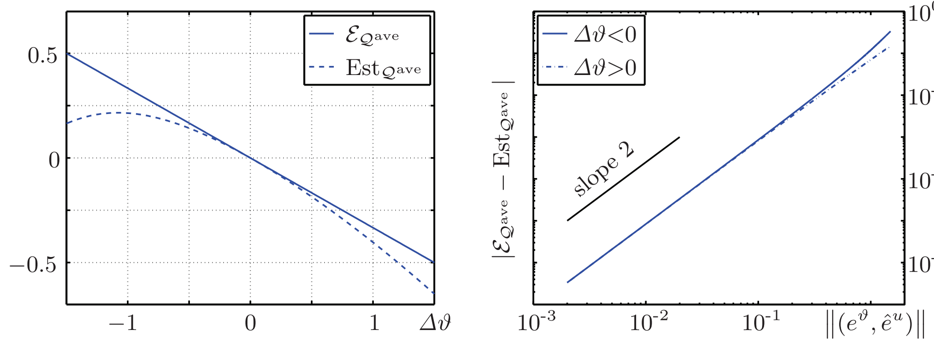

FIG. 6. *True goal error* $\mathcal{E}_{\mathcal{Q}^{\rm ave}}$ *and dual-based error estimate* $\mathrm{Est}_{\mathcal{Q}^{\rm ave}}$ *for the* $\Delta\vartheta$*-family of approximations* $(\vartheta^{\mathsf{h}}, u^{\mathsf{h}})$ *given in* (6.1) *(left). Convergence of the error in the error estimate with respect to the norm* $\|(e^\vartheta, \hat{e}^u)\|$ *(right).*

6.2. Two-dimensional application. Next, we turn to the two-dimensional case. We denote coordinates by $(x, y) \in \mathbb{R}^2$. In the following examples, we compute approximations $(\theta^{\mathsf{h}}, u^{\mathsf{h}})$ of (2.2) based on piecewise-linear finite elements on triangles. Accordingly, the approximate free boundary is a piecewise-linear curve composed of the edges of adjacent elements. The nonlinear problem is solved using a fixed point iteration similar to the explicit Neumann scheme in [14], where we allow the vertices of the free boundary to move only vertically. Hence, $\theta_1^{\mathsf{h}} = 0$ and $\theta_2^{\mathsf{h}} = \alpha_{\theta^{\mathsf{h}}}$ on Γ_0.

The dual problem (5.3) is solved on the same mesh as the approximation but with quadratic shape functions. That is, z is piecewise-quadratic and vanishes on $\Gamma_{\mathcal{D}}$, and the test functions δu are piecewise-quadratic shape functions that are zero on $\partial\hat{\Omega}$. Furthermore, the test functions $\delta\theta$ in (5.3b) are suitable extensions of vertical-perturbation fields $\delta\vartheta$ on $\hat{\Gamma}$:

$$\delta\theta_2(x, y) = \frac{y - y^{\mathrm{b}}(x)}{y^{\hat{\Gamma}}(x) - y^{\mathrm{b}}(x)}\, \delta\vartheta_2\big(x, y^{\hat{\Gamma}}(x)\big) \qquad \forall (x, y) \in \hat{\Omega}\ ,$$

where y^b represents the bottom of the domain and $y^{\hat{\Gamma}} = y^{\Gamma_0} + \alpha_{\theta^{\mathsf{h}}}$ describes the position of the approximate free boundary. Moreover, for $\delta\vartheta_2$ we use piecewise-quadratic shape functions which vanish on $\partial\hat{\Gamma}$.

6.2.1. Effectivity for the parabolic free-boundary test case. First, we investigate the effectivity of the dual-based error estimate under uniform mesh refinement. We consider a test problem with a geometric lay-out and solution as depicted in Figure 7. We have $y_b = 0$ and $y^{\Gamma_0} = 1$ and $\Omega_\theta = (0, 2) \times (0, 1 + \alpha_\theta)$. The data $\{f, g, h\}$ of the problem is manufactured to yield the parabolic free-boundary elevation and solution

$$\alpha_\theta(x) = \frac{1}{2}\, x\,(2 - x)\ ,$$
$$u(x, y) = \frac{y}{1 + \alpha_\theta(x)} + \alpha_\theta(x)\, \frac{y}{1 + \alpha_\theta(x)} \left(1 - \frac{y}{1 + \alpha_\theta(x)}\right)\ .$$

Our interest is the average goal functional with $q^{\mathrm{ave}} = 1$. For the exact solution, we have $Q^{\mathrm{ave}}(\theta; u) = 67/45 = 1.4888\ldots$. An illustration of the coarsest mesh approximation is also visible in Figure 7. For this approximation, we find the value $Q^{\mathrm{ave}}(\theta^{\mathsf{h}}; u^{\mathsf{h}}) = 1.1573\ldots$.

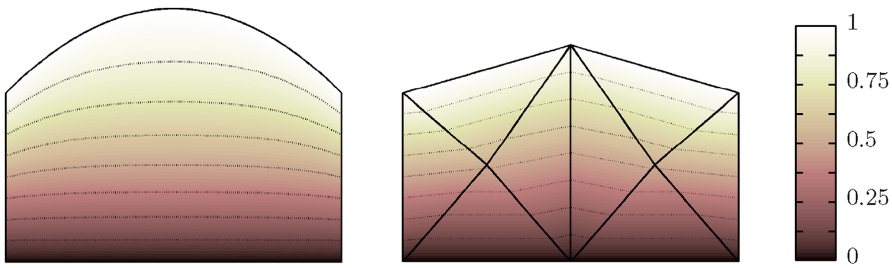

FIG. 7. *Test problem of section* 6.2.1. *The exact domain and solution (contour plot) (left) and the approximate domain and solution corresponding to the coarsest mesh (right).*

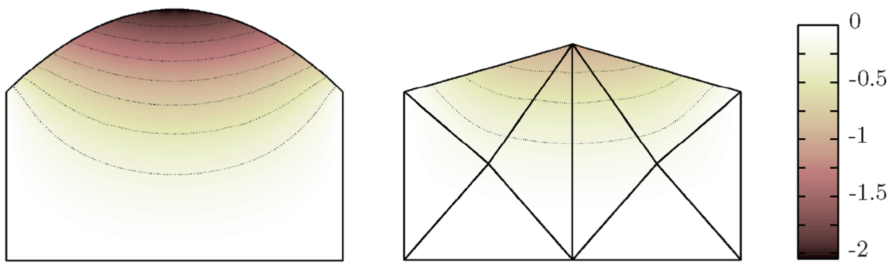

FIG. 8. *Test problem of section* 6.2.1. *The approximate dual solution (contour plot) associated with a very fine mesh (left) and the coarsest mesh (right).*

In Figure 8, we depict the approximate dual solution z for the coarsest mesh and for a very fine mesh. The convergence of the corresponding estimates, $\mathrm{Est}_{\mathcal{Q}^{\mathrm{ave}}} = \mathcal{R}((\theta^{\mathsf{h}}, u^{\mathsf{h}}); z)$, on uniformly refined meshes is reported in Table 2. Note that the effectivity index $\mathrm{Est}_{\mathcal{Q}^{\mathrm{ave}}} / \mathcal{E}_{\mathcal{Q}^{\mathrm{ave}}}$ approaches 1, which clearly demonstrates the consistency of the error estimate.

6.2.2. Goal-oriented adaptivity for free-surface flow over a bump. To investigate the applicability of the dual-based error estimate to drive adaptive mesh refinement, we consider a domain with a reentrant corner at the bottom; see Figure 9 (top). We take $y^{\Gamma_0} = 1$, $\Omega_\theta = (0, 4) \times (y^b, 1 + \alpha_\theta)$, and $f = 0$, $g = 1$. Moreover,

TABLE 2
Convergence of the goal-oriented error estimate $\mathrm{Est}_{\mathcal{Q}^{\mathrm{ave}}}$ *under uniform mesh refinement.*

Elements	DOFs	$\mathcal{Q}^{\mathrm{ave}}(\theta^{\mathsf{h}}; u^{\mathsf{h}})$	$\mathcal{E}_{\mathcal{Q}^{\mathrm{ave}}}$	$\mathrm{Est}_{\mathcal{Q}^{\mathrm{ave}}}$	Effectivity
8	8	1.1573	0.33163	0.22131	0.667
16	15	1.3145	0.17440	0.13852	0.794
32	23	1.3694	0.11947	0.09994	0.836
64	45	1.4284	0.06045	0.05499	0.910
128	77	1.4555	0.03339	0.03055	0.915
256	153	1.4715	0.01740	0.01676	0.963
512	281	1.4803	0.00860	0.00808	0.940
1,024	561	1.4843	0.00458	0.00450	0.984
2,048	1,073	1.4867	0.00217	0.00205	0.947
4,096	2,145	1.4877	0.00117	0.00115	0.991
8,192	4,193	1.4883	0.00054	0.00051	0.949
16,384	8,385	1.4886	0.00029	0.00029	0.993
∞	∞	1.4888	0		

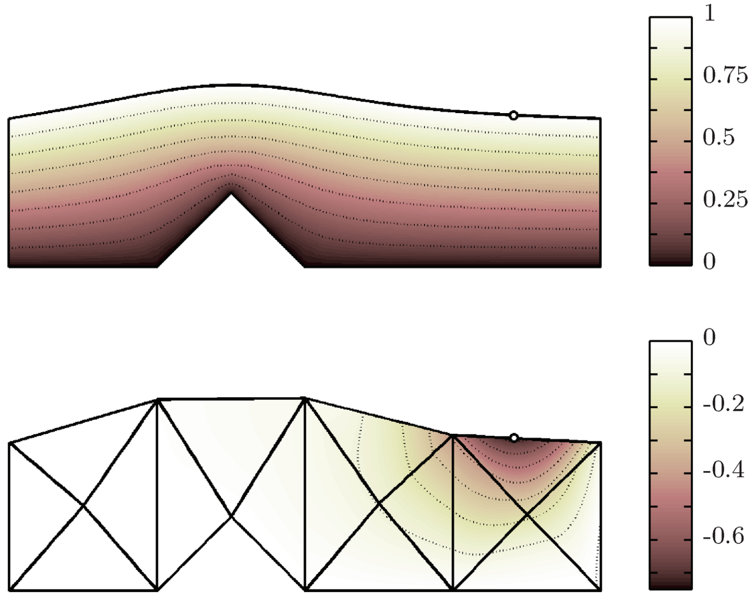

FIG. 9. *Test problem of section* 6.2.2. *The exact domain and solution (contour plot) (top), and the approximate domain and dual solution corresponding to the coarsest mesh (bottom). We have indicated the free-boundary elevation point of interest (at $x_0 = 2 + \sqrt{2}$).*

h is 0 at the bottom and increases linearly to 1 along the sides of the domain. Our interest is the elevation of the free boundary at the specific point $x_0 = 2 + \sqrt{2}$; see Figure 9. This interest corresponds to the elevation goal functional $\mathcal{Q}^{\text{elev}}$ with q^{elev} a Dirac measure at x_0. The linearization of this functional is elaborated in Appendix A. Figure 9 (bottom) displays the corresponding coarsest mesh dual solution.

To drive the adaptivity, element refinement indicators are extracted from the error estimate formula, as usual (see [3], for example). (In particular, we integrate by parts elementwise and assign weighted interior and edge residuals to the associated elements to obtain element contributions. The absolute values of the element contributions are then identified as the element indicators.) Based on these indicators, we mark a set of elements for refinement. This set is the minimal set for which the sum is a fraction of the total sum of indicators (a so-called Dörfler-type marking; see [33]). We take this fraction as 0.4. The marked elements are refined using newest vertex bisection. We introduce additional refinements to preserve a conforming mesh [4, 40].

In Figure 10, we plot the convergence of the error estimate versus the total number of degrees of freedom, which is denoted by n. A plot of the "true" error is also displayed. This true error has been obtained by computing the goal on a uniformly refined mesh with 245,760 elements and $\mathsf{n} = 123{,}585$ resulting in the reference value $\mathcal{Q}^{\text{elev}}(\theta) \approx 0.02271$. The results indicate that the accuracy of this reference value is surpassed on adaptively refined meshes for $\mathsf{n} > 1{,}000$. This explains the drop in the true error for the adaptive case for $\mathsf{n} > 1{,}000$. Furthermore, the plots reveal an asymptotic convergence rate of $\mathcal{O}(\mathsf{n}^{-1})$ for adaptive refinements. This is expected for optimal refinements and should be compared with the suboptimal convergence rate of approximately $\mathcal{O}(\mathsf{n}^{-3/4})$ for uniform refinements. Figure 11 shows several adaptively refined meshes. Apart from the refinement at the reentrant corner, the refinements at the free boundary and particularly near the elevation point of interest are noteworthy.

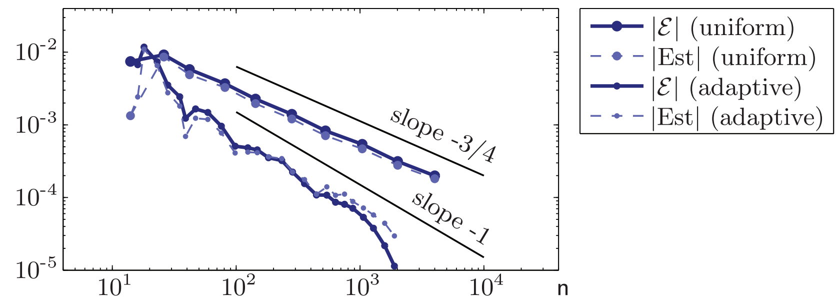

FIG. 10. *Convergence of the "true" error* $\mathcal{E} = \mathcal{E}_{\mathcal{Q}^{\mathrm{elev}}}$ *and error estimate* $\mathrm{Est} = \mathrm{Est}_{\mathcal{Q}^{\mathrm{elev}}}$ *under uniform and adaptive mesh refinement versus the total number of degrees of freedom* n.

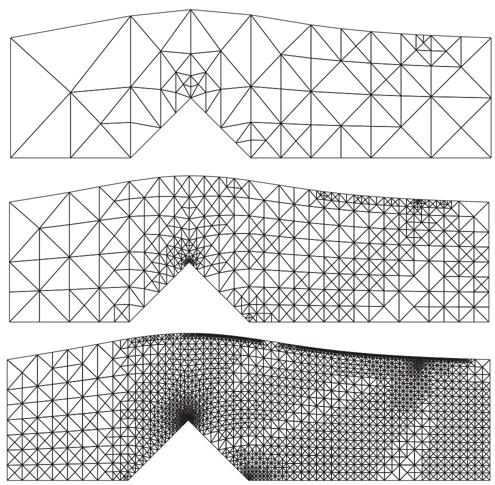

FIG. 11. *Adaptively refined meshes, controlling the error in the free-boundary elevation at* $x_0 = 2 + \sqrt{2}$, *obtained after* 10 *(top),* 18 *(middle), and* 29 *(bottom) iterations with* 120, 793, *and* 5,447 *elements, respectively.*

7. Concluding remarks. We showed that free-boundary problems elude the standard goal-oriented error estimation framework on account of the fact that their typical variational form is noncanonical. To obtain an appropriate dual problem (linearized adjoint), we presented the domain-map linearization approach. In this approach the free-boundary problem is transformed into an equivalent problem on a fixed reference domain which has a canonical variational form. The dual problem is then obtained by linearization with respect to the domain map. We showed that the solution of the dual problem is essentially independent of the selected reference domain: Dual solutions corresponding to distinct reference domains are related by the obvious map between the reference domains.

For a Bernoulli-type free-boundary problem, we showed that the dual problem corresponds to a Poisson problem with a nonlocal Robin-type boundary condition. The nonlocal term depends on the particular extension of boundary perturbations into the domain, but, being of residual type, the nonlocal term vanishes at the exact free-boundary solution. The effectivity of the dual-based error estimate and its usefulness in goal-oriented adaptive mesh refinement was demonstrated by numerical experiments in one and two dimensions.

The presented approach admits several extensions. For example, we considered constant Dirichlet data at the free boundary which means that the data is invariant under domain transformations. Nonconstant Dirichlet data can be included by means of a free-boundary Lagrange multiplier in the variational formulation. Such a formulation, moreover, allows nonconforming trial functions that violate the Dirichlet data.

The domain-map linearization approach bears similarities to the classical material derivative in shape optimization in view of the comparison of functions in a reference domain; see [37]. An alternative in the shape-optimization field is the so-called shape derivative. The shape-linearization approach can also be used to obtain a suitable dual problem for goal-oriented error estimation of free-boundary problems. This is the subject of the companion paper [49]. Moreover, in that paper we present a comparison of the two different approaches.

An extension of both the domain-map and shape-linearization approaches to a fluid-structure-interaction problem is presented in [45, 46].

Appendix A. Linearization of the elevation goal. The elevation goal functional is defined in section 2.4 as

$$\mathcal{Q}^{\mathrm{elev}}(\theta) = \int_{\Gamma_0} q^{\mathrm{elev}}\, \alpha_\theta \ ,$$

where α_θ is, for a specific domain Ω_θ, the vertical deviation of the free boundary Γ_θ from Γ_0. In this section, we present the linearization of $\mathcal{Q}^{\mathrm{elev}}$ at $\theta^{\mathsf{h}} \in \Theta$ by differentiation of α_θ.[6] For the sake of clarity, we consider the two-dimensional case. However, the derivation extends without difficulty to three (and higher) dimensions.

Given $\hat{\Gamma} = \Gamma_{\theta^{\mathsf{h}}}$ and its associated elevation function $\alpha_{\theta^{\mathsf{h}}}$, consider the perturbation $\Gamma_t := \Gamma_{\theta^{\mathsf{h}}+t\,\delta\theta}$ and $\alpha_t := \alpha_{\theta^{\mathsf{h}}+t\,\delta\theta}$; see Figure 12. Without loss of generality, we view θ^{h} and $\delta\theta$ as functions of the horizontal coordinate x only. Next, fixing a particular x, we observe from Figure 12 that the perturbed elevation can be given at a shifted location:

$$\alpha_t\big(x + \theta_1^{\mathsf{h}}(x) + t\,\delta\theta_1(x)\big) = \alpha_0\big(x + \theta_1^{\mathsf{h}}(x)\big) + t\,\delta\theta_2(x)\ .$$

This is the key identity to obtain the derivative of α_θ. By introducing the Γ_0 transformation $T_{\theta_1^{\mathsf{h}},t}(x) := x + \theta_1^{\mathsf{h}}(x) + t\,\delta\theta_1(x)$ and denoting $T_{\theta_1^{\mathsf{h}}} := T_{\theta_1^{\mathsf{h}},0}$, it holds that

$$\big\langle \partial_\theta \alpha_{\theta^{\mathsf{h}}}, \delta\theta \big\rangle = \lim_{t\to 0} \frac{1}{t}\big(\alpha_t - \alpha_0\big) = \delta\theta_2 \circ T^{-1}_{\theta_1^{\mathsf{h}}} + \lim_{t\to 0}\frac{1}{t}\big(\alpha_0 \circ T_{\theta_1^{\mathsf{h}}} \circ T^{-1}_{\theta_1^{\mathsf{h}},t} - \alpha_0\big).$$

As $T_{\theta_1^{\mathsf{h}}} \circ T^{-1}_{\theta_1^{\mathsf{h}},t} = (Id + t\,(\delta\theta_1 \circ T_{\theta_1^{\mathsf{h}}}))^{-1}$, the limit on the right-hand side is equal to $-\alpha'_{\theta^{\mathsf{h}}}\,\delta\theta_1 \circ T^{-1}_{\theta_1^{\mathsf{h}}}$ (for a.e. x). Hence, we obtain

$$\boxed{\big\langle \partial_\theta \alpha_{\theta^{\mathsf{h}}}, \delta\theta \big\rangle = \big(\delta\theta \circ T^{-1}_{\theta_1^{\mathsf{h}}}\big) \cdot \big(-\alpha'_{\theta^{\mathsf{h}}}, 1\big)\ .}$$

[6] Alternatively, one could reformulate $\mathcal{Q}^{\mathrm{elev}}$ as a shape functional involving a domain integral and use a standard shape derivative [37].

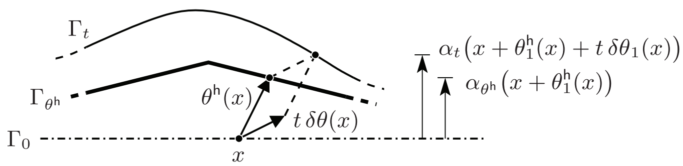

FIG. 12. *Perturbation of the free boundary and associated perturbation of the elevation.*

The elevation derivative, $\alpha'_{\theta^{\mathsf{h}}}$, can be written in terms of θ^{h} by differentiating the identity $\alpha_{\theta^{\mathsf{h}}} \circ T_{\theta_1^{\mathsf{h}}} = \theta_2^{\mathsf{h}}$, yielding $\alpha'_{\theta^{\mathsf{h}}} = \theta_2^{\mathsf{h}\prime}/(1+\theta_1^{\mathsf{h}\prime}) \circ T^{-1}_{\theta_1^{\mathsf{h}}}$. Subsequently, we have $\mathcal{Q}^{\mathrm{elev}\prime}(\theta^{\mathsf{h}})(\delta\theta) = \int_{\Gamma_0} q^{\mathrm{elev}}\,(\delta\theta\cdot(-\theta_2^{\mathsf{h}\prime}/(1+\theta_1^{\mathsf{h}\prime}),1))\circ T^{-1}_{\theta_1^{\mathsf{h}}}$. Performing a change of variables through the Γ_0-map $T_{\theta_1^{\mathsf{h}}}$, thereby picking up a Jacobian $(1+\theta_1^{\mathsf{h}\prime})$, we obtain the expression

$$\mathcal{Q}^{\mathrm{elev}\prime}(\theta^{\mathsf{h}})(\delta\theta) = \int_{\Gamma_0} \big(q^{\mathrm{elev}} \circ T_{\theta_1^{\mathsf{h}}}\big)\,\delta\theta \cdot \big(-\theta_2^{\mathsf{h}\prime}, 1+\theta_1^{\mathsf{h}\prime}\big)\ .$$

This Γ_0-supported integral can be transformed to $\hat{\Gamma}$ by the transformation $T_{\theta^{\mathsf{h}}}$. Carrying out this transformation, we pick up the Jacobian $((\theta_2^{\mathsf{h}\prime})^2 + (1+\theta_1^{\mathsf{h}\prime})^2)^{-1/2} \circ T^{-1}_{\theta^{\mathsf{h}}}$ which nicely combines with $(-\theta_2^{\mathsf{h}\prime}, 1+\theta_1^{\mathsf{h}\prime}) \circ T^{-1}_{\theta^{\mathsf{h}}}$ to form the unit normal vector n. Furthermore, recalling $\hat{\delta\theta} = \delta\theta \circ T^{-1}_{\theta^{\mathsf{h}}}$, we finally obtain the concise result:

$$\boxed{\mathcal{Q}^{\mathrm{elev}\prime}(\theta^{\mathsf{h}})(\delta\theta) = \int_{\hat{\Gamma}} q^{\mathrm{elev}}(x)\,\hat{\delta\theta}\cdot n\ .}$$

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REFERENCES

[1] M. Ainsworth and J. T. Oden, *A Posteriori Error Estimation in Finite Element Analysis*, Pure Appl. Math., Wiley, New York, 2000.
[2] Y. Bazilevs, V. M. Calo, T. J. R. Hughes, and Y. Zhang, *Isogeometric fluid–structure interaction: Theory, algorithms, and computations*, Comput. Mech., 43 (2008), pp. 3–37.
[3] R. Becker and R. Rannacher, *An optimal control approach to a posteriori error estimation in finite element methods*, Acta Numer., 10 (2001), pp. 1–102.
[4] P. Binev, W. Dahmen, and R. DeVore, *Adaptive finite element methods with convergence rates*, Numer. Math., 97 (2004), pp. 219–268.
[5] F. Bouchon, S. Clain, and R. Touzani, *A perturbation method for the numerical solution of the Bernoulli problem*, J. Comput. Math., 26 (2008), pp. 23–36.
[6] C. Cuvelier and R. M. S. M. Schulkes, *Some numerical methods for the computation of capillary free boundaries governed by the Navier–Stokes equations*, SIAM Rev., 32 (1990), pp. 355–423.
[7] M. C. Delfour and J.-P. Zolésio, *Structure of shape derivatives for nonsmooth domains*, J. Funct. Anal., 104 (1992), pp. 1–33.
[8] M. C. Delfour and J.-P. Zolésio, *Shapes and Geometries: Analysis, Differential Calculus, and Optimization*, SIAM Ser. Adv. Design and Control 4, Society for Industrial and Applied Mathematics, Philadelphia, 2001.
[9] M. C. Delfour and J.-P. Zolésio, *Tangential calculus and shape derivatives*, in Shape Optimization and Optimal Design: Proceedings of the IFIP Conference, Lect. Notes Pure Appl. Math. 216, J. Cagnol, M. P. Polis, and J.-P. Zolésio, eds., Marcel Dekker, New York, 2001, pp. 37–60.

[10] T. Dunne, *An Eulerian approach to fluid–structure interaction and goal-oriented mesh adaptation*, Internat. J. Numer. Methods Fluids, 51 (2006), pp. 1017–1039.

[11] K. Eppler and H. Harbrecht, *Efficient treatment of stationary free boundary problems*, Appl. Numer. Math., 56 (2006), pp. 1326–1339.

[12] K. Eppler, H. Harbrecht, and R. Schneider, *On convergence in elliptic shape optimization*, SIAM J. Control Optim., 46 (2007), pp. 61–83.

[13] M. A. Fernández and M. Moubachir, *A Newton method using exact Jacobians for solving fluid–structure interaction*, Comput. & Structures, 83 (2005), pp. 127–142.

[14] M. Flucher and M. Rumpf, *Bernoulli's free-boundary problem, qualitative theory and numerical approximation*, J. Reine Angew. Math., 486 (1997), pp. 165–204.

[15] A. Friedman, *Variational Principles and Free-Boundary Problems*, Pure Appl. Math., Wiley, New York, 1982.

[16] M. B. Giles and E. Süli, *Adjoint methods for PDEs: A posteriori error analysis and postprocessing by duality*, Acta Numer., 11 (2002), pp. 145–236.

[17] P. Grisvard, *Elliptic Problems in Nonsmooth Domains*, Monogr. Stud. Math. 24, Pitman Publishing, London, 1985.

[18] S. C. Gupta, *The Classical Stefan Problem: Basic Concepts, Modelling and Analysis*, North-Holland Ser. Appl. Math. Mech. 45, Elsevier, Amsterdam, 2003.

[19] R. Hartmann, *Multitarget error estimation and adaptivity in aerodynamic flow simulations*, SIAM J. Sci. Comput., 31 (2008), pp. 708–731.

[20] R. Hartmann and P. Houston, *Adaptive discontinuous Galerkin finite element methods for nonlinear hyperbolic conservation laws*, SIAM J. Sci. Comput., 24 (2003), pp. 979–1004.

[21] J. Haslinger, T. Kozubek, K. Kunisch, and G. Peichl, *Shape optimization and fictitious domain approach for solving free boundary problems of Bernoulli type*, Comput. Optim. Appl., 26 (2003), pp. 231–251.

[22] J. Haslinger and P. Neittaanmäki, *Finite Element Approximation for Optimal Shape, Material and Topology Design*, 2nd ed., Wiley, New York, 1996.

[23] J. Hoffman, *On duality-based a posteriori error estimation in various norms and linear functionals for large eddy simulation*, SIAM J. Sci. Comput., 26 (2004), pp. 178–195.

[24] P. Houston and E. Süli, hp-*Adaptive discontinuous Galerkin finite element methods for first-order hyperbolic problems*, SIAM J. Sci. Comput., 23 (2001), pp. 1226–1252.

[25] K. T. Kärkkäinen and T. Tiihonen, *Free surfaces: Shape sensitivity analysis and numerical methods*, Internat. J. Numer. Methods Engrg., 44 (1999), pp. 1079–1098.

[26] C. M. Kuster, P. A. Gremaud, and R. Touzani, *Fast numerical methods for Bernoulli free boundary problems*, SIAM J. Sci. Comput., 29 (2007), pp. 622–634.

[27] M. G. Larson, R. Söderlund, and F. Bengzon, *Adaptive finite element approximation of coupled flow and transport problems with applications in heat transfer*, Internat. J. Numer. Methods Fluids, 57 (2008), pp. 1397–1420.

[28] F. Larsson, P. Hansbo, and K. Runesson, *Strategies for computing goal-oriented a posteriori error measures in non-linear elasticity*, Internat. J. Numer. Methods Engrg., 55 (2002), pp. 879–894.

[29] G. Mejak, *Numerical solution of Bernoulli-type free boundary value problems by variable domain method*, Internat. J. Numer. Methods Engrg., 37 (1994), pp. 4219–4245.

[30] H. Melbø and T. Kvamsdal, *Goal oriented error estimators for Stokes equations based on variationally consistent postprocessing*, Comput. Methods Appl. Mech. Engrg., 192 (2003), pp. 613–633.

[31] M. S. Mommer and R. Stevenson, *A goal-oriented adaptive finite element method with convergence rates*, SIAM J. Numer. Anal., 47 (2009), pp. 861–886.

[32] K.-S. Moon, E. von Schwerin, A. Szepessy, and R. Tempone, *Convergence rates for an adaptive dual weighted residual finite element algorithm*, BIT, 46 (2006), pp. 367–407.

[33] P. Morin, R. H. Nochetto, and K. G. Siebert, *Convergence of adaptive finite element methods*, SIAM Rev., 44 (2002), pp. 631–658.

[34] O. Pironneau, *Optimal Shape Design for Elliptic Systems*, Springer Ser. Comput. Phys., Springer, Berlin, 1984.

[35] S. Prudhomme and J. T. Oden, *On goal-oriented error estimation for elliptic problems: Application to the control of pointwise errors*, Comput. Methods Appl. Mech. Engrg., 176 (1999), pp. 313–331.

[36] S. Prudhomme and J. T. Oden, *Computable error estimators and adaptive techniques for fluid flow problems*, in Error Estimation and Adaptive Discretization Methods in Computational Fluid Dynamics, Lect. Notes Comput. Sci. Eng., 25, T. J. Barth and H. Deconinck, eds., Springer, Berlin, 2003, pp. 207–268.

[37] J. Sokołowski and J.-P. Zolésio, *Introduction to Shape Optimization: Shape Sensitivity Analysis*, Springer Ser. Comput. Math. 16, Springer, New York, 1992.
[38] P. Šolin and L. F. Demkowicz, *Goal-oriented hp-adaptivity for elliptic problems*, Comput. Methods Appl. Mech. Engrg., 193 (2004), pp. 449–468.
[39] R. Stevenson, *Optimality of a standard adaptive finite element method*, Found. Comput. Math., 7 (2007), pp. 245–269.
[40] R. Stevenson, *The completion of locally refined simplicial partitions created by bisection*, Math. Comp., 77 (2008), pp. 227–241.
[41] E. Süli and P. Houston, *Adaptive finite element approximation of hyperbolic problems*, in Error Estimation and Adaptive Discretization Methods in Computational Fluid Dynamics, Lect. Notes Comput. Sci. Eng. 25, T. J. Barth and H. Deconinck, eds., Springer, Berlin, 2003, pp. 269–344.
[42] J. I. Toivanen, J. Haslinger, and R. A. E. Mäkinen, *Shape optimization of systems governed by Bernoulli free boundary problems*, Comput. Methods Appl. Mech. Engrg., 197 (2008), pp. 3802–3815.
[43] E. H. van Brummelen, *Mesh association by projection along smoothed-normal-vector fields: Association of closed manifolds*, Internat. J. Numer. Methods Engrg., 73 (2008), pp. 493–520.
[44] E. H. van Brummelen and A. Segal, *Numerical solution of steady free-surface flows by the adjoint optimal shape design method*, Internat. J. Numer. Methods Fluids, 41 (2003), pp. 3–27.
[45] K. G. van der Zee, *Goal-Adaptive Discretization of Fluid–Structure Interaction*, Ph.D. thesis, Technische Universiteit Delft, Delft, The Netherlands, June 2009. Available online from http://repository.tudelft.nl.
[46] K. G. van der Zee, E. H. van Brummelen, I. Akkerman, and R. de Borst, *Goal-oriented error estimation and adaptivity for fluid–structure interaction using exact linearized adjoints*, Comput. Methods Appl. Mech. Engrg., submitted.
[47] K. G. van der Zee, E. H. van Brummelen, and R. de Borst, *Dual-based a-posteriori error estimation for fluid–structure interaction by the embedded domain method*, in ECCOMAS CFD 06: Proceedings of the European Conference on Computational Fluid Dynamics, Egmond aan Zee, The Netherlands, 2006, P. Wesseling, E. Oñate, and J. Périaux, eds., CD-ROM (paper 588), TU Delft, The Netherlands, 2006.
[48] K. G. van der Zee, E. H. van Brummelen, and R. de Borst, *Goal-oriented error estimation for Stokes flow interacting with a flexible channel*, Internat. J. Numer. Methods Fluids, 56 (2008), pp. 1551–1557.
[49] K. G. van der Zee, E. H. van Brummelen, and R. de Borst, *Goal-oriented error estimation and adaptivity for free-boundary problems: The shape-linearization approach*, SIAM J. Sci. Comput., 32 (2010), pp. 1093–1118.
[50] R. Verfürth, *A Review of A Posteriori Error Estimation and Adaptive Mesh-Refinement Techniques*, Adv. Numer. Math., Wiley-Teubner, New York, Stuttgart, 1996.
[51] Z. Zhang and I. Babuška, *A numerical method for steady state free boundary problems*, SIAM J. Numer. Anal., 33 (1996), pp. 2184–2214.