A priori and *a posteriori* error identities for the scalar Signorini problem

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Abstract

In this paper, on the basis of a (Fenchel) duality theory on the continuous level, we derive an *a posteriori* error identity for arbitrary conforming approximations of the primal formulation and the dual formulation of the scalar Signorini problem. In addition, on the basis of a (Fenchel) duality theory on the discrete level, we derive an *a priori* error identity that applies to the approximation of the primal formulation using the Crouzeix–Raviart element and to the approximation of the dual formulation using the Raviart–Thomas element, and leads to quasi-optimal error decay rates without imposing additional assumptions on the contact set and in arbitrary space dimensions.

Keywords: Scalar Signorini problem; convex duality; Crouzeix–Raviart element; Raviart–Thomas element; *a priori* error identity; *a posteriori* error identity.

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1. Introduction

The *scalar Signorini problem* is a model problem that captures non-trivial effects present in elastic contact problems. It is a non-linear problem as it contains a non-linear boundary condition: in a bounded domain $\Omega \subseteq \mathbb{R}^d$, $d \in \mathbb{N}$, the solution $u\colon \overline{\Omega} \to \mathbb{R}$ of the scalar Signorini problem (*i.e.*, the *displacement field*) on a part of the (topological) boundary $\Gamma_C \subseteq \partial\Omega$ (*i.e.*, the *contact set*) is greater or equal to $\chi\colon \Gamma_C \to \mathbb{R}$ (*i.e.*, the *obstacle*) (*cf.* [41]). It can be expressed in form of a convex minimization problem with an optimality condition given via variational inequality (*cf.* [26]).

1.1 Related contributions

Finite element approximation as well as its *a priori* and *a posteriori* error analysis for unilateral contact problems is an active area of research for many decades. There is a vast literature on this topic; including conforming, non-conforming, and hybrid finite element methods (*cf.* [7, 11, 8, 9]), mixed (*cf.* [40]), and mortar finite element methods (*cf.* [12]). These methods typically employ element-wise affine or quadratic polynomial finite elements, due to limited regularity of the solution of these nonlinear contact problems (*cf.* Remark 3.3).

Due to scarcity, we refer to a few articles and references therein on this topic:

- In the context of *a posteriori* error analyses that provide reliable and efficient error bounds, we refer the reader to the contributions [29, 46, 10, 34].
- In the context of *a priori* error analyses, in [32], assuming that the solution lies in $H^{s+1}(\Omega)$, $s \in (\frac{1}{2}, 1]$, and that the contact set Γ_C has a certain regularity, quasi-optimal *a priori* error estimates are derived; in [30], assuming, again, that the solution lies in $H^{s+1}(\Omega)$, $s \in (\frac{1}{2}, 1]$,

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but no additional regularity of the contact set Γ_C, improved quasi-optimal *a priori* error estimates are derived; recently, in [22], important and interesting results are established to obtain quasi-optimal *a priori* error estimates for conforming finite element methods in two and three space dimensions without additional assumptions on the contact set Γ_C when the solution lies in $H^{s+1}(\Omega)$, $s \in (\frac{1}{2}, \frac{1}{2}+\frac{k}{2}]$, where $k \in \{1,2\}$ is the polynomial degree being used; in [15, 17], Nitsche's type methods with symmetric and non-symmetric variants are proposed and analyzed for the contact problem with $H^{s+1}(\Omega)$, $s \in (\frac{1}{2}, 1]$, regular solution and derived optimal order convergence in H^1-norm. A penalty method is formulated and its convergence at continuous and discrete level are studied in [16] for the two dimensional contact problem with $H^{s+1}(\Omega)$, $s \in (\frac{1}{2}, 1]$, regular solution but without any assumption on the contact set Γ_C, and further therein, the authors have established optimal convergence rates by deriving necessary relation between penalty parameter and the mesh size.

1.2 New contributions

The contributions of the present paper to the existing literature are two-fold:

- On the basis of (Fenchel) duality theory on the continuous level (combining approaches from [39], [14], and [4]), we derive an *a posteriori* error identity that applies to arbitrary conforming approximations of the primal formulation and the dual formulation of the scalar Signorini problem. More precisely, denoting by $u \in K$ and $z \in K^*$ the primal and dual solution, respectively, for admissible approximations $v \in K$ and $y \in K^*$, it holds that

$$\begin{aligned} &\tfrac{1}{2}\|\nabla v - \nabla u\|_{\Omega}^2 + \langle z\cdot n, v-\chi\rangle_{\partial\Omega} - \langle g, v-\chi\rangle_{\Gamma_N} \\ &\quad + \tfrac{1}{2}\|y - z\|_{\Omega}^2 + \langle y\cdot n, u-\chi\rangle_{\partial\Omega} - \langle g, u-\chi\rangle_{\Gamma_N} \\ &= \tfrac{1}{2}\|\nabla v - y\|_{\Omega}^2 + \langle y\cdot n, v-\chi\rangle_{\partial\Omega} - \langle g, v-\chi\rangle_{\Gamma_N}\,, \end{aligned} \tag{1.1}$$

  In addition, the induced local refinement indicators of the primal-dual gap (*a posteriori*) error estimator (*i.e.*, the right-hand side of) can be employed in adaptive mesh-refinement.
- On the basis of (Fenchel) duality theory on the discrete level, analogously to the *a posteriori* error identity on the continuous level (1.1), we derive an *a priori* error identity that applies to the approximation of the primal formulation using the Crouzeix–Raviart element (*cf.* [19]) and the approximation of the dual formulation using the Raviart–Thomas element (*cf.* [38]). More precisely, denoting by $u_h^{cr} \in K_h^{cr}$ and $z_h^{rt} \in K_h^{rt,*}$ the discrete primal and discrete dual solution, respectively, for admissible approximations $v_h \in K_h^{cr}$ and $y_h \in K_h^{rt,*}$, it holds that

$$\begin{aligned} &\tfrac{1}{2}\|\nabla_h v_h - \nabla_h u_h^{cr}\|_{\Omega}^2 + (z_h^{rt}\cdot n, \pi_h v_h - \chi_h)_{\Gamma_C} \\ &\quad + \tfrac{1}{2}\|\Pi_h y_h - \Pi_h z_h^{rt}\|_{\Omega}^2 + (y_h\cdot n, \pi_h u_h^{cr} - \chi_h)_{\Gamma_C} \\ &= \tfrac{1}{2}\|\nabla_h v_h - y_h\|_{\Omega}^2 + (y_h\cdot n, \pi_h v_h - \chi_h)_{\Gamma_C}\,. \end{aligned} \tag{1.2}$$

  From the *a priori* error identity (1.2), we derive quasi-optimal error decay rates without imposing additional assumptions on the regularity of the contact set Γ_C for arbitrary dimensions. This improves the existing literature (*cf.* [45, 31, 35]) on *a priori* error analyses for approximations of the scalar Signorini problem using the Crouzeix–Raviart element.

1.3 Outline

This article is organized as follows: In Section 2, we introduce the notation, the relevant function spaces and finite element spaces. In Section 3, a (Fenchel) duality theory for the continuous scalar Signorini problem is developed. This (Fenchel) duality theory is used in Section 4 in the derivation of an *a posteriori* error identity. In Section 5, a discrete (Fenchel) duality theory for the discrete scalar Signorini problem is developed. This discrete (Fenchel) duality theory, in turn, is used in Section 6 in the derivation of an *a priori* error identity, which, in turn, is used to derive error decay rates given only fractional regularity assumptions on the solution and the obstacle. In Section 7, we carry out numerical experiments that support the findings of Section 4 and Section 6.

2. Preliminaries

Throughout the article, let $\Omega \subseteq \mathbb{R}^d$, $d \in \mathbb{N}$, be a bounded simplicial Lipschitz domain such that $\partial\Omega$ is divided into three disjoint (relatively) open sets: a Dirichlet part $\Gamma_D \subseteq \partial\Omega$ with $|\Gamma_D| > 0$[1], a Neumann part $\Gamma_N \subseteq \partial\Omega$, and a contact part $\Gamma_C \subseteq \partial\Omega$ such that $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N \cup \overline{\Gamma}_C$.

2.1 Standard function spaces

For a (Lebesgue) measurable set $\omega \subseteq \mathbb{R}^n$, $n \in \mathbb{N}$, and (Lebesgue) measurable functions or vector fields $v, w : \omega \to \mathbb{R}^\ell$, $\ell \in \mathbb{N}$, we employ the inner product $(v, w)_\omega := \int_\omega v \odot w \,\mathrm{d}x$, whenever the right-hand side is well-defined, where $\odot : \mathbb{R}^\ell \times \mathbb{R}^\ell \to \mathbb{R}$ either denotes scalar multiplication or the Euclidean inner product. The integral mean over a (Lebesgue) measurable set $\omega \subseteq \mathbb{R}^n$, $n \in \mathbb{N}$, with $|\omega| > 0$ of an integrable function or vector field $v : \omega \to \mathbb{R}^\ell$, $\ell \in \mathbb{N}$, is defined by $\langle v \rangle_\omega := \frac{1}{|\omega|} \int_\omega v \,\mathrm{d}x$.

For $m \in \mathbb{N}$ and an open set $\omega \subseteq \mathbb{R}^n$, $n \in \mathbb{N}$, we define the spaces

$$
\begin{aligned}
H^m(\omega) &:= \left\{ v \in L^2(\omega) \quad \mid \mathrm{D}^{\boldsymbol{\alpha}} v \in L^2(\omega) \text{ for all } \boldsymbol{\alpha} \in (\mathbb{N}_0)^n \text{ with } |\boldsymbol{\alpha}| \le m \right\} , \\
H(\operatorname{div}; \omega) &:= \left\{ y \in (L^2(\omega))^n \mid \operatorname{div} y \in L^2(\omega) \right\} ,
\end{aligned}
$$

where $\mathrm{D}^{\boldsymbol{\alpha}} := \frac{\partial^{|\boldsymbol{\alpha}|}}{\partial x_1^{\alpha_1} \cdot \ldots \cdot \partial x_n^{\alpha_n}}$ and $|\boldsymbol{\alpha}| := \sum_{i=1}^n \alpha_i$ for each multi-index $\boldsymbol{\alpha} := (\alpha_1, \ldots, \alpha_n) \in (\mathbb{N}_0)^n$, and the *Sobolev norm* $\|\cdot\|_{m,\omega} := \|\cdot\|_\omega + |\cdot|_{m,\omega}$, where $\|\cdot\|_\omega := ((\cdot,\cdot)_\omega)^{\frac{1}{2}}$ and

$$
|\cdot|_{m,\omega} := \Bigg(\sum_{\boldsymbol{\alpha} \in (\mathbb{N}_0)^n \,:\, 0 < |\boldsymbol{\alpha}| \le m} \|\mathrm{D}^{\boldsymbol{\alpha}}(\cdot)\|_\omega^2 \Bigg)^{\frac{1}{2}} ,
$$

turns $H^m(\omega)$ into a Hilbert space.

For $s \in (0, \infty) \setminus \mathbb{N}$ and an open set $\omega \subseteq \mathbb{R}^n$, $n \in \mathbb{N}$, the *Sobolev–Slobodeckij semi-norm*, for every $v \in H^m(\omega)$, is defined by

$$
|v|_{s,\omega} := \Bigg(\sum_{|\boldsymbol{\alpha}| = m} \int_\omega \int_\omega \frac{|(\mathrm{D}^{\boldsymbol{\alpha}} v)(x) - (\mathrm{D}^{\boldsymbol{\alpha}} v)(y)|^2}{|x - y|^{2\theta + d}} \,\mathrm{d}x \,\mathrm{d}y \Bigg)^{\frac{1}{2}} ,
$$

where $m \in \mathbb{N}_0$ and $\theta \in (0, 1)$ are such that $s = m + \theta$. Then, for $s \in (0, \infty) \setminus \mathbb{N}$ and an open set $\omega \subseteq \mathbb{R}^n$, $n \in \mathbb{N}$, the *Sobolev–Slobodeckij space* is defined by

$$
H^s(\omega) := \left\{ v \in H^m(\omega) \mid |v|_{s,\omega} < \infty \right\} ,
$$

where $m \in \mathbb{N}_0$ and $\theta \in (0, 1)$ are such that $s = m + \theta$ and the *Sobolev–Slobodeckij norm*

$$
\|\cdot\|_{s,\omega} := \|\cdot\|_{m,\omega} + |\cdot|_{s,\omega}
$$

turns $H^s(\omega)$ into a Hilbert space.

Denote by $\operatorname{tr}(\cdot) : H^1(\Omega) \to H^{\frac{1}{2}}(\partial\Omega)$ the trace operator and by $\operatorname{tr}((\cdot) \cdot n) : H(\operatorname{div}; \Omega) \to H^{-\frac{1}{2}}(\partial\Omega)$ the normal trace operator, where $n : \partial\Omega \to \mathbb{S}^{d-1}$ denotes the outward unit normal vector field to $\partial\Omega$. Then, for every $v \in H^1(\Omega)$ and $y \in H(\operatorname{div}; \Omega)$, there holds the integration-by-parts formula (*cf.* [24, Sec. 4.3, (4.12)])

$$
(\nabla v, y)_\Omega + (v, \operatorname{div} y)_\Omega = \langle \operatorname{tr}(y) \cdot n, \operatorname{tr}(v) \rangle_{\partial\Omega} , \tag{2.1}
$$

where, for every $\widehat{y} \in H^{-\frac{1}{2}}(\gamma)$, $\widehat{v} \in H^{\frac{1}{2}}(\gamma)$, and $\gamma \in \{\Gamma_D, \Gamma_N, \Gamma_C, \partial\Omega\}$, we abbreviate

$$
\langle \widehat{y}, \operatorname{tr}(\widehat{v}) \rangle_\gamma := \langle \widehat{y}, \operatorname{tr}(\widehat{v}) \rangle_{H^{\frac{1}{2}}(\gamma)} . \tag{2.2}
$$

More precisely, in (2.2), for every subset $\gamma \subseteq \partial\Omega$ and $s > 0$, the Hilbert space $H^s(\gamma)$ is defined as the range of the restricted trace operator $\operatorname{tr}(\cdot)|_\gamma$ defined on $H^{s+\frac{1}{2}}(\Omega)$ endowed with the image norm, for every $w \in H^s(\gamma)$, defined by

$$
\|w\|_{s,\gamma} := \inf_{v \in H^{s+\frac{1}{2}}(\Omega) \,:\, \operatorname{tr}(v)|_\gamma = w} \|v\|_{s+\frac{1}{2},\Omega} ,
$$

and $H^{-s}(\gamma) := (H^s(\gamma))^*$ is defined as the corresponding topological dual space.

[1] For a (Lebesgue) measurable set $M \subseteq \mathbb{R}^d$, $d \in \mathbb{N}$, we denote by $|M|$ its d-dimensional Lebesgue measure. For a $(d-1)$-dimensional submanifold $M \subseteq \mathbb{R}^d$, $d \in \mathbb{N}$, we denote by $|M|$ its $(d-1)$-dimensional Hausdorff measure.

Eventually, we employ the notation

$$H^1_D(\Omega) \coloneqq \left\{ v \in H^1(\Omega) \mid \operatorname{tr}(v) = 0 \text{ a.e. on } \Gamma_D \right\},$$

$$H^2_N(\operatorname{div};\Omega) \coloneqq \left\{ y \in H(\operatorname{div};\Omega) \;\middle|\; \begin{aligned} &\langle \operatorname{tr}(y)\cdot n, \operatorname{tr}(v)\rangle_{\partial\Omega} = 0 \text{ for all } v \in H^1_D(\Omega) \\ &\text{with } \operatorname{tr}(v) = 0 \text{ a.e. on } \Gamma_C \end{aligned} \right\}.$$

In what follows, we omit writing both $\operatorname{tr}(\cdot)$ and $\operatorname{tr}((\cdot)\cdot n)$ in this context.

2.2 *Triangulations and standard finite element spaces*

Throughout the article, we denote by $\{\mathcal{T}_h\}_{h>0}$ a family of uniformly shape regular triangulations of $\Omega \subseteq \mathbb{R}^d$, $d \in \mathbb{N}$, (*cf.* [24]). Here, $h > 0$ refers to the *averaged mesh-size*, *i.e.*, $h = (\frac{|\Omega|}{\operatorname{card}(\mathcal{N}_h)})^{\frac{1}{d}}$, where $\mathcal{N}_h$ contains the vertices of the triangulation $\mathcal{T}_h$. We define the following sets of sides:

$$\begin{aligned}
\mathcal{S}_h &\coloneqq \mathcal{S}_h^i \cup \mathcal{S}_h^{\partial\Omega}, \\
\mathcal{S}_h^i &\coloneqq \left\{ T \cap T' \mid T, T' \in \mathcal{T}_h, \dim_{\mathscr{H}}(T \cap T') = d-1 \right\}, \\
\mathcal{S}_h^{\partial\Omega} &\coloneqq \left\{ T \cap \partial\Omega \mid T \in \mathcal{T}_h, \dim_{\mathscr{H}}(T \cap \partial\Omega) = d-1 \right\}, \\
\mathcal{S}_h^{\gamma} &\coloneqq \left\{ S \in \mathcal{S}_h^{\partial\Omega} \mid \operatorname{int}(S) \subseteq \gamma \right\} \text{ for } \gamma \in \left\{ \Gamma_D, \Gamma_N, \Gamma_C \right\},
\end{aligned}$$

where the Hausdorff dimension is defined by $\dim_{\mathscr{H}}(M) \coloneqq \inf\{d' \geq 0 \mid \mathscr{H}^{d'}(M) = 0\}$ for all $M \subseteq \mathbb{R}^d$. It is also assumed that the triangulations $\{\mathcal{T}_h\}_{h>0}$ and boundary parts Γ_D, Γ_C, and Γ_N are chosen such that $\mathcal{S}_h^{\partial\Omega} = \mathcal{S}_h^{\Gamma_D} \dot\cup \mathcal{S}_h^{\Gamma_C} \dot\cup \mathcal{S}_h^{\Gamma_N}$, *e.g.*, in the case $d = 2$, $\overline{\Gamma}_D$, $\overline{\Gamma}_C$, and $\overline{\Gamma}_N$ touch only in vertices.

For $k \in \mathbb{N}_0$ and $T \in \mathcal{T}_h$, let $\mathbb{P}^k(T)$ denote the set of polynomials of maximal degree k on T. Then, for $k \in \mathbb{N}_0$, the set of element-wise polynomial functions is defined by

$$\mathcal{L}^k(\mathcal{T}_h) \coloneqq \left\{ v_h \in L^\infty(\Omega) \mid v_h|_T \in \mathbb{P}^k(T) \text{ for all } T \in \mathcal{T}_h \right\}.$$

For $\ell \in \mathbb{N}$, the (local) L^2-projection $\Pi_h \colon (L^1(\Omega))^\ell \to (\mathcal{L}^0(\mathcal{T}_h))^\ell$ onto element-wise constant functions or vector fields, respectively, for every $v \in (L^1(\Omega))^\ell$ is defined by $\Pi_h v|_T \coloneqq \langle v\rangle_T$ for all $T \in \mathcal{T}_h$.

For $m \in \mathbb{N}_0$ and $S \in \mathcal{S}_h$, let $\mathbb{P}^m(S)$ denote the set of polynomials of maximal degree m on S. Then, for $m \in \mathbb{N}_0$ and $\mathcal{M}_h \in \{\mathcal{S}_h, \mathcal{S}_h^i, \mathcal{S}_h^{\partial\Omega}, \mathcal{S}_h^{\Gamma_D}, \mathcal{S}_h^{\Gamma_C}, \mathcal{S}_h^{\Gamma_N}\}$, the set of side-wise polynomial functions is defined by

$$\mathcal{L}^m(\mathcal{M}_h) \coloneqq \left\{ v_h \in L^\infty(\cup\mathcal{M}_h) \mid v_h|_S \in \mathbb{P}^m(S) \text{ for all } S \in \mathcal{M}_h \right\}.$$

For $\ell \in \mathbb{N}$, the (local) L^2-projection $\pi_h \colon (L^1(\cup\mathcal{S}_h))^\ell \to (\mathcal{L}^0(\mathcal{S}_h))^\ell$ onto side-wise constant functions or vector fields, respectively, for every $v_h \in (L^1(\cup\mathcal{S}_h))^\ell$ is defined by $\pi_h v_h|_S \coloneqq \langle v_h\rangle_S$ for all $S \in \mathcal{S}_h$.

For every $v_h \in \mathcal{L}^m(\mathcal{T}_h)$, $m \in \mathbb{N}_0$, and $S \in \mathcal{S}_h$, the *jump across* S is defined by

$$[\![v_h]\!]_S \coloneqq \begin{cases} v_h|_{T_+} - v_h|_{T_-} & \text{if } S \in \mathcal{S}_h^i, \text{ where } T_+, T_- \in \mathcal{T}_h \text{ satisfy } \partial T_+ \cap \partial T_- = S, \\ v_h|_T & \text{if } S \in \mathcal{S}_h^{\partial\Omega}, \text{ where } T \in \mathcal{T}_h \text{ satisfies } S \subseteq \partial T. \end{cases}$$

For every $y_h \in (\mathcal{L}^m(\mathcal{T}_h))^d$, $m \in \mathbb{N}_0$, and $S \in \mathcal{S}_h$, the *normal jump across* S is defined by

$$[\![y_h \cdot n]\!]_S \coloneqq \begin{cases} y_h|_{T_+} \cdot n_{T_+} + y_h|_{T_-} \cdot n_{T_-} & \text{if } S \in \mathcal{S}_h^i, \text{ where } T_+, T_- \in \mathcal{T}_h \text{ satisfy } \partial T_+ \cap \partial T_- = S, \\ y_h|_T \cdot n & \text{if } S \in \mathcal{S}_h^{\partial\Omega}, \text{ where } T \in \mathcal{T}_h \text{ satisfies } S \subseteq \partial T, \end{cases}$$

where, for every $T \in \mathcal{T}_h$, we denote by $n_T \colon \partial T \to \mathbb{S}^{d-1}$ the outward unit normal vector field to T.

2.2.1 *Crouzeix–Raviart element*

The *Crouzeix–Raviart finite element space* (*cf.* [19]) is defined as the space of element-wise affine functions that are continuous in the barycenters of interior sides, *i.e.*,

$$\mathcal{S}^{1,cr}(\mathcal{T}_h) \coloneqq \left\{ v_h \in \mathcal{L}^1(\mathcal{T}_h) \mid \pi_h[\![v_h]\!] = 0 \text{ a.e. on } \cup\mathcal{S}_h^i \right\}.$$

The Crouzeix–Raviart finite element space with homogeneous Dirichlet boundary condition on Γ_D is defined by

$$\mathcal{S}^{1,cr}_D(\mathcal{T}_h) \coloneqq \big\{ v_h \in \mathcal{S}^{1,cr}(\mathcal{T}_h) \mid \pi_h v_h = 0 \text{ a.e. on } \cup \mathcal{S}_h^{\Gamma_D} \big\} \,.$$

A basis of $\mathcal{S}^{1,cr}(\mathcal{T}_h)$ is given via $\varphi_S \in \mathcal{S}^{1,cr}(\mathcal{T}_h)$, $S\in\mathcal{S}_h$, satisfying $\varphi_S(x_{S'}) = \delta_{S,S'}$ for all $S,S'\in\mathcal{S}_h$. The *(Fortin) quasi-interpolation operator* $\Pi_h^{cr}\colon H^1(\Omega)\to\mathcal{S}^{1,cr}(\mathcal{T}_h)$ (*cf.* [25, Secs. 36.2.1, 36.2.2]), for every $v\in H^1(\Omega)$ defined by

$$\Pi_h^{cr} v \coloneqq \sum_{S\in\mathcal{S}_h} \langle v\rangle_S \, \varphi_S \,, \tag{2.3}$$

preserves averages of gradients and of moments (on sides), *i.e.*, for every $v\in H^1(\Omega)$, it holds that

$$\nabla_h \Pi_h^{cr} v = \Pi_h \nabla v \quad \text{ a.e. in } \Omega \,, \tag{2.4}$$

$$\pi_h \Pi_h^{cr} v = \pi_h v \quad \text{ a.e. on } \cup\mathcal{S}_h \,. \tag{2.5}$$

Here, $\nabla_h\colon \mathcal{L}^1(\mathcal{T}_h)\to(\mathcal{L}^0(\mathcal{T}_h))^d$, defined by $(\nabla_h v_h)|_T \coloneqq \nabla(v_h|_T)$ for all $v_h\in\mathcal{L}^1(\mathcal{T}_h)$ and $T\in\mathcal{T}_h$, denotes the element-wise gradient operator.

For every $s\in[0,1]$, there exists a constant $c>0$ (*cf.* [25, Lem. 36.1]), independent of $h>0$, such that for every $v\in H^{1+s}(\Omega)$ and $T\in\mathcal{T}_h$, it holds that

$$\|v-\Pi_h^{cr}v\|_T + h_T\,\|\nabla v - \nabla\Pi_h^{cr} v\|_T \le c\, h_T^{1+s}\,|v|_{1+s,T} \,. \tag{2.6}$$

2.2.2 Raviart–Thomas element

The *(lowest order) Raviart–Thomas finite element space* (*cf.* [38]) is defined as the space of element-wise affine vector fields that have continuous constant normal components on interior sides, *i.e.*,

$$\mathcal{R}T^0(\mathcal{T}_h) \coloneqq \left\{ y_h \in (\mathcal{L}^1(\mathcal{T}_h))^d \;\middle|\; \begin{aligned} & y_h|_T\cdot n_T = \text{const on } \partial T \text{ for all } T\in\mathcal{T}_h\,, \\ & [\![y_h\cdot n]\!]_S = 0 \text{ on } S \text{ for all } S\in\mathcal{S}_h^i \end{aligned} \right\} .$$

The Raviart–Thomas finite element space with homogeneous normal boundary condition on Γ_N is defined by

$$\mathcal{R}T^0_N(\mathcal{T}_h) \coloneqq \big\{ y_h\in\mathcal{R}T^0(\mathcal{T}_h) \mid y_h\cdot n = 0 \text{ a.e. on } \Gamma_N \big\} \,.$$

A basis of $\mathcal{R}T^0(\mathcal{T}_h)$ is given via vector fields $\psi_S\in\mathcal{R}T^0(\mathcal{T}_h)$, $S\in\mathcal{S}_h$, satisfying $\psi_S|_{S'}\cdot n_{S'} = \delta_{S,S'}$ on S' for all $S'\in\mathcal{S}_h$, where $n_S\in\mathbb{S}^{d-1}$ for all $S\in\mathcal{S}_h$ is the fixed unit normal vector on S pointing from T_- to T_+ if $T_+\cap T_- = S\in\mathcal{S}_h$. For every $s>\frac{1}{2}$, the *(Fortin) quasi-interpolation operator* $\Pi_h^{rt}\colon (H^s(\Omega))^d\to\mathcal{R}T^0(\mathcal{T}_h)$ (*cf.* [24, Sec. 16.1]), for every $y\in(H^s(\Omega))^d$ defined by

$$\Pi_h^{rt} y \coloneqq \sum_{S\in\mathcal{S}_h} \langle y\cdot n_S\rangle_S\,\psi_S \,, \tag{2.7}$$

preserves averages of divergences and of normal traces, *i.e.*, for every $y\in(H^s(\Omega))^d\cap H(\operatorname{div};\Omega)$, it holds that

$$\operatorname{div}\Pi_h^{rt} y = \Pi_h \operatorname{div} y \quad \text{ a.e. in } \Omega \,, \tag{2.8}$$

$$\Pi_h^{rt} y\cdot n = \pi_h y\cdot n \quad \text{ a.e on } \cup\mathcal{S}_h \,. \tag{2.9}$$

For every $s\in(\frac{1}{2},1]$, there exists a constant $c>0$ (*cf.* [24, Thms. 16.4, 16.6]), independent of $h>0$, such that for every $y\in(H^s(\Omega))^d\cap H(\operatorname{div};\Omega)$ and $T\in\mathcal{T}_h$, it holds that

$$\|y-\Pi_h^{rt}y\|_T \le c\,h_T^s\,|y|_{s,T} \,. \tag{2.10}$$

For every $v_h\in\mathcal{S}^{1,cr}(\mathcal{T}_h)$ and $y_h\in\mathcal{R}T^0(\mathcal{T}_h)$, we have the *discrete integration-by-parts formula*

$$(\nabla_h v_h, \Pi_h y_h)_\Omega + (\Pi_h v_h,\, \operatorname{div} y_h)_\Omega = (\pi_h v_h, y_h\cdot n)_{\partial\Omega} \,. \tag{2.11}$$

3. Scalar Signorini problem

In this section, we discuss the (continuous) scalar Signorini problem.

• *Primal problem.* Given $f \in L^2(\Omega)$, $g \in H^{-\frac{1}{2}}(\Gamma_N)$, $u_D \in H^{\frac{1}{2}}(\Gamma_D)$, and $\chi \in H^1(\Omega)$ with $\chi = u_D$ a.e. on Γ_D, the *scalar Signorini problem* is given via the minimization of $I\colon H^1(\Omega) \to \mathbb{R} \cup \{+\infty\}$, for every $v \in H^1(\Omega)$ defined by

$$\begin{aligned} I(v) &\coloneqq \tfrac{1}{2}\|\nabla v\|_\Omega^2 - (f,v)_\Omega - \langle g, v\rangle_{\Gamma_N} + I_K(v) \\ &= \tfrac{1}{2}\|\nabla v\|_\Omega^2 - (f,v)_\Omega - \langle g, v\rangle_{\Gamma_N} + I_{\{u_D\}}^{\Gamma_D}(v) + I_+^{\Gamma_C}(v-\chi)\,, \end{aligned} \tag{3.1}$$

where

$$K \coloneqq \big\{ v \in H^1(\Omega) \mid v = u_D \text{ a.e. on } \Gamma_D\,,\ v \geq \chi \text{ a.e. on } \Gamma_C \big\}\,,$$

and $I_K \coloneqq I_{\{u_D\}}^{\Gamma_D} + I_+^{\Gamma_C}((\cdot)-\chi)$, $I_{\{u_D\}}^{\Gamma_D}, I_+^{\Gamma_C}\colon H^1(\Omega) \to \mathbb{R}\cup\{+\infty\}$, for every $\widehat{v} \in H^1(\Omega)$ are defined by

$$I_{\{u_D\}}^{\Gamma_D}(\widehat{v}) \coloneqq \begin{cases} 0 & \text{if } \widehat{v} = u_D \text{ a.e. on } \Gamma_D\,, \\ +\infty & \text{else}\,, \end{cases}$$

$$I_+^{\Gamma_C}(\widehat{v}) \coloneqq \begin{cases} 0 & \text{if } \widehat{v} \geq 0 \text{ a.e. on } \Gamma_C\,, \\ +\infty & \text{else}\,. \end{cases}$$

Throughout the article, we refer to the minimization of the functional (3.1) as the *primal problem.* Since the functional (3.1) is proper, strictly convex, weakly coercive, and lower semi-continuous, the direct method in the calculus of variations yields the existence of a unique minimizer $u \in K$, called *primal solution.* In what follows, we reserve the notation $u \in K$ for the primal solution.

• *Primal variational inequality.* The primal solution $u \in K$ equivalently is the unique solution of the following variational inequality: for every $v \in K$, it holds that

$$(\nabla u, \nabla u - \nabla v)_\Omega \leq (f, u-v)_\Omega + \langle g, u-v\rangle_{\Gamma_N}\,. \tag{3.2}$$

• *Dual problem.* A *(Fenchel) dual problem* to the scalar Signorini problem is given via the maximization of $D\colon H(\operatorname{div};\Omega) \to \mathbb{R} \cup \{-\infty\}$, for every $y \in H(\operatorname{div};\Omega)$ defined by

$$\begin{aligned} D(y) &\coloneqq -\tfrac{1}{2}\|y\|_\Omega^2 + \langle y\cdot n, \chi\rangle_{\partial\Omega} - \langle g,\chi\rangle_{\Gamma_N} - I_{K^*}(y) \\ &= -\tfrac{1}{2}\|y\|_\Omega^2 + \langle y\cdot n, \chi\rangle_{\partial\Omega} - \langle g,\chi\rangle_{\Gamma_N} - I_{\{-f\}}^{\Omega}(\operatorname{div} y) - I_{\{g\}}^{\Gamma_N}(y\cdot n) - I_+^{\Gamma_C}(y\cdot n)\,, \end{aligned} \tag{3.3}$$

where

$$K^* \coloneqq \big\{ y \in H(\operatorname{div};\Omega) \mid I_{\{-f\}}^{\Omega}(\operatorname{div} y) = I_{\{g\}}^{\Gamma_N}(y\cdot n) = I_+^{\Gamma_C}(y\cdot n) = 0 \big\}\,,$$

$I_{K^*} \coloneqq I_{\{-f\}}^{\Omega}(\operatorname{div}\cdot) + (I_{\{g\}}^{\Gamma_N} + I_+^{\Gamma_C})((\cdot)\cdot n)\colon H(\operatorname{div};\Omega) \to \mathbb{R}\cup\{+\infty\}$, $I_{\{-f\}}^{\Omega}\colon L^2(\Omega) \to \mathbb{R}\cup\{+\infty\}$, for every $\widehat{y} \in L^2(\Omega)$ is defined by

$$I_{\{-f\}}^{\Omega}(\widehat{y}) \coloneqq \begin{cases} 0 & \text{if } \widehat{y} = -f \text{ a.e. in } \Omega\,, \\ +\infty & \text{else}\,, \end{cases}$$

and $I_{\{g\}}^{\Gamma_N}, I_+^{\Gamma_C}\colon H^{-\frac{1}{2}}(\partial\Omega) \to \mathbb{R}\cup\{+\infty\}$, for every $\widehat{y} \in H^{-\frac{1}{2}}(\partial\Omega)$, are defined by

$$I_{\{g\}}^{\Gamma_N}(\widehat{y}) \coloneqq \begin{cases} 0 & \text{if } \langle \widehat{y}, v\rangle_{\partial\Omega} = \langle g, v\rangle_{\Gamma_N} \text{ for all } v \in H_D^1(\Omega) \text{ with } v = 0 \text{ a.e. on } \Gamma_C\,, \\ +\infty & \text{else}\,, \end{cases}$$

$$I_+^{\Gamma_C}(\widehat{y}) \coloneqq \begin{cases} 0 & \text{if } \langle \widehat{y}, v\rangle_{\Gamma_C} \geq 0 \text{ for all } v \in H_D^1(\Omega) \\ & \text{with } v = 0 \text{ a.e. on } \Gamma_N \text{ and } v \geq 0 \text{ a.e. on } \Gamma_C\,, \\ +\infty & \text{else}\,. \end{cases}$$

The identification of the (Fenchel) dual problem (in the sense of [23, Rem. 4.2, p. 60/61]) to the minimization of (3.1) with the maximization of (3.3) can be found in the proof of the following result that also establishes the validity of a strong duality relation and convex optimality relations.

Proposition 3.1 (strong duality and convex duality relations)**.** *The following statements apply:*

(i) A (Fenchel) dual problem to the scalar Signorini problem is given via the maximization of (3.3)*.*

(ii) There exists a unique maximizer $z \in H(\mathrm{div};\Omega)$ of (3.3) *satisfying the* admissibility conditions

$$\operatorname{div} z = -f \qquad \text{a.e. in } \Omega\,, \tag{3.4}$$

$$I_{\{g\}}^{\Gamma_N}(z\cdot n) = 0\,, \tag{3.5}$$

$$I_{+}^{\Gamma_C}(z\cdot n) = 0\,. \tag{3.6}$$

In addition, there holds a strong duality relation*, i.e., it holds that*

$$I(u) = D(z)\,. \tag{3.7}$$

(iii) There hold convex optimality relations*, i.e., it holds that*

$$z = \nabla u \qquad \text{a.e. in } \Omega\,, \tag{3.8}$$

$$\langle z\cdot n, u-\chi\rangle_{\partial\Omega} = \langle g, u-\chi\rangle_{\Gamma_N}\,. \tag{3.9}$$

Remark 3.2. *(i) If $g \in L^1(\Gamma_N)$, then* (3.5) *is equivalent to $z\cdot n = g$ a.e. on Γ_N;*
(ii) If $z\cdot n|_{\Gamma_C} \in L^1(\Gamma_C)$, then (3.6) *is equivalent to $z \cdot n \geq 0$ a.e. on Γ_C.*

Proof (of Proposition 3.1). ad (i). First, if we introduce the proper, lower semi-continuous, and convex functionals $G\colon (L^2(\Omega))^d \to \mathbb{R}$ and $F\colon H^1(\Omega) \to \mathbb{R}\cup\{+\infty\}$, for every $y \in (L^2(\Omega))^d$ and $v \in H^1(\Omega)$, defined by

$$\begin{aligned} G(y) &\coloneqq \tfrac{1}{2}\|y\|_\Omega^2\,,\\ F(v) &\coloneqq -(f,v)_\Omega - \langle g, v\rangle_{\Gamma_N} + I_{\{u_D\}}^{\Gamma_D}(v) + I_{+}^{\Gamma_C}(v-\chi)\,, \end{aligned}$$

then, for every $v \in H^1(\Omega)$, we have that

$$I(v) = G(\nabla v) + F(v)\,.$$

Thus, in accordance with [23, Rem. 4.2, p. 60/61], the (Fenchel) dual problem to the minimization of (3.1) is given via the maximization of $D\colon (L^2(\Omega))^d \to \mathbb{R}\cup\{-\infty\}$, for every $y \in (L^2(\Omega))^d$ defined by

$$D(y) \coloneqq -G^*(y) - F^*(-\nabla^* y)\,, \tag{3.10}$$

where $\nabla^*\colon (L^2(\Omega))^d \to (H^1(\Omega))^*$ is the adjoint operator to the gradient operator $\nabla\colon H^1(\Omega)\to(L^2(\Omega))^d$. Due to [23, Prop. 4.2, p. 19], for every $y \in (L^2(\Omega))^d$, we have that

$$G^*(y) = \tfrac{1}{2}\|y\|_\Omega^2\,. \tag{3.11}$$

Since $v+\chi \in H^1(\Omega)$ with $v+\chi = u_D$ a.e. on Γ_D for all $v \in H^1_D(\Omega)$, for every $y \in (L^2(\Omega))^d$, using the integration-by-parts formula (2.1), we find that

$$\begin{aligned} F^*(-\nabla^* y) &= \sup_{v\in H^1(\Omega)} \big\{ -(y,\nabla v)_\Omega + (f,v)_\Omega + \langle g,v\rangle_{\Gamma_N} - I_{\{u_D\}}^{\Gamma_D}(v) - I_{+}^{\Gamma_C}(v-\chi)\big\}\\ &= \sup_{v\in H^1_D(\Omega)} \big\{ -(y,\nabla v)_\Omega + (f,v)_\Omega + \langle g,v\rangle_{\Gamma_N} - I_{+}^{\Gamma_C}(v)\big\}\\ &\quad - (y,\nabla\chi)_\Omega + (f,\chi)_\Omega + \langle g,\chi\rangle_{\Gamma_N}\\ &= \begin{cases} \left.\begin{aligned} &I_{\{-f\}}^{\Omega}(\operatorname{div} y) + I_{\{g\}}^{\Gamma_N}(y\cdot n) + I_{+}^{\Gamma_C}(y\cdot n)\\ &\qquad -(y,\nabla\chi)_\Omega + (f,\chi)_\Omega + \langle g,\chi\rangle_{\Gamma_N}\end{aligned}\right\} & \text{if } y \in H(\mathrm{div};\Omega)\,,\\ +\infty & \text{else}\,.\end{cases}\\ &= \begin{cases} \left.\begin{aligned} &I_{\{-f\}}^{\Omega}(\operatorname{div} y) + I_{\{g\}}^{\Gamma_N}(y\cdot n) + I_{+}^{\Gamma_C}(y\cdot n)\\ &\qquad -\langle y\cdot n,\chi\rangle_{\partial\Omega} + \langle g,\chi\rangle_{\Gamma_N}\end{aligned}\right\} & \text{if } y \in H(\mathrm{div};\Omega)\,,\\ +\infty & \text{else}\,.\end{cases} \end{aligned} \tag{3.12}$$

Using (3.11) and (3.12) in (3.10), for every $y \in H(\mathrm{div};\Omega)$, we arrive at the representation (3.3). Eventually, since $D = -\infty$ in $(L^2(\Omega))^d \setminus H(\mathrm{div};\Omega)$, it is enough to restrict (3.10) to $H(\mathrm{div};\Omega)$.

ad (ii). Since both $G\colon (L^2(\Omega))^d \to \mathbb{R}$ and $F\colon H^1(\Omega) \to \mathbb{R} \cup \{+\infty\}$ are proper, convex, and lower semi-continuous and since $G\colon (L^2(\Omega))^d \to \mathbb{R}$ is continuous at $\chi \in \operatorname{dom}(F) \cap \operatorname{dom}(G \circ \nabla)$, *i.e.*,

$$G(y) \to G(\nabla\chi) \quad \big(y \to \nabla\chi \quad \text{in } (L^2(\Omega))^d\big)\,,$$

by the celebrated Fenchel duality theorem (*cf.* [23, Rem. 4.2, (4.21), p. 61]), there exists a maximizer $z \in (L^2(\Omega))^d$ of (3.10) and a strong duality relation applies, *i.e.*,

$$I(u) = D(z)\,. \tag{3.13}$$

Since $D = -\infty$ in $(L^2(\Omega))^d \setminus H(\operatorname{div};\Omega)$, from (3.13), we infer that $z \in H(\operatorname{div};\Omega)$. Moreover, since (3.3) is strictly concave, the maximizer $z \in H(\operatorname{div};\Omega)$ is uniquely determined.

ad (iii). By the standard (Fenchel) convex duality theory (*cf.* [23, Rem. 4.2, (4.24), (4.25), p. 61]), there hold the convex optimality relations

$$-\nabla^* z \in \partial F(u)\,, \tag{3.14}$$

$$z \in \partial G(\nabla u)\,. \tag{3.15}$$

While the inclusion (3.15) is equivalent to the convex optimality relation (3.8), the inclusion (3.14), by the standard equality condition in the Fenchel–Young inequality (*cf.* [23, Prop. 5.1, p. 21]) and the admissibility condition (3.4), is equivalent to

$$\begin{aligned}
-(z, \nabla u)_\Omega &= (-\nabla^* z, u)_\Omega \\
&= F^*(-\nabla^* z) + F(u) \\
&= -\langle z \cdot n, \chi\rangle_{\partial\Omega} + \langle g, \chi\rangle_{\Gamma_N} - (f, u)_\Omega - \langle g, u\rangle_{\Gamma_N} \\
&= -\langle z \cdot n, \chi\rangle_{\partial\Omega} - \langle g, u - \chi\rangle_{\Gamma_N} + (\operatorname{div} z, u)_\Omega \\
&= \langle z \cdot n, u - \chi\rangle_{\partial\Omega} - \langle g, u - \chi\rangle_{\Gamma_N} + (\operatorname{div} z, u)_\Omega - \langle z \cdot n, u\rangle_{\partial\Omega}\,,
\end{aligned}$$

which, by the integration-by-parts formula (2.1), is equivalent to the claimed convex optimality relation (3.9). □

• *Dual variational inequality.* A dual solution $z \in K^*$ equivalently is the unique solution of the following variational inequality: for every $y \in K^*$, it holds that

$$(z, z - y)_\Omega \le \langle z \cdot n - y \cdot n, \chi\rangle_{\partial\Omega}\,. \tag{3.16}$$

• *Augmented problem.* There exists a Lagrange multiplier $\Lambda^* \in (H^1_D(\Omega))^*$ such that for every $v \in H^1_D(\Omega)$, there holds the *augmented problem*

$$(\nabla u, \nabla v)_\Omega + \langle \Lambda^*, v\rangle_{H^1_D(\Omega)} = (f, v)_\Omega + \langle g, v\rangle_{\Gamma_N}\,. \tag{3.17}$$

With the convex optimality relations (3.8),(3.9) and the integration-by-parts formula (2.1), for every $v \in H^1_D(\Omega)$, we find that

$$\langle \Lambda^*, v\rangle_{H^1_D(\Omega)} = \langle z \cdot n, v\rangle_{\partial\Omega} - \langle g, v\rangle_{\Gamma_N}\,.$$

In particular, the convex optimality relation (3.9) then also reads as the *complementarity condition*

$$\langle \Lambda^*, u - \chi\rangle_{H^1_D(\Omega)} = 0\,.$$

Remark 3.3 (regularity in 2D)**.** *In the two-dimensional case, the following regularity results apply:*

(i) If $\Omega \subseteq \mathbb{R}^2$ is a bounded domain with smooth boundary, $\Gamma_C = \partial\Omega$, and $\chi \in H^{\frac{3}{2}}(\partial\Omega)$, then $u \in H^2(\Omega)$ (cf. [42, Lem. 2.2]).

(ii) If $\Omega \subseteq \mathbb{R}^2$ is a polygonal, convex, and bounded domain, $\Gamma_C = \partial\Omega$, and $\chi \in H^{\frac{3}{2}}(\partial\Omega)$, then $u \in H^2(\Omega)$ (cf. [27, Thm. 4.1]).

(iii) If $\Omega \subseteq \mathbb{R}^2$ is a polygonal bounded domain, $\Gamma_C \neq \partial\Omega$, and $\chi \in H^{\frac{3}{2}}(\partial\Omega)$, then $u \in H^2(U) \cap C^{1,\lambda}(U)$ for $\lambda \in (1, \frac{1}{2})$ (cf. [37] or [1, Thm. 2.1]), where $U \subseteq \mathbb{R}^2$ is a neighborhood of the critical points, i.e., the points where the boundary condition changes and that are corners of the domain. In addition, in [1, Thm. 3.1], a description of possible singular behavior close to the critical points can be found.

4. *A posteriori* error analysis

In this section, resorting to convex duality arguments, we derive an *a posteriori* error identity for arbitrary conforming approximations of the primal problem (3.1) and the dual problem (3.3) at the same time. To this end, we introduce the *primal-dual gap estimator* $\eta^2_{\mathrm{gap}} \colon K \times K^* \to \mathbb{R}$, for every $v \in K$ and $y \in K^*$ defined by

$$\eta^2(v,y) \coloneqq I(v) - D(y)\,. \tag{4.1}$$

The primal-dual gap estimator (4.1) can be decomposed into two contributions that precisely measure the violation of the convex optimality relations (3.8),(3.9), respectively.

Lemma 4.1. *For every $v \in K$ and $y \in K^*$, we have that*

$$\begin{aligned} \eta^2_{\mathrm{gap}}(v,y) &\coloneqq \eta^2_A(v,y) + \eta^2_B(v,y)\,,\\ \eta^2_{\mathrm{gap},A}(v,y) &\coloneqq \tfrac{1}{2}\|\nabla v - y\|^2_\Omega\,,\\ \eta^2_{\mathrm{gap},B}(v,y) &\coloneqq \langle y\cdot n, v-\chi\rangle_{\partial\Omega} - \langle g, v-\chi\rangle_{\Gamma_N}\,. \end{aligned}$$

Remark 4.2 (interpretation of the components of the primal-dual gap estimator)**.**

(i) The estimator $\eta^2_{\mathrm{gap},A}$ measures the violation of the convex optimality relation (3.8);

(ii) The estimator $\eta^2_{\mathrm{gap},B}$ measures the violation of the convex optimality relation (3.9).

Proof (of Lemma 4.1). Using the admissibility conditions (3.4)–(3.6), the integration-by-parts formula (2.1), and the binomial formula, for every $v \in K$ and $y \in K^*$, we find that

$$\begin{aligned} I(v) - D(y) &= \tfrac{1}{2}\|\nabla v\|^2_\Omega - (f,v)_\Omega - \langle g, v\rangle_{\Gamma_N} + \tfrac{1}{2}\|y\|^2_\Omega - \langle y\cdot n, \chi\rangle_{\partial\Omega} + \langle g,\chi\rangle_{\Gamma_N}\\ &= \tfrac{1}{2}\|\nabla v\|^2_\Omega + (\operatorname{div} y, v)_\Omega + \tfrac{1}{2}\|y\|^2_\Omega - \langle y\cdot n,\chi\rangle_{\partial\Omega} - \langle g, v-\chi\rangle_{\Gamma_N}\\ &= \tfrac{1}{2}\|\nabla v\|^2_\Omega - (y,\nabla v)_\Omega + \tfrac{1}{2}\|y\|^2_\Omega + \langle y\cdot n, v-\chi\rangle_{\partial\Omega} - \langle g, v-\chi\rangle_{\Gamma_N}\\ &= \tfrac{1}{2}\|\nabla v - y\|^2_\Omega + \langle y\cdot n, v-\chi\rangle_{\partial\Omega} - \langle g, v-\chi\rangle_{\Gamma_N}\,. \end{aligned}$$ □

Next, we identify the *optimal strong convexity measures* for the primal energy functional (3.1) at the primal solution $u \in K$, *i.e.*, $\rho^2_I \colon K \to [0,+\infty)$, for every $v \in K$ defined by

$$\rho^2_I(v) \coloneqq I(v) - I(u)\,, \tag{4.2}$$

and for the negative of the dual energy functional (3.3), *i.e.*, $\rho^2_{-D}\colon K^* \to [0,+\infty)$, for every $y \in K^*$ defined by

$$\rho^2_{-D}(y) \coloneqq -D(y) + D(z)\,, \tag{4.3}$$

which will serve as *'natural'* error quantities in the primal-dual gap identity (*cf.* Theorem 4.5).

Lemma 4.3 (optimal strong convexity measures)**.** *The following statements apply:*

(i) For every $v \in K$, we have that

$$\rho^2_I(v) = \tfrac{1}{2}\|\nabla v - \nabla u\|^2_\Omega + \langle z\cdot n, v-\chi\rangle_{\partial\Omega} - \langle g, v-\chi\rangle_{\Gamma_N}\,.$$

(ii) For every $y \in K^*$, we have that

$$\rho^2_{-D}(z) = \tfrac{1}{2}\|y - z\|^2_\Omega + \langle y\cdot n, u-\chi\rangle_{\partial\Omega} - \langle g, u-\chi\rangle_{\Gamma_N}\,.$$

Remark 4.4.

(i) By the convex optimality relation (3.9), the integration-by-parts formula (2.1), the convex optimality relation (3.8), the admissibility condition (3.4), and the primal variational inequality (3.2), for every $v \in K$, we have that

$$\begin{aligned} \langle z\cdot n, v-\chi\rangle_{\partial\Omega} - \langle g, v-\chi\rangle_{\Gamma_N} &= \langle z\cdot n, v-u\rangle_{\partial\Omega} - \langle g, v-u\rangle_{\Gamma_N}\\ &= (z, \nabla v - \nabla u)_\Omega + (\operatorname{div} z, v-u)_\Omega - \langle g, v-u\rangle_{\Gamma_N}\\ &= (\nabla u, \nabla v - \nabla u)_\Omega - (f, v-u)_\Omega - \langle g, v-u\rangle_{\Gamma_N}\\ &\geq 0\,. \end{aligned}$$

(ii) By the convex optimality relation (3.9)*, the integration-by-parts formula* (2.1)*, the convex optimality relation* (3.8)*, the admissibility condition* (3.4)*, and the dual variational inequality* (3.16)*, for every $y \in K^*$, we have that*

$$\begin{aligned}\langle y\cdot n, u-\chi\rangle_{\partial\Omega} - \langle g, u-\chi\rangle_{\Gamma_N} &= \langle y\cdot n - z\cdot n, u\rangle_{\partial\Omega} - \langle y\cdot n - z\cdot n, \chi\rangle_{\partial\Omega}\\ &= (y-z,\nabla u)_\Omega + (\operatorname{div} y - \operatorname{div} z, u)_\Omega - \langle y\cdot n - z\cdot n,\chi\rangle_{\partial\Omega}\\ &= (y-z,z)_\Omega - \langle y\cdot n - z\cdot n,\chi\rangle_{\partial\Omega}\\ &\geq 0\,.\end{aligned}$$

Proof (of Lemma 4.3). ad (i). Using the binomial formula, the convex optimality relation (3.8), the admissibility condition (3.4), the integration-by-parts formula (2.1), and the convex optimality relation (3.9), for every $v \in K$, we find that

$$\begin{aligned}I(v) - I(u) &= \tfrac{1}{2}\|\nabla v\|_\Omega^2 - \tfrac{1}{2}\|\nabla u\|_\Omega^2 - (f, v-u)_\Omega - \langle g, v-u\rangle_{\Gamma_N}\\ &= \tfrac{1}{2}\|\nabla v - \nabla u\|_\Omega^2 + (\nabla u, \nabla v - \nabla u)_\Omega - (f, v-u)_\Omega - \langle g, v-u\rangle_{\Gamma_N}\\ &= \tfrac{1}{2}\|\nabla v - \nabla u\|_\Omega^2 + (z, \nabla v - \nabla u)_\Omega + (\operatorname{div} z, v-u)_\Omega - \langle g, v-u\rangle_{\Gamma_N}\\ &= \tfrac{1}{2}\|\nabla v - \nabla u\|_\Omega^2 + \langle z\cdot n, v-u\rangle_{\partial\Omega} - \langle g, v-u\rangle_{\Gamma_N}\\ &= \tfrac{1}{2}\|\nabla v - \nabla u\|_\Omega^2 + \langle z\cdot n, v-\chi\rangle_{\partial\Omega} - \langle g, v-\chi\rangle_{\Gamma_N}\,.\end{aligned}$$

ad (ii). Using the binomial formula, the admissibility conditions (3.4)–(3.6), the convex optimality relation (3.8), the integration-by-parts formula (2.1), again, the admissibility condition (3.4), and the convex optimality relation (3.9), for every $y \in K^*$, we find that

$$\begin{aligned}-D(y) + D(z) &= \tfrac{1}{2}\|y\|_\Omega^2 - \tfrac{1}{2}\|z\|_\Omega^2 + \langle z\cdot n - y\cdot n, \chi\rangle_{\partial\Omega}\\ &= \tfrac{1}{2}\|y-z\|_\Omega^2 + (z, y-z)_\Omega + \langle z\cdot n - y\cdot n, \chi\rangle_{\partial\Omega}\\ &= \tfrac{1}{2}\|y-z\|_\Omega^2 + (\nabla u, y-z)_\Omega + \langle z\cdot n - y\cdot n, \chi\rangle_{\partial\Omega}\\ &= \tfrac{1}{2}\|y-z\|_\Omega^2 + (\operatorname{div} z - \operatorname{div} y, u)_\Omega + \langle z\cdot n - y\cdot n, \chi - u\rangle_{\partial\Omega}\\ &= \tfrac{1}{2}\|y-z\|_\Omega^2 + \langle y\cdot n, u-\chi\rangle_{\partial\Omega} - \langle g, u-\chi\rangle_{\Gamma_N}\,.\end{aligned}$$ ☐

Eventually, we have everything at our disposal to establish an *a posteriori* error identity that identifies the *primal-dual total error* $\rho_{\mathrm{tot}}^2 \colon K \times K^* \to [0,+\infty)$, for every $v \in K$ and $y \in K^*$ defined by

$$\rho_{\mathrm{tot}}^2(v,y) \coloneqq \rho_I^2(v) + \rho_{-D}^2(y)\,, \tag{4.4}$$

with the primal-dual gap estimator $\eta_{\mathrm{gap}}^2 \colon K \times K^* \to [0,+\infty)$ (*cf.* (4.1)).

Theorem 4.5 (primal-dual gap identity)**.** *For every $v \in K$ and $y \in K^*$, we have that*

$$\rho_{\mathrm{tot}}^2(v,y) = \eta_{\mathrm{gap}}^2(v,y)\,.$$

Proof. Combining the definitions (4.1), (4.2), (4.3), (4.4), and the strong duality relation (3.7), for every $v \in K$ and $y \in K^*$, we find that

$$\begin{aligned}\rho_{\mathrm{tot}}^2(v,y) &= \rho_I^2(v) + \rho_{-D}^2(y)\\ &= I(v) - I(u) + D(z) - D(y)\\ &= I(v) - D(y)\\ &= \eta_{\mathrm{gap}}^2(v,y)\,.\end{aligned}$$ ☐

Note that the primal-dual gap identity (*cf.* Theorem 4.5) applies to arbitrary conforming approximations of the primal problem (3.1) and the dual problem (3.3). To be numerically practicable it is necessary to have a computationally inexpensive way to approximate the primal and the dual problem at the same time. In Section 5, exploiting orthogonality relations between the Crouzeix–Raviart and the Raviart–Thomas element, we transfer all convex duality relations from Section 3 to a discrete level to arrive at a discrete reconstruction formula that allows us to approximate the primal and the dual problem at the same time using only the Crouzeix–Raviart element.

5. DISCRETE SCALAR SIGNORINI PROBLEM

In this section, we discuss the discrete scalar Signorini problem.

• *Discrete primal problem.* Let $f_h \in \mathcal{L}^0(\mathcal{T}_h)$, $g_h \in \mathcal{L}^0(\mathcal{S}_h^{\Gamma_N})$, $u_D^h \in \mathcal{L}^0(\mathcal{S}_h^{\Gamma_D})$, and $\chi_h \in \mathcal{L}^0(\mathcal{S}_h^{\Gamma_D} \cup \mathcal{S}_h^{\Gamma_C})$ with $\chi_h = u_D^h$ a.e. in Γ_D. Then, the *discrete scalar Signorini problem* is given via the minimization of $I_h^{cr}\colon \mathcal{S}^{1,cr}(\mathcal{T}_h) \to \mathbb{R} \cup \{+\infty\}$, for every $v_h \in \mathcal{S}^{1,cr}(\mathcal{T}_h)$ defined by

$$\begin{aligned} I_h^{cr}(v_h) &\coloneqq \tfrac{1}{2}\|\nabla_h v_h\|_\Omega^2 - (f_h, \Pi_h v_h)_\Omega - (g_h, \pi_h v_h)_{\Gamma_N} + I_{K_h^{cr}}(v_h) \\ &= \tfrac{1}{2}\|\nabla_h v_h\|_\Omega^2 - (f_h, \Pi_h v_h)_\Omega - (g_h, \pi_h v_h)_{\Gamma_N} + I_{\{u_D^h\}}^{\Gamma_D}(\pi_h v_h) + I_+^{\Gamma_C}(\pi_h v_h - \chi_h)\,, \end{aligned} \tag{5.1}$$

where

$$K_h^{cr} \coloneqq \big\{ v_h \in \mathcal{S}^{1,cr}(\mathcal{T}_h) \mid \pi_h v_h = u_D^h \text{ a.e. on } \Gamma_D\,,\ \pi_h v_h \geq \chi_h \text{ a.e. on } \Gamma_C \big\}\,,$$

and $I_{K_h^{cr}} \coloneqq I_{\{u_D^h\}}^{\Gamma_D}(\pi_h(\cdot)) + I_h^{\Gamma_C}(\pi_h(\cdot) - \chi_h)\colon \mathcal{S}^{1,cr}(\mathcal{T}_h) \to \mathbb{R} \cup \{+\infty\}$.

In what follows, we refer to the minimization of the functional (5.1) as the *discrete primal problem.* Since the functional (5.1) is proper, strictly convex, weakly coercive, and lower semi-continuous, the direct method in the calculus of variations yields the existence of a unique minimizer $u_h^{cr} \in K_h^{cr}$, called the *discrete primal solution.* We reserve the notation $u_h^{cr} \in K_h^{cr}$ for the discrete primal solution.

• *Discrete primal variational inequality.* The discrete primal solution $u_h^{cr} \in K_h^{cr}$ equivalently is the unique solution of the following variational inequality: for every $v_h \in K_h^{cr}$, it holds that

$$(\nabla_h u_h^{cr}, \nabla_h u_h^{cr} - \nabla_h v_h)_\Omega \leq (f_h, \Pi_h u_h^{cr} - \Pi_h v_h)_\Omega + (g_h, \pi_h u_h^{cr} - \pi_h v_h)_{\Gamma_N}\,. \tag{5.2}$$

• *Discrete dual problem.* The *(Fenchel) dual problem* to the discrete scalar Signorini problem is given via the maximization of $D_h^{rt}\colon \mathcal{RT}^0(\mathcal{T}_h) \to \mathbb{R} \cup \{-\infty\}$, for every $y_h \in \mathcal{RT}^0(\mathcal{T}_h)$ defined by

$$\begin{aligned} D_h^{rt}(y_h) &\coloneqq -\tfrac{1}{2}\|\Pi_h y_h\|_\Omega^2 + (y_h \cdot n, \chi_h)_{\Gamma_D \cup \Gamma_C} - I_{K_h^{rt,*}}(y_h) \\ &= -\tfrac{1}{2}\|\Pi_h y_h\|_\Omega^2 + (y_h \cdot n, \chi_h)_{\Gamma_D \cup \Gamma_C} - I_{\{-f_h\}}^{\Omega}(\operatorname{div} y_h) - I_{\{g_h\}}^{\Gamma_N}(y_h \cdot n) - I_+^{\Gamma_C}(y_h \cdot n)\,, \end{aligned} \tag{5.3}$$

where

$$K_h^{rt,*} \coloneqq \big\{ y_h \in \mathcal{RT}^0(\mathcal{T}_h) \mid \operatorname{div} y_h = -f_h \text{ a.e. in } \Omega\,,\ y_h \cdot n = g_h \text{ a.e. } \Gamma_N\,,\ y_h \cdot n \geq 0 \text{ a.e. on } \Gamma_C \big\}\,,$$

and $I_{K_h^{rt,*}} \coloneqq I_{\{-f_h\}}^{\Omega}(\operatorname{div}(\cdot)) + (I_{\{g_h\}}^{\Gamma_N} + I_+^{\Gamma_C})((\cdot)\cdot n)\colon \mathcal{RT}^0(\mathcal{T}_h) \to \mathbb{R} \cup \{+\infty\}$.

The identification of the (Fenchel) dual problem (in the sense of [23, Rem. 4.2, p. 60/61]) to the minimization of (5.1) with the maximization of (5.3) can be found in the proof of the following result that also establishes the validity of a discrete strong duality relation and discrete convex optimality relations.

Proposition 5.1 (strong duality and convex duality relations)**.** *The following statements apply:*

(i) The (Fenchel) dual problem to the discrete scalar Signorini problem is defined via the maximization of (5.3)*.*

(ii) There exists a unique maximizer $z_h^{rt} \in \mathcal{RT}^0(\mathcal{T}_h)$ of (5.3) *satisfying the* discrete admissibility conditions

$$\operatorname{div} z_h^{rt} = -f_h \qquad \text{a.e. in } \Omega\,, \tag{5.4}$$

$$z_h^{rt} \cdot n = g_h \qquad \text{a.e. on } \Gamma_N\,, \tag{5.5}$$

$$z_h^{rt} \cdot n \geq 0 \qquad \text{a.e. on } \Gamma_C\,, \tag{5.6}$$

In addition, there holds a discrete strong duality relation*, i.e., we have that*

$$I_h^{cr}(u_h^{cr}) = D_h^{rt}(z_h^{rt})\,. \tag{5.7}$$

(iii) There hold the discrete convex optimality relations*, i.e., we have that*

$$\Pi_h z_h^{rt} = \nabla_h u_h^{cr} \qquad \text{a.e. in } \Omega\,, \tag{5.8}$$

$$z_h^{rt} \cdot n\,(\pi_h u_h^{cr} - \chi_h) = 0 \qquad \text{a.e. on } \Gamma_C\,. \tag{5.9}$$

Proof. ad (i). If we introduce the functionals $G_h\colon (\mathcal{L}^0(\mathcal{T}_h))^d \to \mathbb{R}$ and $F_h\colon \mathcal{S}^{1,cr}(\mathcal{T}_h) \to \mathbb{R}\cup\{+\infty\}$, for every $\overline{y}_h \in (\mathcal{L}^0(\mathcal{T}_h))^d$ and $v_h \in \mathcal{S}^{1,cr}(\mathcal{T}_h)$ defined by

$$\begin{aligned} G_h(\overline{y}_h) &\coloneqq \tfrac{1}{2}\|\overline{y}_h\|_\Omega^2\,,\\ F_h(v_h) &\coloneqq -(f_h,\Pi_h v_h)_\Omega - (g_h,\pi_h v_h)_{\Gamma_N} + I_{\{u_D^h\}}^{\Gamma_D}(\pi_h v_h) + I_+^{\Gamma_C}(\pi_h v_h - \chi_h)\,, \end{aligned}$$

then, for every $v_h \in \mathcal{S}^{1,cr}(\mathcal{T}_h)$, we have that

$$I_h^{cr}(v_h) = G_h(\nabla_h v_h) + F_h(v_h)\,.$$

Thus, in accordance with [23, Rem. 4.2, p. 60], the (Fenchel) dual problem to the minimization of (5.1) is given via the maximization of $D_h^0\colon (\mathcal{L}^0(\mathcal{T}_h))^d \to \mathbb{R}\cup\{-\infty\}$, for every $\overline{y}_h \in (\mathcal{L}^0(\mathcal{T}_h))^d$ defined by

$$D_h^0(\overline{y}_h) \coloneqq -G_h^*(\overline{y}_h) - F_h^*(-\nabla_h^*\overline{y}_h)\,, \tag{5.10}$$

where $\nabla_h^*\colon (\mathcal{L}^0(\mathcal{T}_h))^d \to (\mathcal{S}^{1,cr}(\mathcal{T}_h))^*$ denotes the adjoint operator to $\nabla_h\colon \mathcal{S}^{1,cr}(\mathcal{T}_h) \to (\mathcal{L}^0(\mathcal{T}_h))^d$. For every $\overline{y}_h \in (\mathcal{L}^0(\mathcal{T}_h))^d$, we have that

$$G_h^*(\overline{y}_h) = \tfrac{1}{2}\|\overline{y}_h\|_\Omega^2\,. \tag{5.11}$$

For fixed $\widehat{\chi}_h \in \mathcal{S}^{1,cr}(\mathcal{T}_h)$ with $\pi_h\widehat{\chi}_h = \chi_h$ a.e. on $\Gamma_D\cup\Gamma_C$, due to $\chi_h = u_D^h$ a.e. on Γ_D, for every $\overline{y}_h \in (\mathcal{L}^0(\mathcal{T}_h))^d$, using the lifting lemma (*cf.* Lemma A.1) and the discrete integration-by-parts formula (2.11), we find that

$$\begin{aligned} &F_h^*(-\nabla_h^*\overline{y}_h) \qquad\qquad (5.12)\\ &= \sup_{v_h\in\mathcal{S}^{1,cr}(\mathcal{T}_h)}\big\{-(\overline{y}_h,\nabla_h v_h)_\Omega + (f_h,\Pi_h v_h)_\Omega + (g_h,\pi_h v_h)_{\Gamma_N} + I_{\{u_D^h\}}^{\Gamma_D}(\pi_h v_h) + I_+^{\Gamma_C}(\pi_h v_h - \chi_h)\big\}\\ &= \sup_{v_h\in\mathcal{S}_D^{1,cr}(\mathcal{T}_h)}\big\{-(\overline{y}_h,\nabla_h v_h)_\Omega + (f_h,\Pi_h v_h)_\Omega + (g_h,\pi_h v_h)_{\Gamma_N} + I_+^{\Gamma_C}(\pi_h v_h)\big\}\\ &\quad - (\overline{y}_h,\nabla_h\widehat{\chi}_h)_\Omega + (f_h,\Pi_h\widehat{\chi}_h)_\Omega + (g_h,\pi_h\widehat{\chi}_h)_{\Gamma_N}\\ &= \begin{cases} \left.\begin{array}{c} I_{\{-f_h\}}^\Omega(\operatorname{div} y_h) + I_{\{g_h\}}^{\Gamma_N}(y_h\cdot n) + I_+^{\Gamma_C}(y_h\cdot n)\\ -(\Pi_h y_h,\nabla_h\widehat{\chi}_h)_\Omega + (f_h,\Pi_h\widehat{\chi}_h)_\Omega + (g_h,\pi_h\chi_h)_{\Gamma_N}\end{array}\right\} & \text{if } \overline{y}_h = \Pi_h y_h \text{ for some } y_h\in\mathcal{RT}^0(\mathcal{T}_h)\,,\\ +\infty & \text{else}\,,\end{cases}\\ &= \begin{cases} \left.\begin{array}{r} I_{\{-f_h\}}^\Omega(\operatorname{div} y_h) + I_{\{g_h\}}^{\Gamma_N}(y_h\cdot n) + I_+^{\Gamma_C}(y_h\cdot n)\\ -(y_h\cdot n,\chi_h)_{\Gamma_D\cup\Gamma_C}\end{array}\right\} & \text{if } \overline{y}_h = \Pi_h y_h \text{ for some } y_h\in\mathcal{RT}^0(\mathcal{T}_h)\,,\\ +\infty & \text{else}\,.\end{cases} \end{aligned}$$

Using (5.11) and (5.12) in (5.10), for every $\overline{y}_h = \Pi_h y_h \in \Pi_h(\mathcal{RT}^0(\mathcal{T}_h))$, where $y_h \in \mathcal{RT}^0(\mathcal{T}_h)$, we arrive at the representation (5.3). Since $D_h^0 = -\infty$ in $(\mathcal{L}^0(\mathcal{T}_h))^d \setminus \Pi_h(\mathcal{RT}^0(\mathcal{T}_h))$, it is enough to restrict (5.3) to $\Pi_h(\mathcal{RT}^0(\mathcal{T}_h))$. Then, we have that $D_h^0(\Pi_h y_h) = D_h^{rt}(y_h)$ for all $y_h \in \mathcal{RT}^0(\mathcal{T}_h)$.

ad (ii). Since $G_h\colon (\mathcal{L}^0(\mathcal{T}_h))^d \to \mathbb{R}$ and $F_h\colon \mathcal{S}^{1,cr}(\mathcal{T}_h) \to \mathbb{R}\cup\{+\infty\}$ are proper, convex, and lower semi-continuous and since $G_h\colon (\mathcal{L}^0(\mathcal{T}_h))^d \to \mathbb{R}$ is continuous at $\widehat{\chi}_h \in \operatorname{dom}(F_h)\cap\operatorname{dom}(G_h\circ\nabla_h)$, *i.e.*,

$$G_h(\overline{y}_h) \to G_h(\nabla_h\widehat{\chi}_h) \quad \big(\overline{y}_h \to \nabla_h\widehat{\chi}_h \quad \text{in } (\mathcal{L}^0(\mathcal{T}_h))^d\big)\,,$$

by the celebrated Fenchel duality theorem (*cf.* [23, Rem. 4.2, (4.21), p. 61]), there exists a maximizer $z_h^0 \in (\mathcal{L}^0(\mathcal{T}_h))^d$ of (5.10) and a discrete strong duality relation applies, *i.e.*,

$$I_h^{cr}(u_h^{cr}) = D_h^0(z_h^0)\,.$$

Since $D_h^0 = -\infty$ in $(\mathcal{L}^0(\mathcal{T}_h))^d\setminus\Pi_h(\mathcal{RT}^0(\mathcal{T}_h))$, there exists $z_h^{rt} \in \mathcal{RT}^0(\mathcal{T}_h)$ such that $z_h^0 = \Pi_h z_h^{rt}$ a.e. in Ω. In particular, we have that $D_h^0(z_h^0) = D_h^{rt}(z_h^{rt})$, so that $z_h^{rt} \in \mathcal{RT}^0(\mathcal{T}_h)$ is a maximizer of (5.3) and the discrete strong duality relation (5.7) applies. By the strict convexity of $G_h\colon (\mathcal{L}^0(\mathcal{T}_h))^d \to \mathbb{R}$ and the divergence constraint, the maximizer $z_h^{rt} \in \mathcal{RT}^0(\mathcal{T}_h)$ is uniquely determined.

ad (iii). By the standard (Fenchel) convex duality theory (*cf.* [23, Rem. 4.2, (4.24), (4.25), p. 61]), there hold the convex optimality relations

$$-\nabla_h^*\Pi_h z_h^{rt} \in \partial F_h(u_h)\,, \tag{5.13}$$

$$\Pi_h z_h^{rt} \in \partial G_h(\nabla_h u_h^{cr})\,. \tag{5.14}$$

The inclusion (5.14) is equivalent to the discrete convex optimality relation (5.8). The inclusion (5.13), by the standard equality condition in the Fenchel–Young inequality (*cf.* [23, Prop. 5.1, p. 21]), $\pi_h u_h^{cr} = \chi_h$ a.e. on Γ_D, and the discrete admissibility conditions (5.4),(5.5), is equivalent to

$$\begin{aligned}-(\Pi_h z_h^{rt}, \nabla_h u_h^{cr})_\Omega &= (-\nabla_h^* \Pi_h z_h^{rt}, u_h^{cr})_\Omega\\ &= F_h^*(-\nabla_h^*\Pi_h z_h^{rt}) + F_h(u_h^{cr})\\ &= -(z_h^{rt}\cdot n, \chi_h)_{\Gamma_D\cup\Gamma_C} - (f_h, \Pi_h u_h^{cr})_\Omega - (g_h, \pi_h u_h^{cr})_{\Gamma_N}\\ &= (z_h^{rt}\cdot n, \pi_h u_h^{cr} - \chi_h)_{\Gamma_C} + (\operatorname{div} z_h^{rt}, \Pi_h u_h^{cr})_\Omega - (z_h^{rt}\cdot n, \pi_h u_h^{cr})_{\partial\Omega}\,,\end{aligned}$$

which, by the discrete integration-by-parts formula (2.11), is equivalent to $(z_h^{rt}\cdot n, \pi_h u_h^{cr} - \chi_h)_{\Gamma_C} = 0$. Since $z_h^{rt}\cdot n \geq 0$ a.e. on Γ_C and $\pi_h u_h^{cr} - \chi_h \geq 0$ a.e. on Γ_C, we conclude that (5.8) applies. $\square$

- *Discrete dual variational inequality.* A discrete dual solution $z_h^{rt} \in K_h^{rt,*}$ equivalently is the unique solution of the following variational inequality: for every $y_h \in K_h^{rt,*}$, it holds that

$$(\Pi_h z_h^{rt}, \Pi_h z_h^{rt} - \Pi_h y_h)_\Omega \geq (z_h^{rt}\cdot n - y_h\cdot n, \chi_h)_{\Gamma_N}\,. \tag{5.15}$$

- *Discrete augmented problem.* There exists a discrete Lagrange multiplier $\Lambda_h^{cr,*} \in (\mathcal{S}_D^{1,cr}(\mathcal{T}_h))^*$ such that for every $v_h \in \mathcal{S}_D^{1,cr}(\mathcal{T}_h)$, there holds the *discrete augmented problem*

$$\langle \Lambda_h^{cr,*}, v_h\rangle_{\mathcal{S}_D^{1,cr}(\mathcal{T}_h)} = (\nabla_h u_h^{cr}, \nabla_h v_h)_\Omega - (f_h, \Pi_h v_h)_\Omega - (g_h, \pi_h v_h)_{\Gamma_N}\,. \tag{5.16}$$

With the convex optimality relation (5.8) and the discrete integration-by-parts formula (2.11), introducing the discrete Lagrange multiplier $\overline{\lambda}_h^{cr} \coloneqq z_h^{rt}\cdot n|_{\Gamma_C} \in \mathcal{L}^0(\mathcal{S}_h^{\Gamma_C})$, for every $v_h \in \mathcal{S}_D^{1,cr}(\mathcal{T}_h)$, we find that

$$\langle \Lambda_h^{cr,*}, v_h\rangle_{\mathcal{S}_D^{1,cr}(\mathcal{T}_h)} = (\overline{\lambda}_h^{cr}, \pi_h v_h)_{\Gamma_C}\,.$$

We define the *discrete flux*

$$z_h^{rt} \coloneqq \nabla_h u_h^{cr} - \frac{f_h}{d}(\mathrm{id}_{\mathbb{R}^d} - \Pi_h \mathrm{id}_{\mathbb{R}^d}) \in (\mathcal{L}^1(\mathcal{T}_h))^d\,, \tag{5.17}$$

which is admissible in the discrete dual problem and a discrete dual solution.

Proposition 5.2. *The discrete flux $z_h^{rt} \in (\mathcal{L}^1(\mathcal{T}_h))^d$, defined by (5.17), satisfies $z_h^{rt} \in \mathcal{RT}^0(\mathcal{T}_h)$, the discrete admissibility relations (5.4)–(5.6), the discrete convex optimality relations (5.8),(5.9), and is a discrete dual solution.*

Proof. ad $z_h^{rt} \in \mathcal{RT}^0(\mathcal{T}_h)$ with (5.4)–(5.6) and (5.8). Due to (5.16), the lifting lemma (*cf.* Lemma A.1) implies that $z_h^{rt} \in \mathcal{RT}^0(\mathcal{T}_h)$ with (5.4), (5.5), and (5.8). In addition, for every $v_h \in \mathcal{S}_D^{1,cr}(\mathcal{T}_h)$ with $\pi_h v_h \geq 0$ a.e. on Γ_C, the discrete integration-by-parts formula (2.11) and the discrete primal variational inequality (*cf.* (5.2)) yield that

$$\begin{aligned}(z_h^{rt}\cdot n, \pi_h v_h)_{\Gamma_C} &= (\Pi_h z_h^{rt}, \nabla_h v_h)_\Omega + (\operatorname{div} z_h^{rt}, \Pi_h v_h)_\Omega - (z_h^{rt}\cdot n, \pi_h v_h)_{\Gamma_N}\\ &= (\nabla_h u_h^{cr}, \nabla_h v_h)_\Omega - (f_h, \Pi_h v_h)_\Omega - (g_h, \pi_h v_h)_{\Gamma_N} \geq 0\,.\end{aligned} \tag{5.18}$$

Thus, choosing $v_h = \varphi_S$ for all $S \in \mathcal{S}_h^{\Gamma_C}$ in (5.18) and exploiting that $\pi_h\varphi_S = \chi_S$, for every $S \in \mathcal{S}_h^{\Gamma_C}$, we find that admissibility condition (5.6) is satisfied.

ad (5.9). If $S \in \mathcal{S}_h^{\Gamma_C}$ is such that $\pi_h u_h^{cr} > \chi_h$ on S, then there exists some $\alpha_S < 0$ such that $\pi_h u_h^{cr} + \alpha_S\chi_S \geq \chi_h$ on S. Thus, from $v_h = u_h^{cr} + \alpha_S\varphi_S \in \mathcal{S}_D^{1,cr}(\mathcal{T}_h)$ in (5.2), we get $z_h^{rt}\cdot n = 0$ on S.

ad Maximality. Using the discrete convex optimality relations (5.8),(5.9), the discrete integration-by-parts formula (2.11), and the discrete admissibility conditions (5.4)–(5.6), we observe that

$$\begin{aligned}I_h^{cr}(u_h^{cr}) &= \tfrac{1}{2}\|\nabla_h u_h^{cr}\|_\Omega^2 - (f_h, \Pi_h u_h^{cr})_\Omega - (g_h, \pi_h u_h^{cr})_{\Gamma_N}\\ &= \tfrac{1}{2}\|\nabla_h u_h^{cr}\|_\Omega^2 + (\operatorname{div} z_h^{rt}, \Pi_h u_h^{cr})_\Omega - (z_h^{rt}\cdot n, \pi_h u_h^{cr})_{\Gamma_N}\\ &= \tfrac{1}{2}\|\nabla_h u_h^{cr}\|_\Omega^2 - (\Pi_h z_h^{rt}, \nabla_h u_h^{cr})_\Omega + (z_h^{rt}\cdot n, \pi_h u_h^{cr})_{\Gamma_D\cup\Gamma_C}\\ &= -\tfrac{1}{2}\|\Pi_h z_h^{rt}\|_\Omega^2 + (z_h^{rt}\cdot n, \pi_h u_h^{cr})_{\Gamma_D\cup\Gamma_C}\\ &= D_h^{rt}(z_h^{rt})\,,\end{aligned}$$

which, by the discrete strong duality relation (5.7), shows that $z_h^{rt} \in \mathcal{RT}^0(\mathcal{T}_h)$ is maximal for (5.3). $\square$

6. *A priori* ERROR ANALYSIS

In this section, resorting to the discrete convex duality relations established in Section 5, we derive an *a priori* error identity for the discrete primal problem (5.1) and the discrete dual problem (5.3) at the same time. From this *a priori* error identity, in turn, we derive an *a priori* error estimate with an explicit error decay rate that is quasi-optimal. To this end, we proceed analogously to the continuous setting (*cf.* Section 4) and start with examining the *discrete primal-dual gap estimator* $\eta^2_{\mathrm{gap},h}\colon K_h^{cr}\times K_h^{rt,*}\to[0,+\infty)$, for every $v_h\in K_h^{cr}$ and $y_h\in K_h^{rt,*}$ defined by

$$\eta^2_{\mathrm{gap},h}(v_h,y_h)\coloneqq I_h^{cr}(v_h)-D_h^{rt}(y_h)\,. \tag{6.1}$$

The discrete primal-dual gap estimator (*cf.* (6.1)) can be decomposed into two contributions that precisely measure the violation of the discrete convex optimality relations (5.8),(5.9), respectively.

Lemma 6.1 (discrete primal-dual gap estimator)**.** *For every $v_h\in K_h^{cr}$ and $y_h\in K_h^{rt,*}$, we have that*

$$\begin{aligned}\eta^2_{\mathrm{gap},h}(v_h,y_h)&\coloneqq \eta^2_{A,\mathrm{gap},h}(v_h,y_h)+\eta^2_{B,\mathrm{gap},h}(v_h,y_h)\,,\\ \eta^2_{A,\mathrm{gap},h}(v_h,y_h)&\coloneqq \tfrac{1}{2}\|\nabla_h v_h-\Pi_h y_h\|_\Omega^2\,,\\ \eta^2_{B,\mathrm{gap},h}(v_h,y_h)&\coloneqq (y_h\cdot n,\pi_h v_h-\chi_h)_{\Gamma_C}\,.\end{aligned}$$

Remark 6.2 (interpretation of the components of the discrete primal-dual gap estimator)**.**

(i) The estimator $\eta^2_{A,\mathrm{gap},h}$ measures the violation of the discrete convex optimality relation (5.8)*;*

(ii) The estimator $\eta^2_{B,\mathrm{gap},h}$ measures the violation of the discrete convex optimality relation (5.9).

Proof (of Lemma 6.1). Using the discrete admissibility conditions (5.4)–(5.6), the discrete integration-by-parts formula (2.11), and the binomial formula, for every $v_h\in K_h^{cr}$ and $y_h\in K_h^{rt,*}$, due to $\pi_h v_h=\chi_h$ a.e. on Γ_D, we find that

$$\begin{aligned}I_h^{cr}(v_h)-D_h^{rt}(y_h)&=\tfrac{1}{2}\|\nabla_h v_h\|_\Omega^2-(f_h,\Pi_h v_h)_\Omega-(g_h,\pi_h v_h)_{\Gamma_N}+\tfrac{1}{2}\|\Pi_h y_h\|_\Omega^2-(y_h\cdot n,\chi_h)_{\Gamma_D\cup\Gamma_C}\\ &=\tfrac{1}{2}\|\nabla_h v_h\|_\Omega^2+(\operatorname{div} y_h,\Pi_h v_h)_\Omega+\tfrac{1}{2}\|\Pi_h y_h\|_\Omega^2\\ &\quad-(y_h\cdot n,\pi_h v_h)_{\Gamma_N}-(y_h\cdot n,\chi_h)_{\Gamma_D\cup\Gamma_C}\\ &=\tfrac{1}{2}\|\nabla_h v_h\|_\Omega^2-(\Pi_h y_h,\nabla_h v_h)_\Omega+\tfrac{1}{2}\|\Pi_h y_h\|_\Omega^2+(y_h\cdot n,\pi_h v_h-\chi_h)_{\Gamma_D\cup\Gamma_C}\\ &=\tfrac{1}{2}\|\nabla_h v_h-y_h\|_\Omega^2+(y_h\cdot n,\pi_h v_h-\chi_h)_{\Gamma_C}\,.\end{aligned}$$

∎

Next, we identify the *optimal strong convexity measures* for the discrete primal energy functional (5.1) at the discrete primal solution $u_h^{cr}\in K_h^{cr}$, *i.e.*, $\rho^2_{I_h^{cr}}\colon K_h^{cr}\to[0,+\infty)$, for every $v_h\in K_h^{cr}$ defined by

$$\rho^2_{I_h^{cr}}(v_h)\coloneqq I_h^{cr}(v_h)-I_h^{cr}(u_h^{cr})\,, \tag{6.2}$$

and for the negative of the discrete dual energy functional (5.3), *i.e.*, $\rho^2_{-D_h^{rt}}\colon K_h^{rt,*}\to[0,+\infty)$, for every $y_h\in K_h^{rt,*}$ defined by

$$\rho^2_{-D_h^{rt}}(y_h)\coloneqq -D_h^{rt}(y_h)+D_h^{rt}(z_h^{rt})\,, \tag{6.3}$$

which will serve as *'natural'* error quantities in the discrete primal-dual gap identity (*cf.* Theorem 6.5).

Lemma 6.3 (discrete optimal strong convexity measures)**.** *The following statements apply:*

(i) For every $v_h\in K_h^{cr}$, we have that

$$\rho^2_{I_h^{cr}}(v_h)=\tfrac{1}{2}\|\nabla_h v_h-\nabla_h u_h^{cr}\|_\Omega^2+(z_h^{rt}\cdot n,\pi_h v_h-\chi_h)_{\Gamma_C}\,.$$

(ii) For every $y_h\in K_h^{rt,*}$, we have that

$$\rho^2_{-D_h^{rt}}(y_h)=\tfrac{1}{2}\|\Pi_h y_h-\Pi_h z_h^{rt}\|_\Omega^2+(y_h\cdot n,\pi_h u_h^{cr}-\chi_h)_{\Gamma_C}\,.$$

Remark 6.4. *Note that for every $v_h\in K_h^{cr}$, it holds that $\pi_h v_h-\chi_h\ge 0$ a.e. on Γ_C, and for every $y_h\in K_h^{rt,*}$, we have that $y_h\cdot n\ge 0$ a.e. on Γ_C, so that for every $v_h\in K_h^{cr}$ and $y_h\in K_h^{rt,*}$, we have that*

$$y_h\cdot n\,(\pi_h v_h-\chi_h)\ge 0\qquad\text{a.e. on }\Gamma_C\,.$$

Proof (of Lemma 6.3). ad (i). Using the binomial formula, the discrete admissibility conditions (5.4),(5.5), the discrete convex optimality relation (5.8), the discrete integration-by-parts formula (2.11), and the discrete convex optimality relation (5.9), for every $v_h \in K_h^{cr}$, due to $\pi_h v_h = u_D^h = \pi_h u_D^{cr}$ a.e. on Γ_D, we find that

$$\begin{aligned} I_h^{cr}(v_h) - I_h^{cr}(u_h^{cr}) &= \tfrac{1}{2}\|\nabla_h v_h\|_\Omega^2 - \tfrac{1}{2}\|\nabla_h u_h^{cr}\|_\Omega^2 - (f_h, \Pi_h v_h - \Pi_h u_h^{cr})_\Omega - (g_h, \pi_h v_h - \pi_h u_h^{cr})_{\Gamma_N} \\ &= \tfrac{1}{2}\|\nabla_h v_h - \nabla_h u_h^{cr}\|_\Omega^2 + (\Pi_h z_h^{rt}, \nabla_h v_h - \nabla_h u_h^{cr})_\Omega \\ &\quad - (\operatorname{div} z_h^{rt}, \Pi_h v_h - \Pi_h u_h^{cr})_\Omega - (z_h^{rt}\cdot n, \pi_h v_h - \pi_h u_h^{cr})_{\Gamma_N} \\ &= \tfrac{1}{2}\|\nabla_h v_h - \nabla_h u_h^{cr}\|_\Omega^2 + (z_h^{rt}\cdot n, \pi_h v_h - \pi_h u_h^{cr})_{\Gamma_C} \\ &= \tfrac{1}{2}\|\nabla_h v_h - \nabla_h u_h^{cr}\|_\Omega^2 + (z_h^{rt}\cdot n, \pi_h v_h - \chi_h)_{\Gamma_C}\,. \end{aligned}$$

ad (ii). Using the binomial formula, the admissibility conditions (5.4)–(5.6), the convex optimality relation (5.8), the discrete integration-by-parts formula (2.11), again, the admissibility condition (5.4), and the convex optimality relation (5.9), for every $y_h \in K_h^{rt,*}$, due to $y_h\cdot n = g_h = z_h^{rt}\cdot n$ a.e. on Γ_N and $\pi_h u_h = u_D^h = \chi_h$ a.e. on Γ_D, we find that

$$\begin{aligned} -D_h^{rt}(y_h) + D_h^{rt}(z_h^{rt}) &= \tfrac{1}{2}\|\Pi_h y_h\|_\Omega^2 - \tfrac{1}{2}\|\Pi_h z_h^{rt}\|_\Omega^2 + (z_h^{rt}\cdot n - y_h\cdot n, \chi_h)_{\partial\Omega} \\ &= \tfrac{1}{2}\|\Pi_h y_h - z_h^{rt}\|_\Omega^2 + (\nabla_h u_h^{cr}, \Pi_h y_h - \Pi_h z_h^{rt})_\Omega + (z_h^{rt}\cdot n - y_h\cdot n, \chi_h)_{\partial\Omega} \\ &= \tfrac{1}{2}\|\Pi_h y_h - \Pi_h z_h^{rt}\|_\Omega^2 \\ &\quad + (\operatorname{div} z_h^{rt} - \operatorname{div} y_h, \Pi_h u_h^{cr})_\Omega + (z_h^{rt}\cdot n - y_h\cdot n, \chi_h - \pi_h u_h^{cr})_{\partial\Omega} \\ &= \tfrac{1}{2}\|\Pi_h y_h - \Pi_h z_h^{rt}\|_\Omega^2 + (y_h\cdot n, \pi_h u_h^{cr} - \chi_h)_{\Gamma_C}\,. \end{aligned}$$

□

Eventually, we have everything at our disposal to establish a discrete *a posteriori* error identity that identifies the *discrete primal-dual total error* $\rho_{\mathrm{tot},h}^2\colon K_h^{cr}\times K_h^{rt,*}\to[0,+\infty)$, for every $v_h \in K_h^{cr}$ and $y_h \in K_h^{rt,*}$ defined by

$$\rho_{\mathrm{tot},h}^2(v_h, y_h) \coloneqq \rho_{I_h^{cr}}^2(v_h) + \rho_{-D_h^{rt}}^2(y_h)\,, \tag{6.4}$$

with the discrete primal-dual gap estimator $\eta_{\mathrm{gap},h}^2\colon K_h^{cr}\times K_h^{rt,*}\to[0,+\infty)$ (*cf.* (6.1)).

Theorem 6.5 (discrete primal-dual gap identity)**.** *For every $v_h \in K_h^{cr}$ and $y_h \in K_h^{rt,*}$, we have that*

$$\rho_{\mathrm{tot},h}^2(v_h, y_h) = \eta_{\mathrm{gap},h}^2(v_h, y_h)\,.$$

Proof. Using the definitions (6.1), (6.2), (6.3), (6.4), and the discrete strong duality relation (5.7), for every $v_h \in K_h^{cr}$ and $y_h \in K_h^{rt,*}$, we find that

$$\begin{aligned} \rho_{\mathrm{tot},h}^2(v_h, y_h) &= \rho_{I_h^{cr}}^2(v_h) + \rho_{-D_h^{rt}}^2(y_h) \\ &= I_h^{cr}(v_h) - I_h^{cr}(u_h^{cr}) + D_h^{rt}(z_h^{rt}) - D_h^{rt}(y_h) \\ &= I_h^{cr}(v_h) - D_h^{rt}(y_h) \\ &= \eta_{\mathrm{gap},h}^2(v_h, y_h)\,. \end{aligned}$$

□

Inserting the (Fortin) quasi-interpolations (2.3) and (2.7) of the primal and the dual solution, respectively, in the primal-dual gap identity (*cf.* Theorem 6.5), we arrive at an *a priori* error identity, in which the right-hand side represents the residual in the discrete formulation.

Theorem 6.6 (*a priori* error identity and error decay rates)**.** *If $f_h \coloneqq \Pi_h f \in \mathcal{L}^0(\mathcal{T}_h)$, $g_h \coloneqq \pi_h g \in \mathcal{L}^0(\mathcal{S}_h^{\Gamma_N})$, where $g \in L^2(\Gamma_N)$, $u_D^h \coloneqq \pi_h u_D \in \mathcal{L}^0(\mathcal{S}_h^{\Gamma_D})$, and $\chi_h \coloneqq \pi_h \Pi_h^{cr}\chi \in \mathcal{L}^0(\mathcal{S}_h^{\Gamma_C})$, then the following statements apply:*

(i) If $z \in (L^p(\Omega))^d$, where $p > 2$, then $\Pi_h^{cr} u \in K_h^{cr}$, $\Pi_h^{rt} z \in K_h^{rt,*}$, and

$$\rho_{\mathrm{tot},h}^2(\Pi_h^{cr} u, \Pi_h^{rt} z) = \tfrac{1}{2}\|\Pi_h z - \Pi_h \Pi_h^{rt} z\|_\Omega^2 + (z\cdot n, \pi_h \Pi_h^{cr}(u-\chi) - (u-\chi))_{\Gamma_C}\,.$$

(ii) If $u, \chi \in H^{1+s}(\Omega)$, where $s \in (\frac{1}{2}, 1]$, and if $\Delta\chi \in L^2(\Omega)$ or $d = 2$, then

$$\rho_{\mathrm{tot},h}^2(\Pi_h^{cr} u, \Pi_h^{rt} z) \le c\, h^{2s}\,(\|u\|_{1+s,\Omega}^2 + \|\chi\|_{1+s,\Omega}^2)\,.$$

Remark 6.7. *The a priori error estimate in Theorem 6.6(ii) holds as soon as* $u\in H^1(\partial\Omega)$*:*

(i) According to [6, Cor. 3.7], the trace operator

$$\mathrm{Tr}\coloneqq (\mathrm{tr},\mathrm{tr}\circ\nabla)^\top\colon H_\Delta(\Omega)\coloneqq \big\{v\in H^{\frac{3}{2}}(\Omega)\mid \Delta v\in L^2(\Omega)\big\}\to H^1(\partial\Omega)\times(L^2(\partial\Omega))^d\,,$$

is well-defined, linear, and continuous. Thus, if $u\in H^{\frac{3}{2}}(\Omega)$*, due to* $\Delta u=\operatorname{div} z=-f\in L^2(\Omega)$*, we have that* $u\in H_\Delta(\Omega)$ *and, thus, the traces* $u|_{\partial\Omega}\in H^1(\partial\Omega)$ *and* $(\nabla u)|_{\partial\Omega}\in(L^2(\Omega))^d$*.*

(ii) If $\Omega\subseteq\mathbb{R}^2$ *is polygonal bounded Lipschitz domain and* $s\in(\frac{1}{2},1]$*, then (cf. [28, Thm. 1.5.2.1])* $\mathrm{Tr}\coloneqq(\mathrm{tr},\mathrm{tr}\circ\nabla)^\top\colon H^{1+s}(\Omega)\to H^{s+\frac{1}{2}}(\partial\Omega)\times(H^{s-\frac{1}{2}}(\partial\Omega))^d$ *is well-defined, linear and continuous.*

Proof (of Theorem 6.6). ad (i). First, using (2.5), we observe that

$$\pi_h\Pi_h^{cr}u=\pi_h u\begin{cases}=\pi_h u_D=u_D^h & \text{a.e. on }\Gamma_D\,,\\ \geq \pi_h\chi=\chi_h & \text{a.e. on }\Gamma_C\,,\end{cases}$$

i.e., it holds that $\Pi_h^{cr}u\in K_h^{cr}$. Second, if $z\in(L^p(\Omega))^d$, where $p>2$, according to [24, Sec. 17.1], $\Pi_h^{rt}z\in\mathcal{RT}_N^0(\mathcal{T}_h)$ is well-defined and using (2.8) and (2.9), we observe that

$$\begin{aligned}\operatorname{div}\Pi_h^{rt}z&=\Pi_h\operatorname{div}z=-f_h &&\text{a.e. in }\Omega\,,\\ \Pi_h^{rt}z\cdot n&=\pi_h(z\cdot n)\begin{cases}=\pi_h g=g_h\\ \geq 0\end{cases} &&\begin{matrix}\text{a.e. on }\Gamma_N\,,\\ \text{a.e. on }\Gamma_C\,,\end{matrix}\end{aligned}$$

i.e., it holds that $\Pi_h^{rt}z\in K_h^{rt,*}$. Then, using Theorem 6.5 together with Lemma 6.1 and Lemma 6.3 as well as the convex optimality relation (3.9), (2.4), and (2.9), we find that

$$\begin{aligned}\rho_{\mathrm{tot},h}^2(\Pi_h^{cr}u,\Pi_h^{rt}z)&=\tfrac{1}{2}\|\nabla_h\Pi_h^{cr}u-\Pi_h\Pi_h^{rt}z\|_\Omega^2+(\Pi_h^{rt}z\cdot n,\pi_h\Pi_h^{cr}u-\chi_h)_{\Gamma_C}\\ &=\tfrac{1}{2}\|\Pi_h z-\Pi_h\Pi_h^{rt}z\|_\Omega^2+(z\cdot n,\pi_h\Pi_h^{cr}(u-\chi)-(u-\chi))_{\Gamma_C}\\ &\eqqcolon I_h^1+I_h^2\,.\end{aligned}\tag{6.5}$$

ad (ii). We need to estimate I_h^1 and I_h^2:

ad I_h^1*.* Using the L^2-stability property of Π_h and the fractional approximation properties of Π_h^{rt} (*cf.* (2.10)), we find that

$$I_h^1\leq\tfrac{1}{2}\|z-\Pi_h^{rt}z\|_\Omega^2\leq c\,h^{2s}\,|z|_{s,\Omega}^2\leq c\,h^{2s}\,\|u\|_{1+s,\Omega}^2\,.\tag{6.6}$$

ad I_h^2*.* Abbreviating $\tilde u\coloneqq u-\chi\in H^{1+s}(\Omega)$, we find that

$$\begin{aligned}(z\cdot n,\pi_h\Pi_h^{cr}\tilde u-\tilde u)_{\Gamma_C}&=(z\cdot n,\Pi_h^{cr}\tilde u-\tilde u)_{\Gamma_C}+(z\cdot n,\pi_h\Pi_h^{cr}\tilde u-\Pi_h^{cr}\tilde u)_{\Gamma_C}\\ &\eqqcolon I_h^{2,1}+I_h^{2,2}\,.\end{aligned}\tag{6.7}$$

ad $I_h^{2,1}$*.* Using that $\Pi_h^{cr}\tilde u-\tilde u\perp\mathcal{L}^0(\mathcal{S}_h)$ (*cf.* (2.5)), that $\pi_h(z\cdot n)=(\pi_h z)\cdot n$ a.e. in $\cup\mathcal{S}_h$, a local trace inequality (*cf.* [24, Rem. 12.19, (12.17)]), and the fractional approximation properties of π_h and Π_h^{cr} (*cf.* (2.6)), we obtain

$$\begin{aligned}I_h^{2,1}&=(z\cdot n-\pi_h(z\cdot n),\Pi_h^{cr}\tilde u-\tilde u)_{\Gamma_C}\\ &\leq\|z-\pi_h z\|_{\Gamma_C}\,(h^{-\frac{1}{2}}\,\|\tilde u-\Pi_h^{cr}\tilde u\|_\Omega+h^{\frac{1}{2}}\,\|\nabla\tilde u-\nabla_h\Pi_h^{cr}\tilde u\|_\Omega)\\ &\leq c\,h^{s-\frac{1}{2}}|z|_{s-\frac{1}{2},\Gamma_C}\,h^{s+\frac{1}{2}}|\tilde u|_{s+\frac{1}{2},\Omega}\\ &\leq c\,h^{2s}(\|u\|_{1+s,\Omega}^2+\|\chi\|_{1+s,\Omega}^2)\,.\end{aligned}\tag{6.8}$$

ad $I_h^{2,2}$*.* We decompose $I_h^{2,2}$ into local contributions, *i.e.*, we define

$$I_h^{2,2}=\sum_{S\in\mathcal{S}_h^{\Gamma_C}}(z\cdot n,\pi_h\Pi_h^{cr}\tilde u-\Pi_h^{cr}\tilde u)_S\eqqcolon\sum_{S\in\mathcal{S}_h^{\Gamma_C}}I_S^{2,2}\,.\tag{6.9}$$

Next, we distinguish the cases $|S\setminus(\{\tilde u>0\}\cap\Gamma_C)|=0$ (*i.e.*, no contact), $|S\setminus(\{\tilde u=0\}\cap\Gamma_C)|=0$ (*i.e.*, contact), and $|S\setminus(\{\tilde u=0\}\cap\Gamma_C)|>0$ (*i.e.*, both contact and no contact) (equivalent to $|S\setminus(\{\tilde u>0\}\cap\Gamma_C)|>0$): In doing so, we use the identity

$$\Pi_h^{cr}\tilde u-\pi_h\Pi_h^{cr}\tilde u=\nabla_S\Pi_h^{cr}\tilde u\cdot(\mathrm{id}_{\mathbb{R}^d}-\pi_h\mathrm{id}_{\mathbb{R}^d})\quad\text{ in }S\,,\tag{6.10}$$

where, for each $v\in H^1(S)$, we denote by $\nabla_S v\in(L^2(S))^d$ the tangential gradient, which, for every $v\in H_\Delta(T_S)\cap H^{1+s}(T_S)$, where $T_S\in\mathcal{T}_h$ is such that $S\subseteq\partial T_S$, satisfies (*cf.* [24, Rem. 12.19, (12.17)])

$$\|\nabla_S v\|_S\leq\|(\nabla v)|_S\|_S\leq c\,(h_S^{-\frac{1}{2}}\|\nabla v\|_{T_S}+h_S^{s-\frac{1}{2}}|\nabla v|_{s,T_S})\,.\tag{6.11}$$

In particular, from (6.11) together with the fractional approximation properties of Π_h^{cr} (*cf.* (2.6)) and $|\nabla\Pi_h^{cr}\tilde{u}|_{s,T_S}=0$ since $\nabla\Pi_h^{cr}\tilde{u}|_{T_S}=\mathrm{const}$, it follows that

$$\begin{aligned}\|\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u}\|_S&\le (h_S^{-\frac{1}{2}}\|\nabla\tilde{u}-\nabla\Pi_h^{cr}\tilde{u}\|_{T_S}+h_S^{s-\frac{1}{2}}|\nabla\tilde{u}|_{s,T_S})\\&\le h_S^{s-\frac{1}{2}}|\tilde{u}|_{s+\frac{1}{2},T_S}\,.\end{aligned}\tag{6.12}$$

ad $|S\setminus(\{\tilde{u}>0\}\cap\Gamma_C)|=0$ *(i.e., no contact).* In this case, due to the convex optimality relation (3.9), we have that $z\cdot n=0$ a.e. on S and, thus,

$$I_S^{2,2}=0\,.\tag{6.13}$$

ad $|S\setminus(\{\tilde{u}=0\}\cap\Gamma_C)|=0$ *(i.e., contact).* In this case, we have that $\tilde{u}=0$ a.e. on S, which implies that $\nabla_S\tilde{u}=0$ a.e. on S. Therefore, using that $\pi_h\Pi_h^{cr}\tilde{u}-\Pi_h^{cr}\tilde{u}\perp\mathcal{L}^0(\mathcal{S}_h)$, (6.10), the fractional approximation properties of π_h (*cf.* [24, Rem. 18.17]), and (6.12), we obtain

$$\begin{aligned}I_S^{2,2}&=(z\cdot n-\pi_h(z\cdot n),\pi_h\Pi_h^{cr}\tilde{u}-\Pi_h^{cr}\tilde{u})_S\\&=(z\cdot n-\pi_h(z\cdot n),(\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u})\cdot(\mathrm{id}_{\mathbb{R}^d}-\pi_h\mathrm{id}_{\mathbb{R}^d}))_S\\&\le h_S\,\|z-\pi_hz\|_S\|\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u}\|_S\\&\le c\,h_S\,h_S^{s-\frac{1}{2}}|z|_{s-\frac{1}{2},S}\,h_S^{s-\frac{1}{2}}|\tilde{u}|_{s+\frac{1}{2},T_S}\\&\le c\,h_S^{2s}\,(\|u\|_{1+s,T_S}^2+\|\chi\|_{1+s,T_S}^2)\,.\end{aligned}\tag{6.14}$$

ad $|S\setminus(\{\tilde{u}=0\}\cap\Gamma_C)|>0$ *(i.e., both contact and no contact).* On the one hand, we have that $\tilde{u}=0$ a.e. on $S\cap\{\tilde{u}=0\}$, which implies that $\nabla_S\tilde{u}=0$ a.e. on $S\cap\{\tilde{u}=0\}$. Using that $\pi_h\Pi_h^{cr}\tilde{u}-\Pi_h^{cr}\tilde{u}\perp\mathcal{L}^0(\mathcal{S}_h)$, (6.10), [20, Lem. 8.2.3], the fractional approximation properties of π_h, that $\pi_h\nabla_S\Pi_h^{cr}\tilde{u}=\nabla_S\Pi_h^{cr}\tilde{u}$, the L^2-stability of π_h, and (6.12), we obtain

$$\begin{aligned}I_S^{2,2}&=(z\cdot n-\pi_h(z\cdot n),(\langle\nabla_S\tilde{u}\rangle_{S\cap\{\tilde{u}=0\}}-\nabla_S\Pi_h^{cr}\tilde{u})\cdot(\mathrm{id}_{\mathbb{R}^d}-\pi_h\mathrm{id}_{\mathbb{R}^d}))_S\\&\le\|z-\pi_hz\|_S\,h_S\,(\|\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u}\|_S+\|\langle\nabla_S\tilde{u}\rangle_{S\cap\{\tilde{u}=0\}}-\nabla_S\tilde{u}\|_S)\\&\le c\,\|z-\pi_hz\|_S\,h_S\,\big(\|\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u}\|_S+\tfrac{|S|}{|S\cap\{\tilde{u}=0\}|}\|\pi_h(\nabla_S\tilde{u})-\nabla_S\tilde{u}\|_S\big)\\&\le c\,\|z-\pi_hz\|_S\,h_S\,\big(\|\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u}\|_S\\&\quad+\tfrac{|S|}{|S\cap\{\tilde{u}=0\}|}(\|\pi_h(\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u})\|_S+\|\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u}\|_S)\big)\\&\le c\,\tfrac{|S|}{|S\cap\{\tilde{u}=0\}|}\,h_S^{2s}\,(\|u\|_{1+s,T_S}^2+\|\chi\|_{1+s,T_S}^2)\,.\end{aligned}\tag{6.15}$$

On the other hand, we have that $z\cdot n=0$ a.e. in $S\cap\{\tilde{u}>0\}$. Using that $\pi_h\Pi_h^{cr}\tilde{u}-\Pi_h^{cr}\tilde{u}\perp\mathcal{L}^0(\mathcal{S}_h)$, that $\langle z\cdot n\rangle_{S\cap\{\tilde{u}>0\}}=\langle z\rangle_{S\cap\{\tilde{u}>0\}}\cdot n$ a.e. in S, (6.10), [20, Lem. 8.2.3], the fractional approximation properties of π_h, and (6.12), we obtain

$$\begin{aligned}I_S^{2,2}&=(z\cdot n,(\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u})\cdot(\mathrm{id}_{\mathbb{R}^d}-\pi_h\mathrm{id}_{\mathbb{R}^d}))_S\\&=(z\cdot n-\langle z\cdot n\rangle_{S\cap\{\tilde{u}>0\}},(\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u})\cdot(\mathrm{id}_{\mathbb{R}^d}-\pi_h\mathrm{id}_{\mathbb{R}^d}))_S\\&\le\|z-\langle z\rangle_{S\cap\{\tilde{u}>0\}}\|_S\,h_S\,\|\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u}\|_S\\&\le c\,\tfrac{|S|}{|S\cap\{\tilde{u}>0\}|}\,\|z-\pi_hz\|_S\,h_S\,\|\nabla_S\tilde{u}-\nabla_S\Pi_h^{cr}\tilde{u}\|_S\\&\le c\,\tfrac{|S|}{|S\cap\{\tilde{u}>0\}|}\,h_S^{2s}\,(\|u\|_{1+s,T_S}^2+\|\chi\|_{1+s,T_S}^2)\,.\end{aligned}\tag{6.16}$$

Since $S=(S\cap\{\tilde{u}>0\})\dot\cup(S\cap\{\tilde{u}=0\})$, we have that $|S\cap\{\tilde{u}>0\}|\ge\frac{1}{2}|S|$ or $|S\cap\{\tilde{u}=0\}|\ge\frac{1}{2}|S|$. Using in the first case (6.15) and in the second case (6.16), we arrive at

$$I_S^{2,2}\le c\,h_S^{2s}\,(\|u\|_{1+s,T_S}^2+\|\chi\|_{1+s,T_S}^2)\,.\tag{6.17}$$

Combining (6.13), (6.14), and (6.17) in (6.9), we deduce that

$$I_h^{2,2}\le c\,h^{2s}\,(\|u\|_{1+s,\Omega}^2+\|\chi\|_{1+s,\Omega}^2)\,.\tag{6.18}$$

Using (6.8) and (6.18) in (6.7), we infer that

$$I_h^2\le c\,h^{2s}\,(\|u\|_{1+s,\Omega}^2+\|\chi\|_{1+s,\Omega}^2)\,.\tag{6.19}$$

Eventually, using (6.19) and (6.6) in (6.5), we conclude the claimed *a priori* error estimate. □

7. Numerical experiments

In this section, we review the theoretical findings of Section 4 and Section 6 via numerical experiments. All experiments were carried out using the finite element software package FEniCS (version 2019.1.0, *cf.* [36]). All graphics are created using the Matplotlib library (version 3.5.1, *cf.* [33]).

7.1 Implementation details

We compute the discrete primal solution $u_h^{cr}\in\mathcal{S}^{1,cr}_D(\mathcal{T}_h)$ and the associated discrete Lagrange multiplier $\overline{\lambda}_h^{cr}\in\mathcal{L}^0(\mathcal{S}_h^{\Gamma_C})$ jointly satisfying the discrete augmented problem (5.16) via the primal-dual active set strategy interpreted as a semi-smooth Newton method. For sake of completeness, in the case $u_D=0$, we will briefly outline important implementation details related with this strategy.

We fix an ordering of the sides $(S_i)_{i=1,\ldots,N_h^{cr}}$ and an ordering of the elements $(T_i)_{i=1,\ldots,N_h^0}$, where $N_h^{cr}\coloneqq \operatorname{card}(\mathcal{S}_h\setminus\mathcal{S}_h^{\Gamma_D})$, $N_h^{cr,C}=\operatorname{card}(\mathcal{S}_h^{\Gamma_C})$ and $N_h^0\coloneqq\operatorname{card}(\mathcal{T}_h)$ such that[2]

$$
\begin{aligned}
\operatorname{span}(\{\varphi_{S_i}\mid i=1,\ldots,N_h^{cr}\})&=\mathcal{S}^{1,cr}_D(\mathcal{T}_h)\,,\\
\operatorname{span}(\{\chi_{S_i}\mid i=1,\ldots,N_h^{cr,C}\})&=\mathcal{L}^0(\mathcal{S}_h^{\Gamma_C})\,,\\
\operatorname{span}(\{\chi_{T_i}\mid i=1,\ldots,N_h^{cr,0}\})&=\Pi_h(\mathcal{S}^{1,cr}_D(\mathcal{T}_h))\,,
\end{aligned}
$$

where $N_h^{cr,0}=\dim(\Pi_h(\mathcal{S}^{1,cr}_D(\mathcal{T}_h)))\in\{N_h^0,N_h^0-1\}$ because of $\operatorname{codim}_{\mathcal{L}^0(\mathcal{T}_h)}(\Pi_h(\mathcal{S}^{1,cr}_D(\mathcal{T}_h)))\in\{0,1\}$ (*cf.* [5, Cor. 3.2]). Then, if we define the matrices

$$
\begin{aligned}
\mathrm{S}_h^{cr}&\coloneqq((\nabla_h\varphi_{S_i},\nabla_h\varphi_{S_j})_\Omega)_{i,j=1,\ldots,N_h^{cr}}\in\mathbb{R}^{N_h^{cr}\times N_h^{cr}}\,,\\
\mathrm{P}_h^{cr,0}&\coloneqq((\Pi_h\varphi_{S_i},\chi_{T_j})_\Omega)_{i=1,\ldots,N_h^{cr},j=1,\ldots,N_h^{cr,0}}\in\mathbb{R}^{N_h^{cr}\times N_h^{cr,0}}\,,\\
\mathrm{p}_h^{cr,C}&\coloneqq((\Pi_h\varphi_{S_i},\chi_{S_j})_{\Gamma_C})_{i=1,\ldots,N_h^{cr},j=1,\ldots,N_h^{cr,C}}\in\mathbb{R}^{N_h^{cr}\times N_h^{cr,C}}\,,
\end{aligned}
$$

and, assuming for the entire section that $\chi_h\coloneqq\pi_h\Pi_h^{cr}\chi\in\mathcal{L}^0(\mathcal{S}_h)$, the vectors

$$
\begin{aligned}
\mathrm{X}_h^{cr}&\coloneqq((\chi_h,\chi_{S_i})_{\Gamma_C})_{i=1,\ldots,N_h^{cr}}\in\mathbb{R}^{N_h^{cr}}\,,\\
\mathrm{F}_h^{0}&\coloneqq((f_h,\chi_{T_i})_{\Omega})_{i=1,\ldots,N_h^{cr,0}}\in\mathbb{R}^{N_h^{cr,0}}\,,\\
\mathrm{G}_h^{cr}&\coloneqq((g_h,\chi_{S_i})_{\Gamma_N})_{i=1,\ldots,N_h^{cr}}\in\mathbb{R}^{N_h^{cr}}\,,
\end{aligned}
$$

the same argumentation as in [3, Lem. 5.3] shows that the discrete augmented problem (5.16) is equivalent to finding vectors $(\mathrm{U}_h^{cr},\overline{\Lambda}_h^{cr})^\top\in\mathbb{R}^{N_h^{cr}}\times\mathbb{R}^{N_h^{cr,C}}$ such that

$$
\begin{aligned}
\mathrm{S}_h^{cr}\mathrm{U}_h^{cr}+\mathrm{p}_h^{cr,C}\overline{\Lambda}_h^{cr}&=\mathrm{P}_h^{cr,0}\mathrm{F}_h^0+\mathrm{G}_h^{cr}&&\text{in }\mathbb{R}^{N_h^{cr}}\,,\\
\mathscr{C}_h(\mathrm{U}_h^{cr},\overline{\Lambda}_h^{cr})&=0_{\mathbb{R}^{N_h^{cr,C}}}&&\text{in }\mathbb{R}^{N_h^{cr,C}}\,,
\end{aligned}
\tag{7.1}
$$

where for given $\alpha>0$, the mapping $\mathscr{C}_h\colon\mathbb{R}^{N_h^{cr}}\times\mathbb{R}^{N_h^{cr,C}}\to\mathbb{R}^{N_h^{cr,C}}$ for every $(\mathrm{U}_h,\overline{\Lambda}_h)^\top\in\mathbb{R}^{N_h^{cr}}\times\mathbb{R}^{N_h^{cr,C}}$ is defined by[3]

$$
\mathscr{C}_h(\mathrm{U}_h,\overline{\Lambda}_h)\coloneqq\overline{\Lambda}_h-\min\big\{0_{\mathbb{R}^{N_h^{cr,C}}},\overline{\Lambda}_h+\alpha\,(\mathrm{p}_h^{cr,0})^\top(\mathrm{U}_h-\mathrm{X}_h^{cr})\big\}\quad\text{ in }\mathbb{R}^{N_h^{cr,C}}\,.
$$

More precisely, the discrete primal solution $u_h^{cr}\in\mathcal{S}^{1,cr}_D(\mathcal{T}_h)$ and the associated discrete Lagrange multiplier $\overline{\lambda}_h^{cr}\in\mathcal{L}^0(\mathcal{S}_h^{\Gamma_C})$ jointly satisfying the discrete augmented problem (5.16) as well as the vectors $(\mathrm{U}_h^{cr},\overline{\Lambda}_h^{cr})^\top\in\mathbb{R}^{N_h^{cr}}\times\mathbb{R}^{N_h^{cr,C}}$ satisfying (7.1), respectively, are related by[4]

$$
u_h^{cr}=\sum_{i=1}^{N_h^{cr}}(\mathrm{U}_h^{cr}\cdot\mathrm{e}_i)\varphi_{S_i}\in\mathcal{S}^{1,cr}_D(\mathcal{T}_h)\,,\qquad\overline{\lambda}_h^{cr}=\sum_{i=1}^{N_h^{cr,C}}(\overline{\Lambda}_h^{cr}\cdot\mathrm{e}_i)\chi_{S_i}\in\mathcal{L}^0(\mathcal{S}_h^{\Gamma_C})\,.
$$

[2] In practice, the element $\widehat{T}\in\mathcal{T}_h$ for which $\mathbb{R}\chi_{\widehat{T}}\perp\Pi_h(\mathcal{S}^{1,cr}_D(\mathcal{T}_h))$ is found via searching and erasing a zero column (if existent) in the matrix $((\Pi_h\varphi_{S_i},\chi_T)_\Omega)_{i=1,\ldots,N_h^{cr},T\in\mathcal{T}_h}\in\mathbb{R}^{N_h^{cr}\times N_h^0}$ leading to $\mathrm{P}_h^{cr,0}\in\mathbb{R}^{N_h^{cr}\times N_h^{cr,0}}$.

[3] Here, for $a=(a_i)_{i=1,\ldots,n},b=(b_i)_{i=1,\ldots,n}\in\mathbb{R}^n$, $n\in\mathbb{N}$, we define $\min\{a,b\}=(\min\{a_i,b_i\})_{i=1,\ldots,n}\in\mathbb{R}^n$.

[4] Here, for each $i=1,\ldots,N$, $N\in\mathbb{N}$, we denote by $\mathrm{e}_i=(\delta_{ij})_{j=1,\ldots,N}\in\mathbb{R}^N$, the i-th unit vector.

Next, define the mapping $\mathscr{F}_h : \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}} \to \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$ for every $(\mathrm{U}_h, \overline{\Lambda}_h)^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$ by

$$\mathscr{F}_h(\mathrm{U}_h, \overline{\Lambda}_h) := \begin{bmatrix} \mathrm{S}_h^{cr}\mathrm{U}_h + \mathrm{p}_h^{cr,C}\overline{\Lambda}_h - \mathrm{P}_h^{cr,0}\mathrm{F}_h^0 - \mathrm{G}_h^{cr} \\ \mathscr{C}_h(\mathrm{U}_h, \overline{\Lambda}_h) \end{bmatrix} \quad \text{in } \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}} .$$

Then, the non-linear system (7.1) is equivalent to finding $(\mathrm{U}_h^{cr}, \overline{\Lambda}_h^{cr})^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$ such that

$$\mathscr{F}_h(\mathrm{U}_h^{cr}, \overline{\Lambda}_h^{cr}) = 0_{\mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}} \quad \text{in } \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}} .$$

By analogy with [3, Thm. 5.11], one finds that the mapping $\mathscr{F}_h : \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}} \to \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$ is Newton-differentiable at every $(\mathrm{U}_h, \overline{\Lambda}_h)^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$ and with the (active) set

$$\mathscr{A}_h := \mathscr{A}_h(\mathrm{U}_h, \overline{\Lambda}_h) := \big\{ i \in \{1, \dots, N_h^{cr,C}\} \mid (\overline{\Lambda}_h + \alpha(\mathrm{p}_h^{cr,C})^\top(\mathrm{U}_h - \mathrm{X}_h^{cr})) \cdot \mathrm{e}_i < 0 \big\} ,$$

for every $(\mathrm{U}_h, \overline{\Lambda}_h)^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$, we have that

$$\mathrm{D}\mathscr{F}_h(\mathrm{U}_h, \overline{\Lambda}_h) := \begin{bmatrix} \mathrm{S}_h^{cr} & \mathrm{p}_h^{cr,C} \\ \mathrm{I}_{\mathscr{A}_h}(\mathrm{p}_h^{cr,C})^\top & \mathrm{I}_{\mathscr{A}_h^c} \end{bmatrix} \quad \text{in } \mathbb{R}^{N_h^{cr}+N_h^{cr,C}} \times \mathbb{R}^{N_h^{cr}+N_h^{cr,C}} ,$$

where $\mathrm{I}_{\mathscr{A}_h}, \mathrm{I}_{\mathscr{A}_h^c} := \mathrm{I}_{N_h^{cr,C} \times N_h^{cr,C}} - \mathrm{I}_{\mathscr{A}_h} \in \mathbb{R}^{N_h^{cr,C}} \times \mathbb{R}^{N_h^{cr,C}}$ for every $i, j \in \{1, \dots, N_h^{cr,0}\}$ are defined by $(\mathrm{I}_{\mathscr{A}_h})_{ij} := 1$ if $i = j \in \mathscr{A}_h$ and $(\mathrm{I}_{\mathscr{A}_h})_{ij} := 0$ else.

For a given iterate $(\mathrm{U}_h^{k-1}, \overline{\Lambda}_h^{k-1})^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$, one step of the semi-smooth Newton method determines a direction $(\delta\mathrm{U}_h^{k-1}, \delta\overline{\Lambda}_h^{k-1})^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$ such that

$$\mathrm{D}\mathscr{F}_h(\mathrm{U}_h^{k-1}, \overline{\Lambda}_h^{k-1})(\delta\mathrm{U}_h^{k-1}, \delta\overline{\Lambda}_h^{k-1})^\top = -\mathscr{F}_h(\mathrm{U}_h^{k-1}, \overline{\Lambda}_h^{k-1}) \quad \text{in } \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}} . \tag{7.2}$$

Setting the update $(\mathrm{U}_h^k, \overline{\Lambda}_h^k)^\top := (\mathrm{U}_h^{k-1} + \delta\mathrm{U}_h^{k-1}, \overline{\Lambda}_h^{k-1} + \delta\overline{\Lambda}_h^{k-1})^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$ and the active set $\mathscr{A}_h^{k-1} := \mathscr{A}_h(\mathrm{U}_h^{k-1}, \overline{\Lambda}_h^{k-1})$, the linear system (7.2) can equivalently be re-written as

$$\begin{aligned} \mathrm{S}_h^{cr}\mathrm{U}_h^k + \mathrm{p}_h^{cr,C}\overline{\Lambda}_h^k &= \mathrm{P}_h^{cr,0}\mathrm{F}_h^0 && \text{in } \mathbb{R}^{N_h^{cr}} , \\ \mathrm{I}_{(\mathscr{A}_h^{k-1})^c}\overline{\Lambda}_h^k &= 0_{\mathbb{R}^{N_h^{cr,0}}} && \text{in } \mathbb{R}^{N_h^{cr,C}} , \\ \mathrm{I}_{\mathscr{A}_h^{k-1}}(\mathrm{p}_h^{cr,C})^\top\mathrm{U}_h^k &= \mathrm{I}_{\mathscr{A}_h^{k-1}}(\mathrm{p}_h^{cr,C})^\top\mathrm{X}_h^{cr} && \text{in } \mathbb{R}^{N_h^{cr,C}} . \end{aligned} \tag{7.3}$$

The semi-smooth Newton method (7.2) can, thus, equivalently be formulated in the following form, which is a version of a primal-dual active set strategy.

Algorithm 7.1 (primal-dual active set strategy)**.** *Choose parameters $\alpha > 0$ and $\varepsilon_{\mathrm{STOP}} > 0$. Moreover, let $(\mathrm{U}_h^0, \overline{\Lambda}_h^0)^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$ be an initial guess and set $k = 1$. Then, for every $k \in \mathbb{N}$:*

(i) Define the most recent active set

$$\mathscr{A}_h^{k-1} := \mathscr{A}_h(\mathrm{U}_h^{k-1}, \overline{\Lambda}_h^{k-1}) := \big\{ i \in \{1, \dots, N_h^{cr,C}\} \mid (\overline{\Lambda}_h^{k-1} + \alpha(\mathrm{p}_h^{cr,C})^\top(\mathrm{U}_h^{k-1} - \mathrm{X}_h^{cr})) \cdot \mathrm{e}_i < 0 \big\} .$$

(ii) Compute the iterate $(\mathrm{U}_h^k, \overline{\Lambda}_h^k)^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$ such that

$$\begin{bmatrix} \mathrm{S}_h^{cr} & \mathrm{p}_h^{cr,C} \\ \mathrm{I}_{\mathscr{A}_h^{k-1}}(\mathrm{p}_h^{cr,C})^\top & \mathrm{I}_{(\mathscr{A}_h^{k-1})^c} \end{bmatrix} \begin{bmatrix} \mathrm{U}_h^k \\ \overline{\Lambda}_h^k \end{bmatrix} = \begin{bmatrix} \mathrm{P}_h^{cr,0}\mathrm{F}_h^0 \\ \mathrm{I}_{\mathscr{A}_h^{k-1}}(\mathrm{p}_h^{cr,C})^\top\mathrm{X}_h^{cr} \end{bmatrix} .$$

(iii) Stop if $|\mathrm{U}_h^k - \mathrm{U}_h^{k-1}| \le \varepsilon_{\mathrm{STOP}}$; otherwise, increase $k \to k+1$ and continue with step (i).

Remark 7.2 (Important implementation details)**.** *(i) Algorithm 7.1 converges super-linearly if $(\mathrm{U}_h^0, \overline{\Lambda}_h^0)^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$ is sufficiently close to the solution $(\mathrm{U}_h^{cr}, \overline{\Lambda}_h^{cr})^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$. As the Newton-differentiability only holds in finite-dimensional situations and deteriorates as $N_h^{cr} + N_h^{cr,C} \to \infty$, the condition on the initial guess becomes more critical for $N_h^{cr} + N_h^{cr,C} \to \infty$.*

(ii) The degrees of freedom related to the entries $\overline{\Lambda}_h^k|_{(\mathscr{A}_h^{k-1})^c}$ can be eliminated from the linear system of equations in Algorithm 7.1, step (ii) (see also $(7.3)_2$).

(iii) Since only a finite number of active sets are possible, the algorithm terminates within a finite number of iterations at the exact solution $(\mathrm{U}_h^{cr}, \overline{\Lambda}_h^{cr})^\top \in \mathbb{R}^{N_h^{cr}} \times \mathbb{R}^{N_h^{cr,C}}$. For this reason, in practice, the stopping criterion in step (iii) is reached with $|\mathrm{U}_h^{k^*} - \mathrm{U}_h^{k^*-1}| = 0$ for some $k^* \in \mathbb{N}$, in which case, one has that $\mathrm{U}_h^{k^*} = \mathrm{U}_h^{cr}$, provided $\varepsilon_{\mathrm{STOP}} > 0$ is sufficiently small.

7.2 Numerical experiments concerning the a priori error analysis

In this subsection, we review the theoretical findings of Section 6.

For our numerical experiments, we choose a setup from [43, Sec. 7], [18, §6], or [2, Sec. 5.1]. More precisely, let $\Omega := (0,1)^2$, $\Gamma_C := (0,1)\times\{0\}$, $\Gamma_D := \partial\Omega\setminus\Gamma_C$ (*cf.* Figure 1(*left*)), *i.e.*, $\Gamma_N := \emptyset$, and $\chi := 0 \in H^2(\Omega)$. Then, we compute $f \in L^2(\Omega)$ such that the primal solution $u \in K$, in polar coordinates centered at $(0.5,0)^\top \in \Gamma_C$, *i.e.*, for every $x = (x_1,x_2)^\top \in \Omega$, setting

$$r(x) := \big((x_1 - \tfrac{1}{2})^2 + x_2^2\big)^{\frac{1}{2}}\,, \qquad \theta(x) := \arccos\big(\tfrac{x_1-\frac{1}{2}}{r(x)}\big)\,,$$

for every $x \in \Omega$, is defined by

$$u(x) := -10\,\psi(r(x))\,r(x)^{\frac{3}{2}}\sin\big(\tfrac{3}{2}\theta(x)\big)\,.$$

Here, $\psi\colon [0,\infty) \to \mathbb{R}$ (*cf.* Figure 1(*right*)) is the zero extension of a ninth-order spline with respect to the single element partition of $[0, 0.45]$ which satisfies $\psi(r) > 0$ for all $r \in (0.05, 0.045)$, $\psi(r) = 0$ for all $r \in [0.45,\infty)$, and

$$1 - \psi(0) = \psi(0.45) = \psi^i(0) = \psi^i(0.45) = 0 \quad \text{ for all } i = 1,\dots,4\,.$$

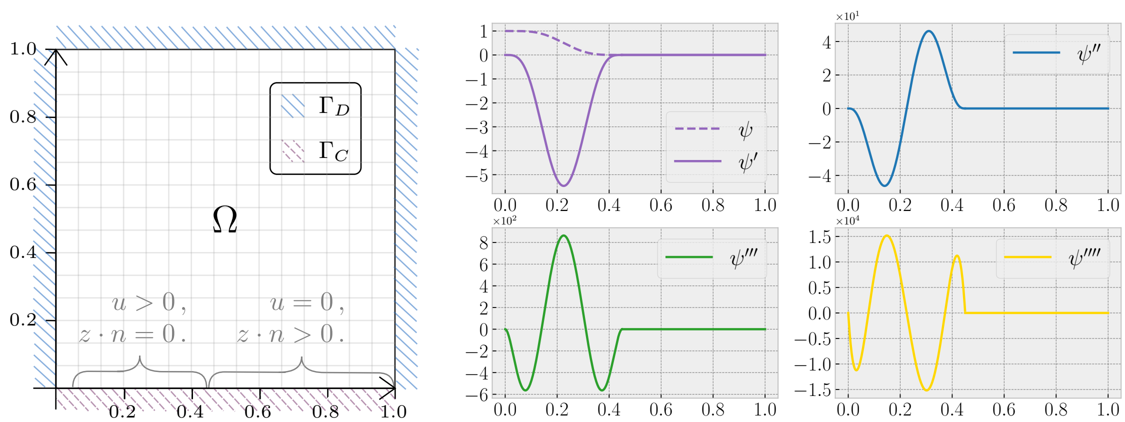

Figure 1: *left*: Ω, Γ_C, Γ_D, $\{u>0\}\cap\Gamma_C = \{z\cdot n = 0\}\cap\Gamma_C$, and $\{u=0\}\cap\Gamma_C = \{z\cdot n>0\}\cap\Gamma_C$; *right*: $\psi,\psi',\psi'',\psi''',\psi''''\colon [0,1]\to\mathbb{R}$.

In this example, we have that $u \in H^2(\Omega)$, so that Theorem 6.6(ii) suggests an experimental convergence rate of about $\mathcal{O}(h_k^2) = \mathcal{O}(N_k)$, where $N_k := \dim(\mathcal{S}^{1,cr}_D(\mathcal{T}_{h_k})) + \dim(\mathcal{L}^0(\mathcal{S}^{\Gamma_C}_{h_k}))$, $k\in\mathbb{N}$, for the discrete primal-dual total errors (*cf.* (6.4)), which are equal to the discrete primal-dual gap estimators (*cf.* (6.1)), *i.e.*, we expect (*cf.* Theorem 6.6(i))

$$\rho^2_{\mathrm{tot},h_k}(\Pi^{cr}_{h_k}u, \Pi^{rt}_{h_k}z) = \rho^2_{\mathrm{gap},h_k}(\Pi^{cr}_{h_k}u, \Pi^{rt}_{h_k}z) = \mathcal{O}(h_k^2) = \mathcal{O}(N_k)\,.$$

An initial triangulation $\mathcal{T}_{h_0}$, $h_0 = \sqrt{2}$, is constructed by subdividing the unit square Ω along its diagonal from $(0,0)^\top$ to $(1,1)^\top$ into two triangles. Refined triangulations $\mathcal{T}_{h_k}$, $k = 1,\dots,7$, where $h_{k+1} = \frac{h_k}{2}$ for all $k = 1,\dots,7$, are obtained by applying the red-refinement routine (*cf.* [44]).

For the resulting series of triangulations $\mathcal{T}_{h_k}$, $k = 1,\dots,7$, we apply the primal-dual active set strategy (*cf.* Algorithm 7.1) to compute the discrete primal solution $u^{cr}_{h_k} \in K^{cr}_{h_k}$, $k = 1,\dots,7$, the discrete Lagrange multiplier $\overline{\lambda}^{cr}_{h_k} \in \mathcal{L}^0(\mathcal{S}^{\Gamma_C}_{h_k})$, $k=1,\dots,7$, and, subsequently, resorting to (5.17), the discrete dual solution $z^{rt}_{h_k} \in K^{rt,*}_{h_k}$, $k = 1,\dots,7$. Then, we compute the error quantities

$$\left.\begin{aligned} e_k^{\mathrm{tot}} &:= \rho^2_{\mathrm{tot},h_k}(\Pi^{cr}_{h_k}u, \Pi^{rt}_{h_k}z)\,,\\ e_k^{\mathrm{gap}} &:= \rho^2_{\mathrm{gap},h_k}(\Pi^{cr}_{h_k}u, \Pi^{rt}_{h_k}z)\,,\\ e_k^{\Delta} &:= |\rho^2_{\mathrm{tot},h_k}(\Pi^{cr}_{h_k}u, \Pi^{rt}_{h_k}z) - \rho^2_{\mathrm{gap},h_k}(\Pi^{cr}_{h_k}u, \Pi^{rt}_{h_k}z)|\,, \end{aligned}\right\} \quad k = 1,\dots,7\,. \tag{7.4}$$

For determining the convergence rates, the experimental order of convergence (EOC), *i.e.*,

$$\texttt{EOC}_k(e_k) := \frac{\log(e_k) - \log(e_{k-1})}{\log(h_k) - \log(h_{k-1})}\,, \quad k = 1,\dots,7\,,$$

where, for every $k = 1,\dots,7$, we denote by e_k, either e_k^{gap}, e_k^{tot}, or e_k^{Δ}, respectively, is recorded.

In Figure 3, we report the expected optimal convergence rate of $\texttt{EOC}_k(e_k^{\mathrm{tot}}) \approx \texttt{EOC}_k(e_k^{\mathrm{gap}}) \approx 2$, $k = 1, \ldots, 7$, *i.e.*, an error decay of order $\mathcal{O}(h_k^2) = \mathcal{O}(N_k)$, $k = 1, \ldots, 7$. In addition, we observe that the *a priori* error identity in Theorem 6.6(i) is asymptotically satisfied. More precisely, for the error between the discrete primal-dual total error (*cf.* (6.4)) and the discrete primal-dual gap estimator (*cf.* (6.1)), we report a convergence rate of about $\texttt{EOC}_k(e_k^{\Delta}) \approx 3.7$, $k = 1, \ldots, 7$, *i.e.*, an error decay of order $\mathcal{O}(h_k^{3.7}) = \mathcal{O}(N_k^{1.85})$, $k = 1, \ldots, 7$, which is the quadrature error involved in the computation of the quasi-interpolants $\Pi_{h_k}^{cr} u \in K_{h_k}^{cr}$, $k = 1, \ldots, 7$, and $\Pi_{h_k}^{rt} z \in K_{h_k}^{rt,*}$, $k = 1, \ldots, 7$.

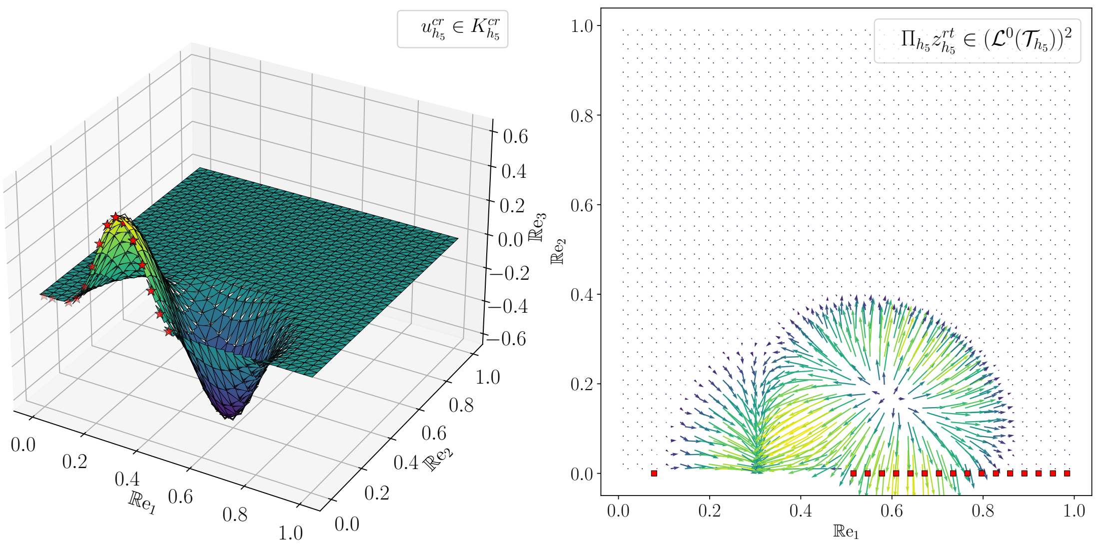

Figure 2: *left*: discrete primal solution $u_{h_5}^{cr} \in K_{h_5}^{cr}$, where red stars mark sides $S \in \mathcal{T}_{h_5}$ with $\pi_{h_5} u_{h_5}^{cr}|_S > 0$; *right*: (local) L^2-projection (onto $(\mathcal{L}^0(\mathcal{T}_{h_5}))^d$) of discrete dual solution $z_{h_5}^{rt} \in K_{h_5}^{rt,*}$, where red squares mark sides $S \in \mathcal{T}_{h_5}$ with $z_{h_5}^{rt} \cdot n|_S > 0$. We find that $z_{h_5}^{rt} \cdot n\, \pi_{h_5} u_{h_5}^{cr} = 0$ a.e. on Γ_C.

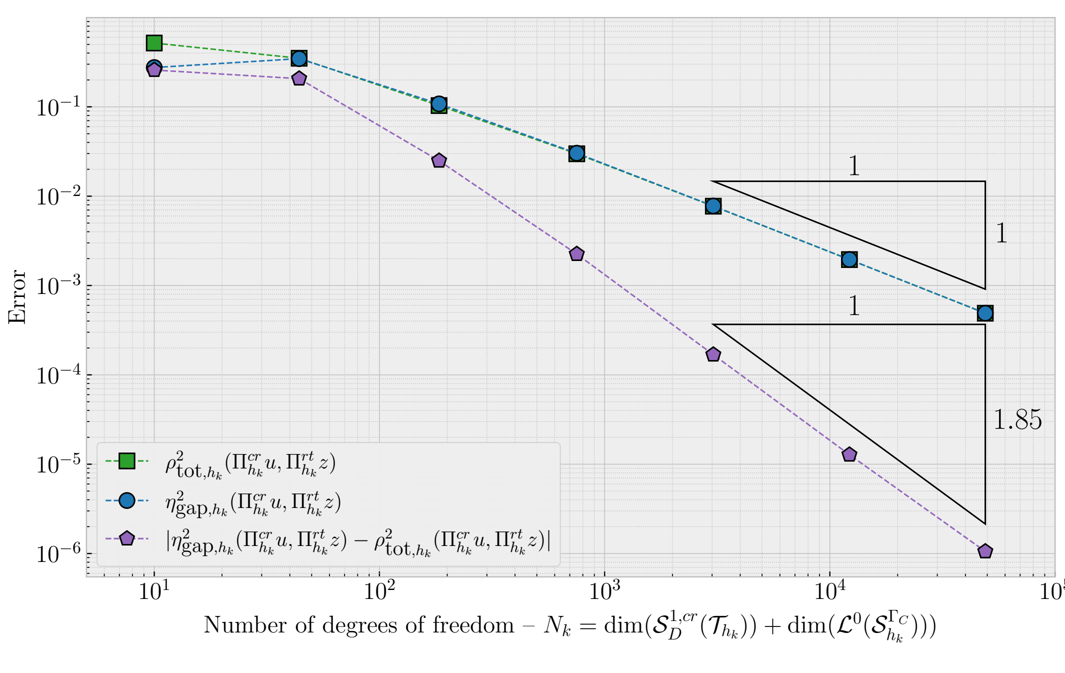

Figure 3: Logarithmic plots of the experimental convergence rates of the error quantities (7.4). We observe the experimental orders of convergence $\texttt{EOC}_k(e_k^{\mathrm{tot}}) \approx \texttt{EOC}_k(e_k^{\mathrm{gap}}) \approx 2$, $k = 1, \ldots, 7$, and $\texttt{EOC}_k(e_k^{\Delta}) \approx 3.7$, $k = 1, \ldots, 7$.

7.3 Numerical experiments concerning a posteriori error analysis

In this subsection, we review the theoretical findings of Section 4.

More precisely, we employ the local refinement indicators $\eta^2_{\mathrm{gap},T}\colon K\times K^*_{\mathrm{tr}_n\in L^2(\Gamma_C)}\to[0,+\infty)$, $T\in\mathcal{T}_h$, where

$$K^*_{\mathrm{tr}_n\in L^2(\Gamma_C)}\coloneqq\left\{y\in K^*\mid y\cdot n\in L^2(\Gamma_C)\right\},$$

induced by the primal-dual gap estimator (*cf.* (4.1)), for every $v\in K$, $y\in K^*_{\mathrm{tr}_n\in L^2(\Gamma_C)}$, and $T\in\mathcal{T}_h$, defined by

$$\eta^2_{\mathrm{gap},T}(v,y)\coloneqq\tfrac{1}{2}\|\nabla v-y\|^2_T+(y\cdot n,v-\chi)_{\partial T\cap\Gamma_C}\,, \tag{7.5}$$

in an adaptive mesh-refinement scheme. The definition of the local refinement indicators (*cf.* (7.5)) is motivated by the representation of the primal-dual gap estimator (*cf.* (4.1)) in Lemma 4.1.

The numerical experiments are based on the following *adaptive algorithm*:

Algorithm 7.3 (AFEM)**.** *Let $\varepsilon_{\mathrm{STOP}}>0$, $\theta\in(0,1)$, and $\mathcal{T}_0$ an initial triangulation of Ω. Then, for every $k\in\mathbb{N}\cup\{0\}$:*

('Solve') *Compute the discrete primal solution $u^{cr}_{h_k}\in K^{cr}_{h_k}$ and the discrete dual solution $z^{rt}_{h_k}\in K^{rt,*}_{h_k}$. Post-process $u^{cr}_{h_k}\in K^{cr}_{h_k}$ and $z^{rt}_{h_k}\in K^{rt,*}_{h_k}$ to obtain a conforming approximations $\overline{u}^{cr}_{h_k}\in K$ and $\overline{z}^{rt}_{h_k}\in K^*$ of the primal solution $u\in K$ and the dual solution $z\in K^*$, respectively;*

('Estimate') *Compute the resulting local refinement primal-dual indicators $\{\eta^2_{\mathrm{gap},T}(\overline{u}^{cr}_{h_k},\overline{z}^{rt}_{h_k})\}_{T\in\mathcal{T}_{h_k}}$. If $\eta^2_{\mathrm{gap}}(\overline{u}^{cr}_{h_k},\overline{z}^{rt}_{h_k})\le\varepsilon_{\mathrm{STOP}}$, then* STOP*; otherwise, continue with step ('Mark');*

('Mark') *Choose a minimal (in terms of cardinality) subset $\mathcal{M}_{h_k}\subseteq\mathcal{T}_{h_k}$ such that*

$$\sum_{T\in\mathcal{M}_{h_k}}\eta^2_{\mathrm{gap},T}(\overline{u}^{cr}_{h_k},\overline{z}^{rt}_{h_k})\ge\theta^2\sum_{T\in\mathcal{T}_{h_k}}\eta^2_{\mathrm{gap},T}(\overline{u}^{cr}_{h_k},\overline{z}^{rt}_{h_k})\,;$$

('Refine') *Perform a conforming refinement of $\mathcal{T}_{h_k}$ to obtain $\mathcal{T}_{h_{k+1}}$ such that each element $T\in\mathcal{M}_{h_k}$ is 'refined' in $\mathcal{T}_{h_{k+1}}$. Increase $k\mapsto k+1$ and continue with step ('Solve').*

Remark 7.4 (Implementation details)**.** *(i) The discrete primal solution $u^{cr}_{h_k}\in K^{cr}_{h_k}$ and the discrete Lagrange multiplier $\overline{\lambda}^{cr}_{h_k}\in\mathcal{L}^0(\mathcal{S}^{\Gamma_C}_{h_k})$ in step ('Solve') are computed using the primal-dual active set strategy (cf. Algorithm 7.1) for the parameter $\alpha=1$;*

(ii) The computation of the discrete dual solution in step ('Solve') is based on the reconstruction formula (5.17)*. Note that $z^{rt}_{h_k}\in K^*$ if and only if $f=f_{h_k}\in\mathcal{L}^0(\mathcal{T}_{h_k})$ and $g=g_{h_k}\in\mathcal{L}^0(\mathcal{S}^{\Gamma_N}_{h_k})$;*

(iii) If $\chi|_{\Gamma_D\cup\Gamma_C}\in\mathcal{L}^1(\mathcal{S}^{\Gamma_D}_{h_k}\cup\mathcal{S}^{\Gamma_C}_{h_k})$, i.e., $u_D\in\mathcal{L}^1(\mathcal{S}^{\Gamma_D}_{h_k})$, then as an admissible approximation $\overline{u}^{cr}_{h_k}\in K$ in step ('Solve'), we employ a contact boundary modified node-averaging quasi-interpolant, i.e.,

$$\overline{u}^{cr}_{h_k}\coloneqq\sum_{\nu\in\mathcal{N}_{h_k}}\{u^{cr}_{h_k}\}_\nu\,\varphi_\nu\in K\,,$$

$$\textit{where }\{u^{cr}_{h_k}\}_\nu\coloneqq\begin{cases}\frac{1}{\mathrm{card}(\mathcal{T}_{h_k}(\nu))}\sum_{T\in\mathcal{T}_{h_k}(\nu)}(u^{cr}_{h_k}|_T)(\nu) & \textit{if }\nu\in\Omega\cup\Gamma_N\,,\\ \max\left\{\chi(\nu),\frac{1}{\mathrm{card}(\mathcal{T}_{h_k}(\nu))}\sum_{T\in\mathcal{T}_{h_k}(\nu)}(u^{cr}_{h_k}|_T)(\nu)\right\} & \textit{if }\nu\in\Gamma_C\,,\\ u_D(\nu) & \textit{if }\nu\in\Gamma_D\,,\end{cases}$$

where $(\varphi_\nu)_{\nu\in\mathcal{N}_{h_k}}\subseteq\mathcal{S}^1(\mathcal{T}_{h_k})$ denotes the shape basis of $\mathcal{S}^1(\mathcal{T}_{h_k})\coloneqq\mathcal{L}^1(\mathcal{T}_{h_k})\cap H^1(\Omega)$ and, for every $\nu\in\mathcal{N}_{h_k}$, we denote by $\mathcal{T}_{h_k}(\nu)\coloneqq\{T\in\mathcal{T}_{h_k}\mid\nu\in T\}$ the set of elements containing ν;

(iv) By the primal-dual gap identity (cf. Theorem 4.5), the stopping criterion in step ('Estimate') guarantees accuracy of $\overline{u}^{cr}_{h_k}\in K$ and $z^{rt}_{h_k}\in K^*$ in terms of the primal-dual total error (cf. (4.4) *with Lemma 6.3), i.e., $\rho^2_{\mathrm{tot}}(\overline{u}^{cr}_k,\overline{z}^{rt}_k)=\eta^2_{\mathrm{gap}}(\overline{u}^{cr}_{h_k},\overline{z}^{rt}_{h_k})\le\varepsilon_{\mathrm{STOP}}$ in step ('Estimate').*

(i) If not otherwise specified, we employ the parameter $\theta=\frac{1}{2}$ in step ('Mark').

(ii) To find the set $\mathcal{M}_{h_k}\subseteq\mathcal{T}_{h_k}$ in step ('Mark'), we resort to the Dörfler marking strategy (cf. [21]).

(iii) The (minimal) conforming refinement of $\mathcal{T}_{h_k}$ with respect to $\mathcal{M}_{h_k}$ in step ('Refine') is obtained by deploying the red-green-blue-refinement algorithm (cf. [13]).

7.3.1 Example with unknown primal and dual solution

In this example, let $\Omega \coloneqq (-1,1)^2$, $\Gamma_C \coloneqq (-1,1)\times\{-1\}$, $\Gamma_D \coloneqq ((-1,1)\times\{1\})\cup(\{1\}\times(0,1))$ (*cf.* Figure 4(*left*)), *i.e.*, $\Gamma_N \coloneqq \partial\Omega\setminus(\Gamma_D\cup\Gamma_C)$, $f=-1\in L^2(\Omega)$, $g=0\in L^2(\Gamma_N)$, and $\chi\in H^1_D(\Omega)$ with $\chi(x)\coloneqq \min\{\frac{1}{2}(|x_1|-\frac{1}{2}),0\}$ for all $x=(x_1,x_2)^\top\in\Gamma_C$. In this case, the primal solution $u\in K$ is not known and since the Dirichlet part Γ_D and the Neumann part Γ_N touch in $(1,0)^\top$ with interior angle π (*cf.* Figure 4(*left*)), it cannot be expected to satisfy $u\in H^2(\Omega)$, so that uniform mesh refinement is expected to yield a reduced error decay rate compared to the quasi-optimal linear error decay rate.

Algorithm 7.3 refines the mesh towards the contact set Γ_C and $(1,0)^\top$ (*cf.* Figure 5), where we expect a singularity. In Figure 4(*right*), one finds that uniform mesh refinement (*i.e.*, $\theta=1$ in Algorithm 7.3) yields the reduced convergence rate $h_k\sim N_k^{-\frac{2}{3}}$, $k=0,\dots,4$, while adaptive mesh refinement (*i.e.*, $\theta=\frac{1}{2}$ in Algorithm 7.3) yields the optimal convergence rate $h_k^2\sim N_k^{-1}$, $k=0,\dots,20$.

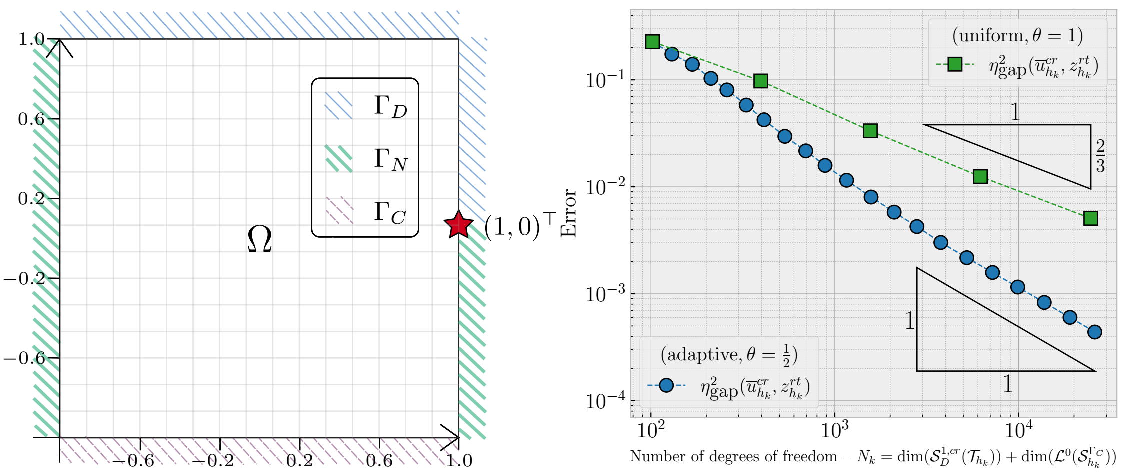

Figure 4: *left*: Ω, Γ_C, Γ_D, Γ_N, and $(1,0)^\top$; *right*: primal-dual gap estimator $\eta^2_{\mathrm{gap}}(\overline{u}^{cr}_{h_k}, z^{rt}_{h_k})$ for $k=0,\dots,20$, when employing adaptive mesh refinement (*i.e.*, $\theta=\frac{1}{2}$ in Algorithm 7.3), and for $k=0,\dots,4$, when employing uniform mesh refinement (*i.e.*, $\theta=1$ in Algorithm 7.3).

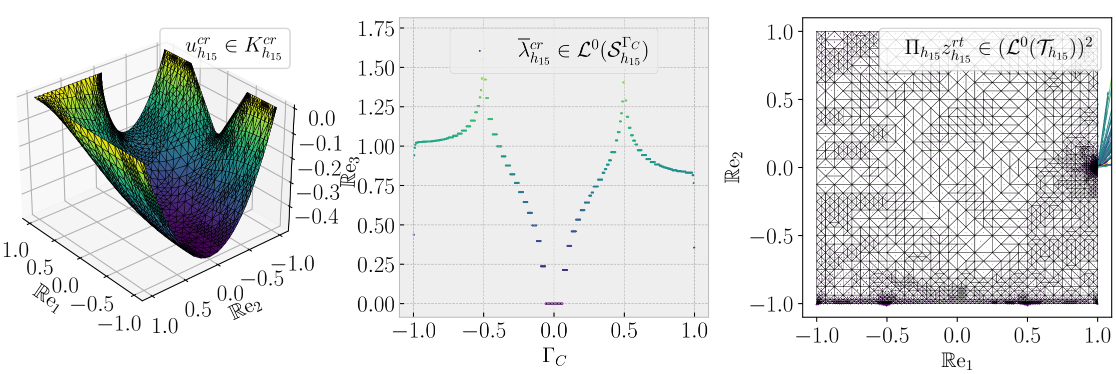

Figure 5: *left*: discrete primal solution $u^{cr}_{h_{15}}\in K^{cr}_{h_{15}}$; MIDDLE: discrete Lagrange multiplier $\overline{\lambda}^{cr}_{h_{15}}\in\mathcal{L}^0(\mathcal{S}^{\Gamma_C}_{h_{15}})$; *right*: (local) L^2-projection of the discrete dual solution $z^{rt}_{h_{15}}\in K^{rt,*}_{h_{15}}$.

A. Appendix

In this appendix, we prove a lifting lemma that for a given element-wise constant vector field, a given element-wise constant function, and a given side-wise constant function defined on Neumann sides, jointly satisfying a compatibility condition, provides a Raviart–Thomas vector field whose (local) L^2-projection coincides with the element-wise constant vector field, whose divergence coincides with the element-wise constant function, and whose normal traces coincide with the side-wise constant function on Neumann sides.

Lemma A.1 (lifting). *Let $\overline{y}_h \in (\mathcal{L}^0(\mathcal{T}_h))^d$, $f_h \in \mathcal{L}^0(\mathcal{T}_h)$, and $g_h \in \mathcal{L}^0(\mathcal{S}_h^{\Gamma_N})$ be such that for every $v_h \in \mathcal{S}^{1,cr}_D(\mathcal{T}_h)$ with $\pi_h v_h = 0$ a.e. on Γ_C, there holds the* compatibility condition

$$(\overline{y}_h, \nabla_h v_h)_\Omega - (f_h, \Pi_h v_h)_\Omega - (g_h, \pi_h v_h)_{\Gamma_N} = 0\,. \tag{A.1}$$

Then, the vector field $y_h \in (\mathcal{L}^1(\mathcal{T}_h))^d$ defined by

$$y_h \coloneqq \overline{y}_h - \frac{f_h}{d}(\mathrm{id}_{\mathbb{R}^d} - \Pi_h \mathrm{id}_{\mathbb{R}^d}) \qquad a.e.\ in\ \Omega\,, \tag{A.2}$$

satisfies $y_h \in \mathcal{RT}^0(\mathcal{T}_h)$ and

$$\Pi_h y_h = \overline{y}_h \qquad a.e.\ in\ \Omega\,, \tag{A.3}$$

$$\operatorname{div} y_h = -f_h \qquad a.e.\ in\ \Omega\,, \tag{A.4}$$

$$y_h \cdot n = g_h \qquad a.e.\ on\ \Gamma_N\,. \tag{A.5}$$

Proof. From the definition (A.2), it follows directly that (A.3) is satisfied. Since, due to $|\Gamma_D| > 0$, $\operatorname{div}\colon \mathcal{RT}^0(\mathcal{T}_h) \to \mathcal{L}^0(\mathcal{T}_h)$ is surjective, there exists $\widehat{y}_h \in \mathcal{RT}^0(\mathcal{T}_h)$ such that $\operatorname{div} \widehat{y}_h = -f_h$ a.e. in Ω. Then, using the discrete integration-by-parts formula (2.11) and (A.1), for every $v_h \in \mathcal{S}^{1,cr}_D(\mathcal{T}_h)$ with $\pi_h v_h = 0$ a.e. on $\Gamma_N \cup \Gamma_C$, we find that

$$\begin{aligned}(\Pi_h \widehat{y}_h, \nabla_h v_h)_\Omega &= -(\operatorname{div} \widehat{y}_h, \Pi_h v_h)_\Omega \\ &= (f_h, \Pi_h v_h)_\Omega \\ &= (\overline{y}_h, \nabla_h v_h)_\Omega\,.\end{aligned} \tag{A.6}$$

Using (A.3) in (A.6), for every $v_h \in \mathcal{S}^{1,cr}_D(\mathcal{T}_h)$ with $\pi_h v_h = 0$ a.e. on $\Gamma_N \cup \Gamma_C$, we arrive at

$$(y_h - \widehat{y}_h, \nabla_h v_h)_\Omega = (\Pi_h y_h - \Pi_h \widehat{y}_h, \nabla_h v_h)_\Omega = 0\,. \tag{A.7}$$

On the other hand, due to $\operatorname{div}(y_h - \widehat{y}_h) = 0$ in T for all $T \in \mathcal{T}_h$, we have that $y_h - \widehat{y}_h \in (\mathcal{L}^0(\mathcal{T}_h))^d$. By (A.7) and the discrete Helmholtz–Weyl decomposition (*cf.* [5, Sec. 2.4]), we conclude that

$$y_h - \widehat{y}_h \in \ker(\operatorname{div}|_{\mathcal{RT}^0(\mathcal{T}_h)})\,,$$

and, thus, $y_h \in \mathcal{RT}^0(\mathcal{T}_h)$ with (A.4). In addition, for every $v_h \in \mathcal{S}^{1,cr}_D(\mathcal{T}_h)$ with $\pi_h v_h = 0$ a.e. on Γ_C, the discrete integration-by-parts formula (2.11) and (A.1) yield that

$$\begin{aligned}(y_h \cdot n, \pi_h v_h)_{\Gamma_N} &= (\Pi_h y_h, \nabla_h v_h)_\Omega + (\operatorname{div} y_h, \Pi_h v_h)_\Omega \\ &= (\overline{y}_h, \nabla_h v_h)_\Omega - (f_h, \Pi_h v_h)_\Omega \\ &= (g_h, \pi_h v_h)_{\Gamma_N}\,.\end{aligned} \tag{A.8}$$

Thus, choosing $v_h = \varphi_S$ for all $S \in \mathcal{S}_h^{\Gamma_N}$ in (A.8) and exploiting that $\pi_h \varphi_S = \chi_S$, for every $S \in \mathcal{S}_h^{\Gamma_N}$, we find that (A.5) is satisfied. ☐

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