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FE–BE COUPLING FOR A TRANSMISSION PROBLEM INVOLVING MICROSTRUCTURE

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Abstract. We analyze a finite element/boundary element procedure for a non-convex contact problem for the double–well potential. After relaxing the associated functional, the degenerate minimization problem is reduced to a boundary/domain variational inequality, a discretized saddle point formulation of which may then be solved numerically. The convergence of the Galerkin approximations to certain macroscopic quantities and a corresponding a posteriori estimate for the approximation error are discussed. Numerical results illustrate the performance of the proposed method.

Keywords. Interface problem; Double–well potential; FE-BE coupling.

1. Introduction

Adaptive finite element / boundary element procedures provide an efficient and extensively investigated tool for the numerical solution of uniformly elliptic transmission or contact problems. However, models of strongly nonlinear materials often lead to nonelliptic partial differential equations, where the standard Hilbert space techniques are no longer appropriate to analyze the numerical approximations by coupled finite and boundary element methods. In a previous work [1] we showed that certain mixed $L^2 - L^p$–Sobolev spaces provide a convenient setting to study contact problems for monotone operators like the p–Laplacian. This article extends the approach to nonconvex functionals, discussing the prototypical model case of a double–well potential in Signorini and transmission contact with the linear Laplace equation. As a proof of principle, it intends to clarify the mathematical basis – including well–posedness, convergence, a priori and a simple a posteriori estimate – of adaptive finite element/ boundary element methods involving a non–strictly monotone operator, by clarifying how the analysis in different function spaces of the interior and the exterior problem can be combined.

In particular, in Lemma 2.1 we show that the solution of the exterior problem is reliably computable with boundary integral methods, even if the solution of the interior problem is not

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unique or only exists as a Young measure. More generally, we obtain the well-posedness of a convexified, but not strictly convex problem with a priori and posteriori error estimates for the error of Galerkin solutions in Theorems 3.1 and 4.1. Our estimates generalize those known for the discretization of the Dirichlet or Neumann problem for the double–well potential to contact problems. They allow adaptive approaches similar to those studied for the nonlinear interior problem. Our methods readily extend to certain systems of equations from nonlinear elasticity, or to frictional contact and more elaborate a posteriori estimates as in [1]. The coupling of finite elements and boundary elements is well-known to provide efficient, rapidly convergent methods, which have been thoroughly investigated for elliptic problems [2, 3, 4].

Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain and $\partial\Omega = \overline{\Gamma_t \cup \Gamma_s}$ a decomposition of its boundary into disjoint open subsets, $\Gamma_t \neq \emptyset$. We consider the problem of minimizing the functional

$$\Psi(u_1,u_2) = \int_\Omega W(\nabla u_1) + \frac{1}{2}\int_{\Omega^c} |\nabla u_2|^2 - \int_\Omega f u_1 - \langle t_0, u_2|_{\partial\Omega}\rangle$$

with nonconvex energy density $W(F) = |F-F_1|^2\ |F-F_2|^2$ $(F_1 \neq F_2 \in \mathbb{R}^n)$ over the closed convex set

$$\{(u_1,u_2) \in W^{1,4}(\Omega)\times W^{1,2}_{loc}(\Omega^c) : (u_1-u_2)|_{\Gamma_t} = u_0,\, (u_1-u_2)|_{\Gamma_s} \leq u_0,\, u_2 \in \mathscr{L}_2\},$$

$$\mathscr{L}_2 = \left\{ v \in W^{1,2}_{loc}(\Omega^c) : \Delta v = 0 \text{ in } W^{-1,2}(\Omega^c),\, v = \left\{ \begin{array}{ll} o(1) & ,n=2 \\ \mathscr{O}(|x|^{2-n}) & ,n>2 \end{array} \right\} \right\}.$$

The data $f \in L^{4/3}(\Omega)$, $t_0 \in W^{-\frac{1}{2},2}(\partial\Omega)$ and $u_0 \in W^{\frac{1}{2},2}(\partial\Omega)$ are taken from the appropriate spaces, and $\langle\cdot,\cdot\rangle$ denotes the duality pairing between $W^{-\frac{1}{2},2}(\partial\Omega)$ and $W^{\frac{1}{2},2}(\partial\Omega)$.

Classical exact minimizers of Ψ satisfy a transmission problem involving the derivative DW of W:

$$\begin{aligned} -\operatorname{div} DW(\nabla u_1) = f \quad \text{in } \Omega, \quad \Delta u_2 &= 0 \quad \text{in } \Omega^c, \\ \nu\cdot DW(\nabla u_1) - \partial_\nu u_2 = t_0 \quad \text{on } \partial\Omega,\, u_1 - u_2 &= u_0 \text{ on } \Gamma_t, \\ u_1-u_2 \leq u_0,\ \nu\cdot DW(\nabla u_1) \leq 0,\ \nu\cdot DW(\nabla u_1)(u_1-u_2-u_0) &= 0 \quad \text{on } \Gamma_s, \\ + \text{ radiation condition for } u_2 &\text{ at } \infty. \end{aligned}$$

Here ν denotes the exterior unit normal vector. Therefore, the minimization problem for Ψ is a variational formulation of a contact problem between the double–well potential W and the Laplace equation, with transmission (Γ_t) and Signorini (Γ_s) contact at the interface.

Nonconvex minimization problems of this type arise naturally when a material in Ω passes the critical point of a phase transition into a finely textured mixture of locally energetically equivalent configurations of lower symmetry, the so–called microstructure, see, e.g., [5]. Lacking convexity in Ω, the existence and uniqueness of minimizers for Ψ is not assured, see [6, 7]. In addition, a direct numerical solution of a non-convex variational problem typically faces the challenge of the finite element approximation of rapid oscillations. In order to overcome this difficulty, we follow the idea of [8], see also [9], to consider a relaxed problem by using the quasi-convex envelope of the non-convex functional. The relaxed problem then admits solutions, which are possibly not unique, and related stresses equal to the stress obtained by solving the original problem in a generalized sense involving Young measures [10]. Beyond the stresses, we show that additional average physical properties of the sequences minimizing Ψ can be computed from the relaxed functional: the displacement in the exterior, the region, where minimizing sequences develop microstructure, or also the gradient of the displacement away from the microstructure. Crucially for the use of boundary elements, the exterior boundary value on the interface is not affected by the presence of microstructure.

The increasingly fine length scale of the microstructure often prevents the direct numerical minimization, and starting with works of Carstensen and Plecháč [8, 11] computational approaches based on *relaxed* formulations have been considered. Relaxation amounts to replacing the nonconvex functional by its quasi–convex envelope, in our setting the degenerate functional

$$\Psi^{**}(u_1,u_2) = \int_\Omega W^{**}(\nabla u_1) + \frac{1}{2}\int_{\Omega^c} |\nabla u_2|^2 - \int_\Omega f u_1 - \langle t_0, u_2|_{\partial\Omega}\rangle.$$

If $A = \frac{1}{2}(F_2 - F_1)$ and $B = \frac{1}{2}(F_1+F_2)$, the convex integrand W^{**} is given by the formula (cf. [8])

$$W^{**}(F) = \left(\max\{0, |F-B|^2 - |A|^2\}\right)^2 + 4|A|^2|F-B|^2 - 4(A(F-B))^2.$$

More generally, we consider a stabilized functional

$$\Phi^{**}(u_1,u_2) = \Psi^{**}(u_1,u_2) + \alpha\int_\Omega (u_1 - \bar{f})^2\,, \qquad (\alpha \geq 0,\ \bar{f}\in L^2(\Omega))\,.$$

For $\alpha > 0$ this functional lifts the potential non-uniqueness of solutions by penalizing deviation from a reference displacement $\bar{f}$. The theory of relaxation for nonconvex integrands shows that the weak limit of any minimizing sequence for $\Phi = \Psi + \alpha\int_\Omega (u_1-\bar{f})^2$ minimizes Φ^{**}. Macroscopic quantities like the stress DW^{**} on Ω defined by this weak limit coincide with the averages such as the average stress $\int DW(u)\,\mathrm{d}\mu(u)$ defined by the Young measure μ associated to the minimizing sequence. To extract the average physical properties of sequences minimizing Φ, it is hence sufficient to understand the minimizers of the degenerately convex functional Φ^{**}. Later work [12] showed how also the microstructure itself could be recovered numerically.

We are thus going to analyze a finite element / boundary element scheme which numerically minimizes Φ^{**} and thereby approximates certain macroscopic quantities independent of the particular minimizer. Our approach is based on previous works by Carstensen / Plecháč [8, 11] and Bartels [12] for double–well potentials with Dirichlet or Neumann boundary conditions and shows how to combine them with techniques developed in [1] for strongly nonlinear interface problems. It is readily modified to include the explicit Young measures in the interior part as in Bartels [12]. Section 2 discusses the relaxed problem and identifies several quantities shared by its minimizers. A priori error estimates for their computation and convergence are established in Section 3. Section 4 contains an a posteriori estimate of residual type, on which an adaptive grid refinement strategy may be based.

For later reference, we recall from [8] the following estimates for the relaxed double–well potential ($E, F \in \mathbb{R}^n$):

$$\max\{C_1|F|^4 - C_2, 0\} \leq W^{**}(F) \leq C_3 + C_4|F|^4, \tag{1.1}$$

$$|DW^{**}(F)| \leq C_5(1+|F|^3), \tag{1.2}$$

$$|DW^{**}(F) - DW^{**}(E)|^2 \leq C_6(1+|F|^2+|E|^2)(DW^{**}(F)-DW^{**}(E))(F-E), \tag{1.3}$$

$$\begin{aligned} 8|A|^2|\mathbb{P}F - \mathbb{P}E|^2 + 2\frac{Q(F)+Q(E)}{|A|}|A(F-E)|^2 + 2(Q(F)-Q(E))^2 \\ \leq (DW^{**}(F)-DW^{**}(E))(F-E), \end{aligned} \tag{1.4}$$

where $Q(F) = \max\{0, |F-B|^2 - |A|^2\}$ and $\mathbb{P}$ is the orthogonal projection onto the subspace of vectors orthogonal to A.

2. Analysis of the Relaxed Problem

We first outline how the minimization problem for Φ^{**} can be reduced to a boundary–domain variational inequality. As it involves the exterior problem, it is not affected by the nonconvex part of the functional. See, e.g., [1] for a more detailed exposition.

Recall the Steklov–Poincaré operator

$$S : W^{\frac{1}{2},2}(\partial\Omega) \to W^{-\frac{1}{2},2}(\partial\Omega),$$

a positive and selfadjoint operator (pseudodifferential of order 1, if $\partial\Omega$ is smooth) with defining property

$$\partial_\nu u_2|_{\partial\Omega} = -S(u_2|_{\partial\Omega})$$

for solutions $u_2 \in \mathscr{L}_2$ of the Laplace equation on Ω^c. The operator S may be expressed in terms of the boundary integral operators V, K, K', W as

$$S = \frac{1}{2}(W + (I-K')V^{-1}(I-K)),$$

where

$$V\phi(x) = 2\int_{\partial\Omega} \phi(x')G(x,x')\, ds_{x'}\,, \qquad K\phi(x) = 2\int_{\partial\Omega} \phi(x')\partial_{\nu_{x'}} G(x,x')\, ds_{x'}\,, \tag{2.1}$$

$$K'\phi(x) = 2\partial_{\nu_x}\int_{\partial\Omega} \phi(x')G(x,x')\, ds_{x'}\,, \qquad W\phi(x) = -2\partial_{\nu_x}\int_{\partial\Omega} \phi(x')\partial_{\nu_{x'}} G(x,x')\, ds_{x'}\,. \tag{2.2}$$

G denotes the fundamental solution of the Laplace equation in $\mathbb{R}^n$.

Let

$$\widetilde{W}^{\frac{1}{2},2}(\Gamma_s) = \{v \in W^{\frac{1}{2},2}(\partial\Omega) : \operatorname{supp} v \subset \bar{\Gamma}_s\}, \quad X = W^{1,4}(\Omega) \times \widetilde{W}^{\frac{1}{2},2}(\Gamma_s).$$

The following affine change of variables

$$(u_1, u_2) \mapsto (u, v) = (u_1 - c, u_0 + u_2|_{\partial\Omega} - u_1|_{\partial\Omega}) \in X$$

will be useful. Note that v is indeed supported in $\overline{\Gamma_s}$: The boundary condition $(u_1 - u_2)|_{\Gamma_t} = u_0$ assures $v|_{\Gamma_t} = 0$. Using S and this change of variables for a suitable $c \in \mathbb{R}$, the exterior part of Φ^{**} is reduced to $\Gamma = \partial\Omega$:

$$\begin{aligned}\Phi^{**}(u_1,u_2) &= \int_\Omega W^{**}(\nabla u) + \alpha\int_\Omega u^2 + \frac{1}{2}\langle S(u|_{\partial\Omega} + v), u|_{\partial\Omega} + v\rangle - \lambda(u,v) + C \\ &\equiv J(u,v) + C.\end{aligned}$$

Here $\alpha \geq 0$,

$$\lambda(u,v) = \langle t_0 + Su_0, u|_{\partial\Omega} + v\rangle + \int_\Omega (f + 2\alpha\bar{f} - 2\alpha c)u$$

and $C = C(u_0, t_0)$ is a constant independent of u, v. Therefore, instead of Φ^{**} one may equivalently minimize J over

$$\mathscr{A} = \{(u,v) \in X : v \geq 0 \text{ and } \langle S(u|_{\partial\Omega} + v - u_0), 1\rangle = 0 \text{ if } n = 2\}. \tag{2.3}$$

Here, the condition $\langle S(u|_{\partial\Omega} + v - u_0), 1\rangle = -\langle \partial_\nu u_2, 1\rangle = 0$ for $n = 2$ assures the existence of a harmonic extension u_2 in Ω^c with $u_2 = o(1)$ as $|x| \to \infty$.

A reformulation as a variational inequality reads as follows: Find $(\hat{u},\hat{v}) \in \mathscr{A}$ such that

$$\int_\Omega DW^{**}(\nabla\hat{u})\nabla(u-\hat{u}) + \langle S(\hat{u}|_{\partial\Omega}+\hat{v}),(u-\hat{u})|_{\partial\Omega}+v-\hat{v}\rangle \qquad (2.4)$$
$$+2\alpha\int_\Omega \hat{u}(u-\hat{u}) \geq \lambda(u-\hat{u},v-\hat{v})$$

for all $(u,v)\in\mathscr{A}$.

Convexity and the closedness of $\mathscr{A}$ assure that the relaxed functional J assumes its minimum. Due to the lack of coercivity, the minimizer may fail to be unique, though certain macroscopic quantities are uniquely determined.

Lemma 2.1. *The set of minimizers is nonempty and bounded in X. The stress $DW^{**}(\hat{u})$, the projected gradient $\mathbb{P}\nabla\hat{u}$, the region of microstructure $\{x\in\Omega : Q(\nabla\hat{u})=0\}$ and the boundary value $\hat{u}|_{\partial\Omega}+\hat{v}$ are independent of the minimizer $(\hat{u},\hat{v})\in\mathscr{A}$ of J (up to sets of measure 0). If $\alpha>0$, $\hat{u}$ is unique and belongs to $L^2(\Omega)$.*

For the proof, we recall the variant

$$\|\hat{u}\|_{W^{1,4}(\Omega)} \lesssim \|\nabla\hat{u}\|_{L^4(\Omega)} + \|\hat{u}\|_{W^{\frac{1}{2},2}(\Gamma_t)} \qquad (2.5)$$

of Friedrichs' inequality from [1].

Proof of Lemma 2.1. By (1.1) and the coercivity of S, we have

$$\begin{aligned}
|J(\hat{u},\hat{v})| \quad \geq \quad & C_1\|\nabla\hat{u}\|^4_{L^4(\Omega)} + \alpha\|\hat{u}\|^2_{L^2(\Omega)} - C_2 \mathrm{vol}\,\Omega + \frac{1}{2}C_S\|\hat{u}|_{\Gamma_s}+v\|^2_{W^{\frac{1}{2},2}(\Gamma_s)} \\
& + \frac{1}{2}C_S\|\hat{u}\|^2_{W^{\frac{1}{2},2}(\Gamma_t)} - \|f+2\alpha\bar{f}-2\alpha c\|_{L^{4/3}(\Omega)}\|\hat{u}\|_{W^{1,4}(\Omega)} \\
& - \|t_0+Su_0\|_{W^{-\frac{1}{2},2}(\partial\Omega)}\|\hat{u}|_{\Gamma_s}+\hat{v}\|_{W^{\frac{1}{2},2}(\Gamma_s)} \\
& - \|t_0+Su_0\|_{W^{-\frac{1}{2},2}(\partial\Omega)}\|\hat{u}\|_{W^{\frac{1}{2},2}(\Gamma_t)}
\end{aligned}$$

for any minimizer $(\hat{u},\hat{v})\in\mathscr{A}$ of J. Consequently,

$$\|\nabla\hat{u}\|^4_{L^4(\Omega)} + \alpha\|\hat{u}\|^2_{L^2(\Omega)} + \|\hat{u}|_{\Gamma_s}+\hat{v}\|^2_{W^{\frac{1}{2},2}(\Gamma_s)} + \|\hat{u}\|^2_{W^{\frac{1}{2},2}(\Gamma_t)} - C\|\hat{u}\|_{W^{1,4}(\Omega)}$$

is bounded for some $C>0$. The inequality (2.5) easily yields the boundedness of $\|(\hat{u},\hat{v})\|_X$.

If $(\hat{u}_1,\hat{v}_1),(\hat{u}_2,\hat{v}_2)\in\mathscr{A}$ are two minimizers, J is constant on $\{(\hat{u}_1,\hat{v}_1)+s(\hat{u}_2-\hat{u}_1,\hat{v}_2-\hat{v}_1) : s\in[0,1]\}$: If not, the restriction of J to this set would have a maximum $> J(\hat{u}_1,\hat{v}_1)=J(\hat{u}_2,\hat{v}_2)$ for some $0<s<1$, contradicting the convexity of J. Therefore

$$\langle J'(\hat{u}_2,\hat{v}_2)-J'(\hat{u}_1,\hat{v}_1),(\hat{u}_2-\hat{u}_1,\hat{v}_2-\hat{v}_1)\rangle = 0,$$

or for our particular J

$$\begin{aligned}
0 \quad = \quad & \int_\Omega (DW^{**}(\nabla\hat{u}_2)-DW^{**}(\nabla\hat{u}_1))\nabla(\hat{u}_2-\hat{u}_1) + 2\alpha\int_\Omega(\hat{u}_2-\hat{u}_1)^2 \\
& + \langle S((\hat{u}_2-\hat{u}_1)|_{\partial\Omega}+\hat{v}_2-\hat{v}_1),(\hat{u}_2-\hat{u}_1)|_{\partial\Omega}+\hat{v}_2-\hat{v}_1\rangle.
\end{aligned}$$

The three terms on the right hand side are non–negative, because S is coercive and W^{**} convex, and hence

$$\hat{u}_1|_{\partial\Omega} + \hat{v}_1 = \hat{u}_2|_{\partial\Omega} + \hat{v}_2 \text{ and } (DW^{**}(\nabla\hat{u}_2) - DW^{**}(\nabla\hat{u}_1))\nabla(\hat{u}_2 - \hat{u}_1) = 0$$

almost everywhere, and hence the exterior boundary values $\hat{u}_1|_{\partial\Omega} + \hat{v}_1 = \hat{u}_2|_{\partial\Omega} + \hat{v}_2$ coincide. If $\alpha > 0$, also $\hat{u}_1 = \hat{u}_2$ almost everywhere, independent of the minimizer. The inequality (1.3),

$$|DW^{**}(\nabla\hat{u}_2) - DW^{**}(\nabla\hat{u}_1)|^2 \lesssim (1 + |\nabla\hat{u}_2|^2 + |\nabla\hat{u}_1|^2)(DW^{**}(\nabla\hat{u}_2) - DW^{**}(\nabla\hat{u}_1))\nabla(\hat{u}_2 - \hat{u}_1),$$

implies $DW^{**}(\nabla\hat{u}_1) = DW^{**}(\nabla\hat{u}_2)$ almost everywhere, hence independent of the minimizer. The assertions about the projected gradients and the region of microstructure are immediate consequences of inequality (1.4),

$$|\mathbb{P}\nabla\hat{u}_2 - \mathbb{P}\nabla\hat{u}_1|^2 + (Q(\nabla\hat{u}_2) - Q(\nabla\hat{u}_1))^2 \lesssim (DW^{**}(\nabla\hat{u}_2) - DW^{**}(\nabla\hat{u}_1))\nabla(\hat{u}_2 - \hat{u}_1).$$

□

In particular, the displacement $\hat{u}_2$ on Ω^c is uniquely determined and may be computed from $\hat{u}|_{\partial\Omega} + \hat{v}$ with the help of layer potentials. Due to the lack of convexity of W, neither $\hat{u}$ nor $\nabla\hat{u}$ needs to be unique if $\alpha = 0$. However, Lemma 2.1 allows to identify subsets of Ω, on which these quantities are well–defined.

Corollary 2.1. *a) Let $\Omega_{t,A}$ be the set of points $x \in \Omega$ for which the component of a hyperplane perpendicular to A through x intersects Γ_t. Then the displacement $u|_{\Omega_{t,A}}$ is independent of the minimizer.*
b) The same holds for the gradient $\nabla\hat{u}$ outside the region of microstructure.

Proof. a) The proof is almost identical to the corresponding proof in [8]. Let $(\hat{u}_1, \hat{v}_1)$, $(\hat{u}_2, \hat{v}_2) \in \mathscr{A}$ be two minimizers, and consider $w = \hat{u}_2 - \hat{u}_1$. Because $\mathbb{P}\nabla\hat{u}_1 = \mathbb{P}\nabla\hat{u}_2$ due to Lemma 2.1, $\mathbb{P}\nabla w = 0$ almost everywhere. By definition, $\mathbb{P}$ is the projection onto the orthogonal complement of A, so that ∇w is parallel to A almost everywhere. It is easy to see that, therefore, w may be modified on a set of measure zero to yield an absolutely continuous function which is locally constant along the hyperplanes perpendicular to A. With $w|_{\Gamma_t}$ being 0 by Lemma 2.1, w also has to vanish on almost every hyperplane hitting Γ_t.
b) is a consequence of $\mathbb{P}\nabla\hat{u}_1 = \mathbb{P}\nabla\hat{u}_2$, $DW^{**}(\nabla\hat{u}_1) = DW^{**}(\nabla\hat{u}_2)$ and (1.4):

$$(Q(\nabla\hat{u}_2) + Q(\nabla\hat{u}_1))|A\nabla(\hat{u}_2 - \hat{u}_1)|^2 \lesssim (DW^{**}(\nabla\hat{u}_2) - DW^{**}(\nabla\hat{u}_1))\nabla(\hat{u}_2 - \hat{u}_1) = 0.$$

Outside the region of microstructure $Q(\nabla\hat{u}_1), Q(\nabla\hat{u}_2) \neq 0$, so that $A\nabla\hat{u}_1 = A\nabla\hat{u}_2$. Together with $\mathbb{P}\nabla\hat{u}_1 = \mathbb{P}\nabla\hat{u}_2$, this implies $\nabla\hat{u}_1 = \nabla\hat{u}_2$. □

3. Discretization and A Priori Estimates

We are now going to analyze which quantities can be computed numerically with a Galerkin method. For simplicity, we restrict to $\Omega \subset \mathbb{R}^2$.

Let $\{\mathscr{T}_h\}_{h\in I}$ be a regular triangulation of $\Omega \subset \mathbb{R}^2$ into disjoint open regular triangles K, so that $\overline{\Omega} = \bigcup_{K\in\mathscr{T}_h} \overline{K}$. Each element has at most one edge on $\partial\Omega$, and the closures of any two of them share at most a single vertex or edge. Let h_K denote the diameter of $K \in \mathscr{T}_h$ and ρ_K the diameter of the largest inscribed ball. We assume that $1 \le \max_{K\in\mathscr{T}_h} \frac{h_K}{\rho_K} \le R$ independent of h and that $h = \max_{K\in\mathscr{T}_h} h_K$. The set of all edges of the triangles in $\mathscr{T}_h$ will be denoted by $\mathscr{E}_h$, and the set of nodes by D. Associated to $\mathscr{T}_h$ is the space $W_h^{1,4}(\Omega) \subset W^{1,4}(\Omega)$ of continuous functions whose restrictions to any $K \in \mathscr{T}_h$ are linear.

The boundary $\partial\Omega$ is triangulated by $\{l \in \mathscr{E}_h : \exists K \in \mathscr{T}_h \text{ such that } l \subset \partial K \cap \partial\Omega\}$. The corresponding space of continuous, piecewise linear functions is denoted by $W_h^{\frac{1}{2},2}(\partial\Omega)$, and $\widetilde{W}_h^{\frac{1}{2},2}(\Gamma_s)$ is the subspace of those supported on Γ_s. Finally, $W_h^{-\frac{1}{2},2}(\partial\Omega) \subset W^{-\frac{1}{2},2}(\partial\Omega)$ consists of piecewise constant functions,

$$\mathscr{A}_h = \mathscr{A} \cap (W_h^{1,4}(\Omega) \times W_h^{\frac{1}{2},2}(\partial\Omega))$$

and $X_h^4 = W_h^{1,4}(\Omega) \times \widetilde{W}_h^{\frac{1}{2},2}(\Gamma_s)$.

We denote by $i_h : W_h^{1,4}(\Omega) \hookrightarrow W^{1,4}(\Omega)$, $j_h : \widetilde{W}_h^{\frac{1}{2},2}(\Gamma_s) \hookrightarrow \widetilde{W}^{\frac{1}{2},2}(\Gamma_s)$ and $k_h : W_h^{-\frac{1}{2},2}(\partial\Omega) \hookrightarrow W^{-\frac{1}{2},2}(\partial\Omega)$ the canonical inclusion maps. A discretization of the Steklov–Poincaré operator is defined as

$$S_h = \frac{1}{2}(W + (I-K')k_h(k_h^* V k_h)^{-1} k_h^*(I-K))$$

from the single resp. double layer potentials V and K and the hypersingular integral operator W of the exterior problem. S_h is well–known [2] to be uniformly coercive for small h in the sense that there exists $h_0 > 0$ and an h–independent $\alpha_S > 0$ such that for all $0 < h < h_0$

$$\langle S_h u_h, u_h\rangle \ge \alpha_S \|u_h\|^2_{W^{\frac{1}{2},2}(\partial\Omega)}.$$

Furthermore, in this case

$$\|(S_h - S)u\|_{W^{-\frac{1}{2},2}(\partial\Omega)} \le C_S \operatorname{dist}_{W^{-\frac{1}{2},2}(\partial\Omega)}(V^{-1}(1-K)u, W_h^{-\frac{1}{2},2}(\partial\Omega)) \tag{3.1}$$

for all $u \in W^{\frac{1}{2},2}(\partial\Omega)$ and all $0 < h < h_0$.

As before, $(\hat{u}, \hat{v})$ denotes a minimizer of J over $\mathscr{A}$, while $(\hat{u}_h, \hat{v}_h)$ minimizes the approximate functional

$$J_h(u_h, v_h) = \int_\Omega W^{**}(\nabla u_h) + \alpha \int_\Omega u_h^2 + \frac{1}{2}\langle S_h(u_h|_{\partial\Omega} + v_h), u_h|_{\partial\Omega} + v_h\rangle - \lambda_h(u_h, v_h),$$

$$\lambda_h(u_h, v_h) = \langle t_0 + S_h u_0, u_h|_{\partial\Omega} + v_h\rangle + \int_\Omega (f + 2\alpha\bar{f} - 2\alpha c)u_h,$$

over $\mathscr{A}_h$.

The equivalent variational inequality reads as follows: Find $(\hat{u}_h, \hat{v}_h) \in \mathscr{A}_h$ such that

$$\int_\Omega DW^{**}(\nabla\hat{u}_h)\nabla(u_h - \hat{u}_h) + \langle S_h(\hat{u}_h|_{\partial\Omega} + \hat{v}_h), (u_h - \hat{u}_h)|_{\partial\Omega} + v_h - \hat{v}_h\rangle \tag{3.2}$$
$$+ 2\alpha \int_\Omega \hat{u}_h(u_h - \hat{u}_h) \ge \lambda_h(u_h - \hat{u}_h, v_h - \hat{v}_h)$$

for all $(u_h, v_h) \in \mathscr{A}_h$.

For simplicity, abbreviate the stress $DW^{**}(\nabla\hat{u})$ by σ and the indicator $Q(\nabla\hat{u})$ for microstructure by ξ. Similarly, write σ_h and ξ_h for the corresponding quantities associated to $\hat{u}_h$. The following a priori estimate holds.

Theorem 3.1. *Let $(\hat{u},\hat{v}) \in \mathscr{A}$ be a solution to the variational inequality (2.4), $(\hat{u}_h,\hat{v}_h) \in \mathscr{A}_h$ a solution to the discretization (3.2). Then the resulting approximations of the stress σ, exterior boundary values $u|_{\partial\Omega}+v$ and the other quantities in Lemma 2.1 converge for $h \to 0$.*
a) There is an h–independent $C = C(\alpha) > 0$ such that

$$\begin{aligned}
&\|\sigma-\sigma_h\|^2_{L^{\frac{4}{3}}(\Omega)} + \alpha\|\hat{u}-\hat{u}_h\|^2_{L^2(\Omega)} + \|(\hat{u}-\hat{u}_h)|_{\partial\Omega} + \hat{v}-\hat{v}_h\|^2_{W^{\frac{1}{2},2}(\partial\Omega)} \\
&\quad + \|\mathbb{P}\nabla\hat{u} - \mathbb{P}\nabla\hat{u}_h\|^2_{L^2(\Omega)} + \|(\xi+\xi_h)^{1/2}A\nabla(\hat{u}-\hat{u}_h)\|^2_{L^2(\Omega)} + \|\xi-\xi_h\|^2_{L^2(\Omega)} \\
&\leq C \inf_{(U_h,V_h)\in\mathscr{A}_h} \left\{\|\hat{u}-U_h\|_{W^{1,4}(\Omega)} + \|(\hat{u}-U_h)|_{\partial\Omega} + \hat{v}-V_h\|_{W^{\frac{1}{2},2}(\partial\Omega)}\right\} \\
&\quad + \operatorname{dist}_{W^{-\frac{1}{2},2}(\partial\Omega)}(V^{-1}(1-K)(\hat{u}+\hat{v}-u_0), W_h^{-\frac{1}{2},2}(\partial\Omega))^2.
\end{aligned}$$

b) For pure transmission conditions, $\Gamma_t = \partial\Omega$, the slightly better estimate

$$\begin{aligned}
&\|\sigma-\sigma_h\|^2_{L^{\frac{4}{3}}(\Omega)} + \alpha\|\hat{u}-\hat{u}_h\|^2_{L^2(\Omega)} + \|\hat{u}-\hat{u}_h\|^2_{W^{\frac{1}{2},2}(\partial\Omega)} + \|\mathbb{P}\nabla\hat{u} - \mathbb{P}\nabla\hat{u}_h\|^2_{L^2(\Omega)} \\
&\quad + \|(\xi+\xi_h)^{1/2}A\nabla(\hat{u}-\hat{u}_h)\|^2_{L^2(\Omega)} + \|\xi-\xi_h\|^2_{L^2(\Omega)} \\
&\leq C \inf_{U_h\in W_h^{1,4}(\Omega)} \left\{\|\nabla\hat{u}-\nabla U_h\|^2_{L^4(\Omega)} + \alpha\|\hat{u}-U_h\|^2_{L^2(\Omega)} + \|\hat{u}-U_h\|^2_{W^{\frac{1}{2},2}(\partial\Omega)}\right\} \\
&\qquad + \operatorname{dist}_{W^{-\frac{1}{2},2}(\partial\Omega)}(V^{-1}(1-K)(\hat{u}-u_0), W_h^{-\frac{1}{2},2}(\partial\Omega))^2
\end{aligned}$$

holds.

Note the squared norms on the right hand side of the estimate in b), as compared to a). This corresponds to the reduced convergence rates, by a factor of 2, which are well-known for the numerical approximation of variational inequalities [1, 13].

Proof. We integrate (1.3) and use Hölder's inequality as well as the uniform bound on the norm of minimizers (the first assertion in Lemma 2.1) to obtain

$$\|\sigma-\sigma_h\|^2_{L^{\frac{4}{3}}(\Omega)} \lesssim \int_\Omega (\sigma-\sigma_h)\nabla(\hat{u}-\hat{u}_h). \tag{3.3}$$

Most of the remaining terms on the left hand side are similarly bounded with the help of (1.4):

$$\begin{aligned}
\|\mathbb{P}\nabla\hat{u} - \mathbb{P}\nabla\hat{u}_h\|^2_{L^2(\Omega)} + \|(\xi+\xi_h)^{1/2}A\nabla(\hat{u}-\hat{u}_h)\|^2_{L^2(\Omega)} + \|\xi-\xi_h\|^2_{L^2(\Omega)}& \\
\lesssim \int_\Omega (\sigma-\sigma_h)\nabla(\hat{u}-\hat{u}_h).&
\end{aligned} \tag{3.4}$$

Adding the inequalities (3.3) and (3.4), as well as $\alpha\|\hat{u}-\hat{u}_h\|^2_{L^2(\Omega)}$,

$$\begin{aligned}
LHS^2 \;&:=\; \|\sigma-\sigma_h\|^2_{L^{\frac{4}{3}}(\Omega)}+\alpha\|\hat{u}-\hat{u}_h\|^2_{L^2(\Omega)} \\
&\quad +\|(\hat{u}-\hat{u}_h)|_{\partial\Omega}+\hat{v}-\hat{v}_h\|^2_{W^{\frac{1}{2},2}(\partial\Omega)}+\|\mathbb{P}\nabla\hat{u}-\mathbb{P}\nabla\hat{u}_h\|^2_{L^2(\Omega)} \\
&\quad +\|(\xi+\xi_h)^{1/2}A\nabla(\hat{u}-\hat{u}_h)\|^2_{L^2(\Omega)}+\|\xi-\xi_h\|^2_{L^2(\Omega)} \\
&\lesssim\; \textstyle\int_\Omega(\sigma-\sigma_h)(\nabla\hat{u}-\nabla\hat{u}_h)+2\alpha\|\hat{u}-\hat{u}_h\|^2_{L^2(\Omega)} \\
&\quad +\langle S((\hat{u}-\hat{u}_h)|_{\partial\Omega}+\hat{v}-\hat{v}_h),(\hat{u}-\hat{u}_h)|_{\partial\Omega}+\hat{v}-\hat{v}_h\rangle \\
&=\; -\int_\Omega\sigma\nabla\hat{u}_h-2\alpha\int_\Omega\hat{u}\hat{u}_h-\langle S((\hat{u}|_{\partial\Omega}+\hat{v}),\hat{u}_h|_{\partial\Omega}+\hat{v}_h)\rangle \\
&\quad -\int_\Omega\sigma_h\nabla\hat{u}-2\alpha\int_\Omega\hat{u}_h\hat{u}-\langle S(\hat{u}_h|_{\partial\Omega}+\hat{v}_h),\hat{u}|_{\partial\Omega}+\hat{v}\rangle \\
&\quad +\int_\Omega\sigma\nabla\hat{u}+2\alpha\int_\Omega\hat{u}^2+\langle S(\hat{u}|_{\partial\Omega}+\hat{v}),\hat{u}|_{\partial\Omega}+\hat{v}\rangle \\
&\quad +\int_\Omega\sigma_h\nabla\hat{u}_h+2\alpha\int_\Omega\hat{u}_h^2+\langle S_h(\hat{u}_h|_{\partial\Omega}+\hat{v}_h),\hat{u}_h|_{\partial\Omega}+\hat{v}_h\rangle \\
&\quad +\langle(S-S_h)(\hat{u}_h|_{\partial\Omega}+\hat{v}_h),\hat{u}_h|_{\partial\Omega}+\hat{v}_h\rangle.
\end{aligned}$$

Let $(U,V)\in\mathscr{A}$, $(U_h,V_h)\in\mathscr{A}_h$. Applying the variational inequality (2.4) and its discrete counterpart (3.2) to the third and fourth lines and rearranging terms leads to

$$\begin{aligned}
LHS^2 \;&\lesssim\; \int_\Omega\sigma\nabla(U-\hat{u}_h)+2\alpha\int_\Omega\hat{u}(U-\hat{u}_h) \\
&\quad +\langle S(\hat{u}|_{\partial\Omega}+\hat{v}),U|_{\partial\Omega}+V-\hat{u}_h|_{\partial\Omega}-\hat{v}_h\rangle \\
&\quad +\int_\Omega\sigma_h\nabla(U_h-\hat{u})+2\alpha\int_\Omega\hat{u}_h(U_h-\hat{u}) \\
&\quad +\langle S(\hat{u}_h|_{\partial\Omega}+\hat{v}_h),U_h|_{\partial\Omega}+V_h-\hat{u}|_{\partial\Omega}-\hat{v}\rangle \\
&\quad +\lambda(\hat{u}-U,\hat{v}-V)+\lambda(\hat{u}_h-U_h,\hat{v}_h-V_h) \\
&\quad +\langle(S-S_h)(\hat{u}_h|_{\partial\Omega}+\hat{v}_h-u_0),(\hat{u}_h-U_h)|_{\partial\Omega}+\hat{v}_h-V_h\rangle
\end{aligned}$$

and then

$$\begin{aligned}
LHS^2 \;&\lesssim\; \int_\Omega\sigma\nabla(U-\hat{u}_h)+2\alpha\int_\Omega\hat{u}(U-\hat{u}_h) \\
&\quad +\langle S(\hat{u}|_{\partial\Omega}+\hat{v}),(U-\hat{u}_h)|_{\partial\Omega}+V-\hat{v}_h\rangle \\
&\quad +\int_\Omega\sigma\nabla(U_h-\hat{u})+2\alpha\int_\Omega\hat{u}(U_h-\hat{u}) \\
&\quad +\langle S(\hat{u}|_{\partial\Omega}+\hat{v}),(U_h-\hat{u})|_{\partial\Omega}+V_h-\hat{v}\rangle \\
&\quad +\int_\Omega(\sigma_h-\sigma)\nabla(U_h-\hat{u})+2\alpha\int_\Omega(\hat{u}_h-\hat{u})(U_h-\hat{u}) \\
&\quad +\langle S((\hat{u}_h-\hat{u})|_{\partial\Omega}+\hat{v}_h-\hat{v}),(U_h-\hat{u})|_{\partial\Omega}+V_h-\hat{v}\rangle \\
&\quad +\lambda(\hat{u}-U,\hat{v}-V)+\lambda(\hat{u}_h-U_h,\hat{v}_h-V_h) \\
&\quad +\langle(S-S_h)(\hat{u}|_{\partial\Omega}+\hat{v}-u_0),(\hat{u}_h-U_h)|_{\partial\Omega}+\hat{v}_h-V_h\rangle \\
&\quad +\langle(S-S_h)((\hat{u}_h-\hat{u})|_{\partial\Omega}+\hat{v}_h-\hat{v}),(\hat{u}_h-U_h)|_{\partial\Omega}+\hat{v}_h-V_h\rangle.
\end{aligned} \tag{3.5}$$

Hölder's inequality tells us that

$$\int_\Omega (\sigma_h - \sigma)\nabla(U_h - \hat{u}) \leq \|\sigma_h - \sigma\|_{L^{\frac{4}{3}}(\Omega)} \|\nabla(U_h - \hat{u})\|_{L^4(\Omega)},$$

and the continuity of S allows to bound

$$\langle S((\hat{u}_h - \hat{u})|_{\partial\Omega} + \hat{v}_h - \hat{v}), (U_h - \hat{u})|_{\partial\Omega} + V_h - \hat{v}\rangle$$

by a multiple of

$$\begin{aligned}
&\|(\hat{u}_h - \hat{u})|_{\partial\Omega} + \hat{v}_h - \hat{v}\|_{W^{\frac{1}{2},2}(\partial\Omega)} \|(U_h - \hat{u})|_{\partial\Omega} + V_h - \hat{v}\|_{W^{\frac{1}{2},2}(\partial\Omega)} \\
&\lesssim \quad \varepsilon \|(\hat{u}_h - \hat{u})|_{\partial\Omega} + \hat{v}_h - \hat{v}\|^2_{W^{\frac{1}{2},2}(\partial\Omega)} + \frac{1}{\varepsilon}\|(U_h - \hat{u})|_{\partial\Omega} + V_h - \hat{v}\|^2_{W^{\frac{1}{2},2}(\partial\Omega)}
\end{aligned}$$

for small $\varepsilon > 0$. Similarly, the last two lines of (3.5) are, up to prefactors, bounded by

$$\begin{aligned}
&\varepsilon \|(\hat{u}_h - \hat{u})|_{\partial\Omega} + \hat{v}_h - \hat{v}\|^2_{W^{\frac{1}{2},2}(\partial\Omega)} + (1 + \frac{1}{\varepsilon})\|(U_h - \hat{u})|_{\partial\Omega} + V_h - \hat{v}\|^2_{W^{\frac{1}{2},2}(\partial\Omega)} \\
&+ \|(S - S_h)(\hat{u}|_{\partial\Omega} + \hat{v} - u_0)\|^2_{W^{-\frac{1}{2},2}(\partial\Omega)}.
\end{aligned}$$

We choose $(U,V) = (\hat{u}_h, \hat{v}_h)$. For $\varepsilon > 0$ sufficiently small, the terms of order ε can be combined with the left hand side to obtain

$$\begin{aligned}
LHS^2 \quad \lesssim \quad & \|\sigma_h - \sigma\|_{L^{\frac{4}{3}}(\Omega)} \|\nabla(U_h - \hat{u})\|_{L^4(\Omega)} + 2\alpha \|\hat{u}_h - \hat{u}\|_{L^2(\Omega)} \|U_h - \hat{u}\|_{L^2(\Omega)} \\
& + \|(U_h - \hat{u})|_{\partial\Omega} + V_h - \hat{v}\|^2_{W^{\frac{1}{2},2}(\partial\Omega)} + \|(S - S_h)(\hat{u}|_{\partial\Omega} + \hat{v} - u_0)\|^2_{W^{\frac{1}{2},2}(\partial\Omega)} \\
& + \int_\Omega \sigma \nabla(U_h - \hat{u}) + 2\alpha \int_\Omega \hat{u}(U_h - \hat{u}) \\
& + \langle S(\hat{u}|_{\partial\Omega} + \hat{v}), (U_h - \hat{u})|_{\partial\Omega} + V_h - \hat{v}\rangle - \lambda(U_h - \hat{u}, V_h - \hat{v}). \qquad (3.6)
\end{aligned}$$

If $\Gamma_t = \partial\Omega$, the variational inequality (2.4) becomes an equality, the sum of the last two lines in (3.6) vanishes and b) follows. In the general case, $\Gamma_t \subsetneq \partial\Omega$, we estimate the last two lines of (3.6) by

$$\begin{aligned}
&\|\sigma\|_{L^{\frac{4}{3}}(\Omega)} \|\nabla(U_h - \hat{u})\|_{L^4(\Omega)} + \|f + 2\alpha\bar{f} - 2\alpha c - 2\alpha\hat{u}\|_{L^{\frac{4}{3}}(\Omega)} \|U_h - \hat{u}\|_{L^4(\Omega)} \\
&\quad + \|S(\hat{u}|_{\partial\Omega} + \hat{v} - u_0) - t_0\|_{W^{-\frac{1}{2},2}(\partial\Omega)} \|(U_h - \hat{u})|_{\partial\Omega} + V_h - \hat{v}\|_{W^{\frac{1}{2},2}(\partial\Omega)},
\end{aligned}$$

recalling that

$$\lambda(U_h - \hat{u}, V_h - \hat{v}) = \langle t_0 + Su_0, (U_h - \hat{u})|_{\partial\Omega} + V_h - \hat{v}\rangle + \int_\Omega (f + 2\alpha\bar{f} - 2\alpha c)(U_h - \hat{u}).$$

This shows the estimate in a).
By Lemma (2.1), the set of minimizers is bounded in X, so that all constants may be chosen independent of $(\hat{u}, \hat{v})$. □

4. Adaptive Grid Refinement

In order to set up an adaptive algorithm, we now establish an a posteriori estimate of residual type. It allows to localize the approximation error and leads to an adaptive mesh refinement strategy. A related and somewhat more involved estimate for the linear Laplace operator with unilateral Signorini contact has been considered in [14].

Let $(\hat{u},\hat{v}) \in \mathscr{A}$, $(\hat{u}_h,\hat{v}_h) \in \mathscr{A}_h$ solutions of the continuous resp. discretized variational inequality. We define a simple approximation $(\pi_h\hat{u},\pi_h\hat{v}) \in \mathscr{A}_h$ of $(\hat{u},\hat{v})$ as follows: $\pi_h\hat{u}$ is going to be the Scott-Zhang interpolant of $\hat{u}$, and $\pi_h\hat{v} = \hat{v}_h$.

The next lemma collects the crucial properties of Scott-Zhang interpolation (see, e.g., [15]).

Lemma 4.1. *Let $K \in \mathscr{T}_h$ and $E \in \mathscr{E}_h$. Then with $\omega_K = \bigcup_{\overline{K'}\cap\overline{K}\neq\emptyset} K'$ and $\omega_E = \bigcup_{\overline{E'}\cap E\neq\emptyset} E'$ we have:*

$$\begin{aligned}\|\hat{u}-\pi_h\hat{u}\|_{L^4(K)} &\lesssim h_K\|\hat{u}\|_{W^{1,4}(\omega_K)}\ ,\\ \|\hat{u}-\pi_h\hat{u}\|_{L^2(E)} &\lesssim h_E^{1/2}\|\hat{u}\|_{W^{\frac{1}{2},2}(\omega_E)}.\end{aligned}$$

We are going to prove the following a posteriori estimate:

Theorem 4.1. *Let $(\hat{u},\hat{v}) \in \mathscr{A}$ be a solution to the variational inequality (2.4), $(\hat{u}_h,\hat{v}_h) \in \mathscr{A}_h$ a solution to the discretization (3.2). Then there holds,*

$$\begin{aligned}&\|\sigma-\sigma_h\|^2_{L^{\frac{4}{3}}(\Omega)} + \alpha\|\hat{u}-\hat{u}_h\|^2_{L^2(\Omega)} + \|(\hat{u}-\hat{u}_h)|_{\partial\Omega}+\hat{v}-\hat{v}_h\|^2_{W^{\frac{1}{2},2}(\partial\Omega)}\\ &+\|\mathbb{P}\nabla\hat{u}-\mathbb{P}\nabla\hat{u}_h\|^2_{L^2(\Omega)} + \|(\xi+\xi_h)^{1/2}A\nabla(\hat{u}-\hat{u}_h)\|^2_{L^2(\Omega)} + \|\xi-\xi_h\|^2_{L^2(\Omega)}\\ &\lesssim \eta_\Omega+\eta_C+\eta_S+\operatorname{dist}_{W^{-\frac{1}{2},2}(\partial\Omega)}(V^{-1}(1-K)(\hat{u}_h|_{\partial\Omega}+\hat{v}_h-u_0),W_h^{-\frac{1}{2},2}(\partial\Omega))^2\ ,\end{aligned}$$

where

$$\eta_\Omega = \left(\sum_K h_K^{4/3}\|f+2\alpha(\bar{f}-c-\hat{u}_h)\|^{4/3}_{L^{4/3}(K)}\right)^{3/4} + \left(\sum_{E\cap\partial\Omega=\emptyset} h_E\|[\nu_E\cdot\sigma_h]\|^2_{L^2(E)}\right)^{1/2},$$

$$\eta_C = \eta_{C,1}+\eta_{C,2} = \sum_{E\subset\Gamma_s}\|(\nu_E\cdot\sigma_h)_+\|_{L^2(E)} + \sum_{E\subset\Gamma_s}\int_E(\nu_E\cdot\sigma_h)_-\ \hat{v}_h,$$

and

$$\eta_S = \left(\sum_{E\subset\partial\Omega} h_E\ \|S_h(\hat{u}_h|_{\partial\Omega}+\hat{v}_h-u_0)+(\nu_{\partial\Omega}\cdot\sigma_h)-t_0\|^2_{L^2(E)}\right)^{1/2}.$$

Here, $(\nu_E\cdot\sigma_h)_+ = \max\{\nu_E\cdot\sigma_h,0\}$ and $(\nu_E\cdot\sigma_h)_- = \min\{\nu_E\cdot\sigma_h,0\}$ denote the positive resp. negative part of $\nu_E\cdot\sigma_h$

Remark 4.1. a) The main point of this estimate is to show that the a posteriori estimates for the contact part [14] and the double–well term [8] are compatible. More sophisticated bounds related to a different choice of π_h generalize to our setting in a similar way. For example, in a related setting [14] use a more considerate (sign–preserving) choice of $\pi_h \hat{v}$ to gain a power of h in $\eta_{C,1}$ at the expense of modifying

$$\eta_{C,2} = \sum_{E \subset \Gamma_s} \int_E (\nu_E \cdot \sigma_h)_- \ \pi_h^1 \hat{v}_h \ .$$

b) As in [1], it is straight forward to introduce an additional variable on the boundary to obtain estimates that do not involve the incomputable difference $S_h - S$.

Proof of Theorem 4.1. As in the proof of Theorem 3.1, we start with the inequality

$$\begin{aligned} LHS^2 := & \|\sigma - \sigma_h\|^2_{L^{\frac{4}{3}}(\Omega)} + \alpha \|\hat{u} - \hat{u}_h\|^2_{L^2(\Omega)} + \|(\hat{u} - \hat{u}_h)|_{\partial\Omega} + \hat{v} - \hat{v}_h\|^2_{W^{\frac{1}{2},2}(\partial\Omega)} \\ & + \|\mathbb{P}\nabla\hat{u} - \mathbb{P}\nabla\hat{u}_h\|^2_{L^2(\Omega)} + \|(\xi + \xi_h)^{1/2} A \nabla(\hat{u} - \hat{u}_h)\|^2_{L^2(\Omega)} + \|\xi - \xi_h\|^2_{L^2(\Omega)} \\ \lesssim & \int_\Omega (\sigma - \sigma_h)\nabla(\hat{u} - \hat{u}_h) + 2\alpha \int_\Omega (\hat{u} - \hat{u}_h)^2 \\ & + \langle S((\hat{u} - \hat{u}_h)|_{\partial\Omega} + \hat{v} - \hat{v}_h), (\hat{u} - \hat{u}_h)|_{\partial\Omega} + \hat{v} - \hat{v}_h \rangle. \end{aligned}$$

Using the variational inequality (2.4) and its discretized variant (3.2) results in

$$\begin{aligned} LHS^2 \ \lesssim \ & \lambda(\hat{u} - \hat{u}_h, \hat{v} - \hat{v}_h) - \int_\Omega \sigma_h \nabla(\hat{u} - \hat{u}_h) - 2\alpha \int_\Omega \hat{u}_h(\hat{u} - \hat{u}_h) \\ & - \langle S(\hat{u}_h|_{\partial\Omega} + \hat{v}_h), (\hat{u} - \hat{u}_h)|_{\partial\Omega} + \hat{v} - \hat{v}_h \rangle \\ = \ & \lambda(\hat{u} - \hat{u}_h, \hat{v} - \hat{v}_h) - \int_\Omega \sigma_h \nabla(\hat{u} - \hat{u}_h) - 2\alpha \int_\Omega \hat{u}_h(\hat{u} - \hat{u}_h) \\ & - \langle S_h(\hat{u}_h|_{\partial\Omega} + \hat{v}_h), (\hat{u} - \hat{u}_h)|_{\partial\Omega} + \hat{v} - \hat{v}_h \rangle \\ & + \langle (S_h - S)(\hat{u}_h|_{\partial\Omega} + \hat{v}_h), (\hat{u} - \hat{u}_h)|_{\partial\Omega} + \hat{v} - \hat{v}_h \rangle \\ \leq \ & \lambda_h(\hat{u} - u_h, \hat{v} - v_h) - \int_\Omega \sigma_h \nabla(\hat{u} - u_h) - 2\alpha \int_\Omega \hat{u}_h(\hat{u} - u_h) \\ & - \langle S_h(\hat{u}_h|_{\partial\Omega} + \hat{v}_h), (\hat{u} - u_h)|_{\partial\Omega} + \hat{v} - v_h \rangle \\ & + \langle (S_h - S)(\hat{u}_h|_{\partial\Omega} + \hat{v}_h - u_0), (\hat{u} - \hat{u}_h)|_{\partial\Omega} + \hat{v} - \hat{v}_h \rangle \ . \end{aligned}$$

Explicitly,

$$\begin{aligned} LHS^2 \ \lesssim \ & \int_\Omega (f + 2\alpha\bar{f} - 2\alpha c - 2\alpha\hat{u}_h)(\hat{u} - u_h) - \sum_{E \cap \partial\Omega = \emptyset} \int_E [\nu_E \cdot \sigma_h](\hat{u} - u_h) \\ & - \langle S_h(\hat{u}_h|_{\partial\Omega} + \hat{v}_h - u_0) + (\nu_{\partial\Omega} \cdot \sigma_h) - t_0, (\hat{u} - u_h)|_{\partial\Omega} + \hat{v} - v_h \rangle \\ & + \int_{\Gamma_s} (\nu_{\partial\Omega} \cdot \sigma_h) \ (\hat{v} - v_h) \\ & + \langle (S_h - S)(\hat{u}_h|_{\partial\Omega} + \hat{v}_h - u_0), (\hat{u} - \hat{u}_h)|_{\partial\Omega} + \hat{v} - \hat{v}_h \rangle \end{aligned}$$

for all $(u_h, v_h) \in \mathscr{A}_h$. Here, ν_E and $\nu_{\partial\Omega}$ denote the outward–pointing unit normal vector to an edge $E \subset \overline{K}$, resp. to $\partial\Omega$, and $[\nu_E \cdot \sigma_h]$ is the jump of the discretized normal stress across E. We have used $\mathrm{div}\sigma_h = 0$ for discretization by piecewise linear functions, as well as that $\hat{v}$ and v_h vanish on Γ_t. According to estimate (3.1) for $S_h - S$ and Young's inequality, the last term can be estimated by

$$\mathrm{dist}_{W^{-\frac{1}{2},2}(\partial\Omega)}(V^{-1}(1-K)(\hat{u}_h|_{\partial\Omega} + \hat{v}_h - u_0), W_h^{-\frac{1}{2},2}(\partial\Omega))^2,$$

which is not explicitly computable.

We are going to choose $(u_h, v_h) = (\pi_h \hat{u}, \pi_h \hat{v})$. Then, the first three terms on the right hand side can be estimated with the help of Lemma 4.1 and Hölder's inequality:

$$\int_\Omega (f + 2\alpha(\bar{f} - c - \hat{u}_h))(\hat{u} - \pi_h \hat{u}) \lesssim \|\hat{u}\|_{W^{1,4}(\Omega)} \left(\sum_K h_K^{4/3} \int_K |f + 2\alpha(\bar{f} - c - \hat{u}_h)|^{4/3}\right)^{3/4},$$

$$\Big|\sum_{E \cap \partial\Omega = \emptyset} \int_E [\nu_E \cdot \sigma_h](\hat{u} - \pi_h \hat{u})\Big| \lesssim \|\hat{u}\|_{W^{\frac{1}{2},2}(\partial\Omega)} \Big(\sum_{E \cap \partial\Omega = \emptyset} h_E \int_E |[\nu_E \cdot \sigma_h]|^2\Big)^{1/2}$$

and

$$\begin{aligned} &|\langle S_h(\hat{u}_h|_{\partial\Omega} + \hat{v}_h - u_0) + (\nu_{\partial\Omega} \cdot \sigma_h) - t_0, (\hat{u} - \pi_h \hat{u})|_{\partial\Omega} + \hat{v} - \pi_h \hat{v}\rangle| \\ &\lesssim (\|\hat{u}\|_{W^{\frac{1}{2},2}(\partial\Omega)} + \|\hat{v}\|_{W^{\frac{1}{2},2}(\partial\Omega)} + \|\hat{v}_h\|_{W^{\frac{1}{2},2}(\partial\Omega)}) \\ &\quad \cdot \|S_h(\hat{u}_h|_{\partial\Omega} + \hat{v}_h - u_0) + (\nu_{\partial\Omega} \cdot \sigma_h) - t_0\|_{W^{-\frac{1}{2},2}(\partial\Omega)}. \end{aligned}$$

The trace theorem shows that $\|\hat{u}\|_{W^{\frac{1}{2},2}(\partial\Omega)}$ is bounded by $\|\hat{u}\|_{W^{1,2}(\Omega)}$, and therefore also by $\|\hat{u}\|_{W^{1,4}(\Omega)}$. Note that the boundedness of the set of minimizers, Lemma 2.1, provides an explicit uniform bound on both $\|\hat{u}, \hat{v}\|_X$ and $\|\hat{u}_h, \hat{v}_h\|_X$, including $\|\hat{u}\|_{W^{1,4}(\Omega)}$. The $W^{-\frac{1}{2},2}(\partial\Omega)$–norm leads to η_S [2].

The remaining term requires a slightly more precise analysis. Decompose

$$(\nu_{\partial\Omega} \cdot \sigma_h) = (\nu_{\partial\Omega} \cdot \sigma_h)_+ - (\nu_{\partial\Omega} \cdot \sigma_h)_-$$

into its positive and negative parts. For a classical exact solution, the Signorini condition requires $(\nu_{\partial\Omega} \cdot \sigma)_+ = 0$, and we estimate the corresponding term as above:

$$\Big|\int_{\Gamma_s} (\nu_{\partial\Omega} \cdot \sigma_h)_+ \, (\hat{v} - \pi_h \hat{v})\Big| \lesssim (\|\hat{v}\|_{W^{\frac{1}{2},2}(\partial\Omega)} + \|\hat{v}_h\|_{W^{\frac{1}{2},2}(\partial\Omega)}) \left(\int_{\Gamma_s} |(\nu_E \cdot \sigma_h)_+|^2\right)^{1/2}.$$

For the negative part, we use that $v_h = \hat{v}_h$ and $\hat{v} \geq 0$ from (2.3):

$$\begin{aligned} -\int_{\Gamma_s} (\nu_{\partial\Omega} \cdot \sigma_h)_- \, (\hat{v} - v_h) &= \sum_{E \subset \Gamma_s} (\nu_E \cdot \sigma_h)_- \int_E (v_h - \hat{v}) \\ &\leq \sum_{E \subset \Gamma_s} (\nu_E \cdot \sigma_h)_- \int_E \hat{v}_h. \end{aligned}$$

The a posteriori estimate follows. □

The a posteriori error estimate in Theorem 4.1 leads to an adaptive mesh refinement procedure as in [1]: Given an initial triangulation $\mathscr{T}_h^{(0)}$, the adaptive algorithm generates a sequence $\mathscr{T}_h^{(\ell)}$ of triangulations based on the error indicator $\eta_\Omega + \eta_C + \eta_S$, a refinement criterion and a refinement rule, by following the established sequence of steps:

$$\text{SOLVE} \rightarrow \text{ESTIMATE} \rightarrow \text{MARK} \rightarrow \text{REFINE}.$$

The efficiency of this approach has been shown in [8] for the double–well problem with Dirichlet boundary conditions. The adaptive algorithm was extended to strongly nonlinear interface problems solved by FE-BE procedures in [1], in the case of p-Laplacian-type operators. The estimate in this paper combines these two approaches, which we expect to be similarly efficient.

5. Numerical Experiments

Let $\Omega=(0,1)^2$, $F_1=(-1,0)$, $F_2=(1,0)$ and

$$f_0(x)=-\frac{3}{128}(x-0.5)^5-\frac{1}{3}(x-0.5)^3\ ,$$

$\bar{f}(x,y):=f_0(x)$. We also define

$$\bar{u}(x,y)=\begin{cases} f_0(x), & \text{for } 0\le x\le 1/2,\\ \frac{1}{24}(x-0.5)^3+x-0.5, & \text{for } 1/2\le x\le 1.\end{cases}$$

In problem (2.4) we set $\Gamma_s=\emptyset$, $f\equiv 0$, $u_0:=\bar{u}|_{\partial\Omega}$, $t_0:=\frac{\partial}{\partial n}\bar{u}$ and $\alpha=1$. A similar example with local boundary conditions has been studied in [8].
We obtain the non-linear problem: Find $\hat{u}\in W^{1,4}(\Omega)$ such that

$$\int_\Omega DW^{**}(\nabla\hat{u})\nabla u+2\int_\Omega \hat{u}u+\langle S(\hat{u}|_{\partial\Omega}),u|_{\partial\Omega}\rangle=\langle t_0+Su_0,u|_{\partial\Omega}\rangle+\int_\Omega fu+2\int_\Omega \bar{f}u \tag{5.1}$$

for all $u\in W^{1,4}(\Omega)$. We know that the solution of (5.1) is the minimizer of

$$J(u)=\int_\Omega W^{**}(\nabla u)+\int_\Omega (u-\bar{f})^2+\frac{1}{2}\langle S(u|_{\partial\Omega}),u|_{\partial\Omega}\rangle-\langle t_0+Su_0,u|_{\partial\Omega}\rangle-\int_\Omega fu, \tag{5.2}$$

which we will use to measure the convergence.

Problem (5.1) can be linearized by the Newton-Algorithm.

Algorithm 5.1 (Newton)**.** (1) Choose $u^{(0)}\in W^{1,4}(\Omega)$.

(2) Find $\delta u\in W^{1,4}(\Omega)$ such that

$$\begin{aligned}&\int_\Omega D^2W^{**}(\nabla u^{(n)})(\nabla\delta u,\nabla u)+2\int_\Omega \delta u\cdot u+\langle S\delta u|_{\partial\Omega},u|_{\partial\Omega}\rangle\\ &=-\int_\Omega DW^{**}(\nabla u^{(n)})\nabla u-2\int_\Omega u^{(n)}u\\ &\quad-\langle S(u^{(n)}|_{\partial\Omega}),u|_{\partial\Omega}\rangle+\langle t_0+Su_0,u|_{\partial\Omega}\rangle+\int_\Omega fu+2\int_\Omega \bar{f}u\end{aligned}$$

for all $u\in W^{1,4}(\Omega)$.

(3) Update

$$u^{(n+1)}=u^{(n)}+\delta u.$$

(4) If $\|\delta u\|_{W^{1,4}(\Omega)}>10^{-8}$ goto 2

Table 1 gives the energy error $(J_h(u_h)-J(u))^{1/2}$ and the numerical convergence rate γ for a sequence of uniform meshes (triangular elements). It_{New} is the number of Newton steps and $\tau(s)$ the total computing time for solving the linear systems iteratively using the CG algorithm. The computations have been done using the software framework *maiprogs* on a Xeon E5-2640 processor, 2.4GHz, 256GByte memory.

In Figure 1, we show the indicator for microstructure $\xi:=Q(\nabla\hat{u})$. Recall from Lemma 2.1 that the region of microstructure is given by $\{x\in\Omega:Q(\nabla\hat{u})=0\}$, so that in this example we have microstructure in the left part of the domain. The approximation to the corresponding solution $\hat{u}$ is displayed in Figure 2. Table 1 illustrates the convergence in the energy J to its

DOF	$J_h(u_h)$	$(J_h(u_h)-J(u))^{1/2}$	γ	It_{New}	$\tau(s)$
25	-1.39482	0.16131	—	8	0.0350359
81	-1.41004	0.10394	-0.373940	10	0.0857504
289	-1.41646	0.06622	-0.354421	12	0.3176073
1089	-1.41924	0.04011	-0.377901	12	1.3824396
4225	-1.42023	0.02479	-0.354911	14	10.198651
16641	-1.42060	0.01555	-0.339924	19	117.28788
66049	-1.42075	0.00976	-0.338222	29	1638.0605
263169	-1.42081	0.00613	-0.336551	42	.2661E+05

TABLE 1. Experimental convergence rates γ in the energy, Newton iteration numbers It_{New} and runtime $\tau(s)$ (uniform mesh)

DOF	$\|u_h\|_{L^2(\Omega)}$	$\left\|\|u_h\|_{L^2(\Omega)}-\|u\|_{L^2(\Omega)}\right\|$	γ
25	0.2794074598	0.00065	—
81	0.2790474065	0.00029	-0.694171
289	0.2788991366	0.00014	-0.576218
1089	0.2787571712	.48E-05	-2.522545
4225	0.2787653556	.34E-05	-0.268460
16641	0.2787609993	.10E-05	-0.882613
66049	0.2787623532	.35E-06	-0.755459
263169	0.2787620217	.22E-07	-2.018029

TABLE 2. Experimental convergence rates γ in $L^2(\Omega)$ (uniform mesh)

extrapolated value -1.420846 as the number of degrees of freedom is increased. The convergence rate is around -0.34 with respect to degrees of freedom, or 0.67 with respect to the mesh size h. From the proof of Theorem 3.1, the difference $J_h(u_h)-J(u)$ controls the error

$$\|\sigma-\sigma_h\|^2_{L^{\frac{4}{3}}(\Omega)}+\alpha\|\hat{u}-\hat{u}_h\|^2_{L^2(\Omega)}+\|(\hat{u}-\hat{u}_h)|_{\partial\Omega}+\hat{v}-\hat{v}_h\|^2_{W^{\frac{1}{2},2}(\partial\Omega)}$$
$$+\|\mathbb{P}\nabla\hat{u}-\mathbb{P}\nabla\hat{u}_h\|^2_{L^2(\Omega)}+\|(\xi+\xi_h)^{1/2}A\nabla(\hat{u}-\hat{u}_h)\|^2_{L^2(\Omega)}+\|\xi-\xi_h\|^2_{L^2(\Omega)}.$$

This assures that σ, $\hat{u}$, $\hat{u}|_{\partial\Omega}+\hat{v}$, $\mathbb{P}\nabla\hat{u}$, $\xi^{1/2}A\nabla\hat{u}$ and ξ converge with (at least) this rate, even though the exact solution is not known.

Table 2 confirms the convergence of the $L^2(\Omega)$-norm of the approximate solutions to the extrapolated value $\|u\|_{L^2(\Omega)}\simeq 0.2787620$. Note that the convergence is faster than for J, but the experimental convergence rate is highly variable.

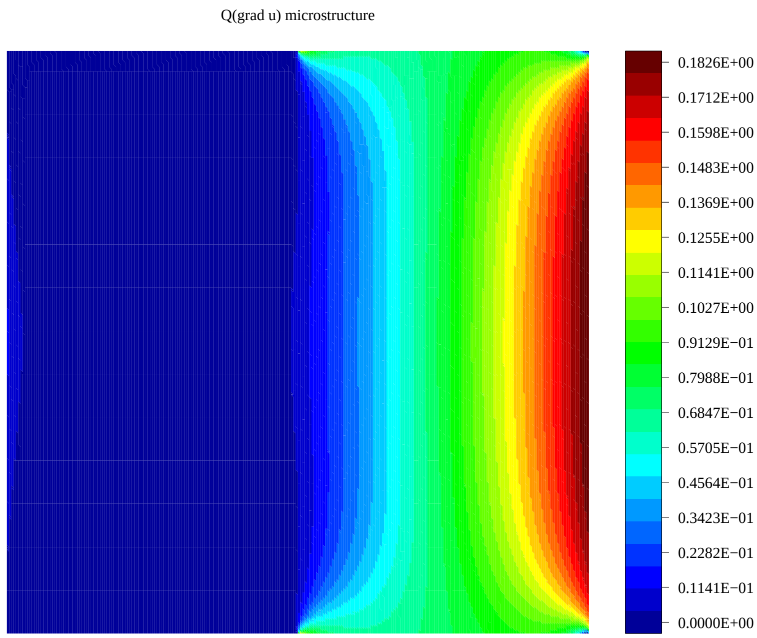

FIGURE 1. Indicator $Q(\nabla \hat{u}_h)$ of microstructure

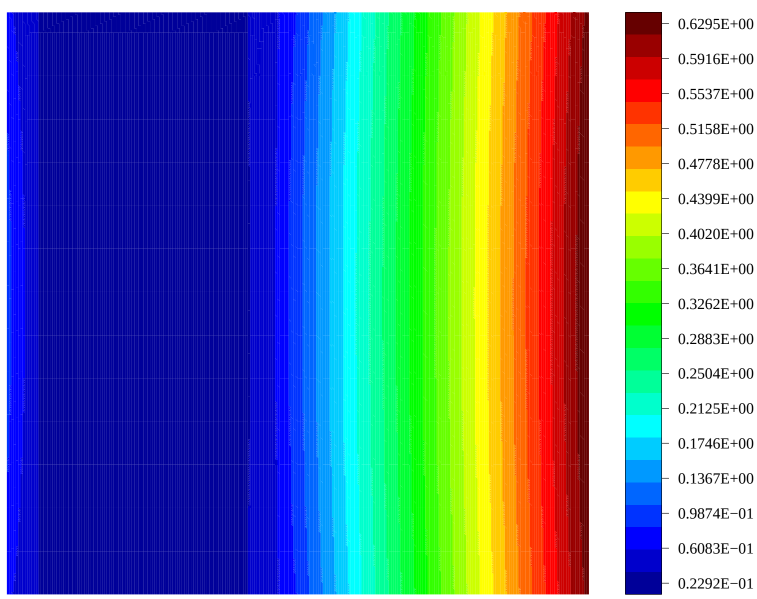

FIGURE 2. Solution $\hat{u}_h$ of relaxed problem

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