THE PRIMAL-DUAL ACTIVE SET METHOD FOR A CRACK PROBLEM WITH NON-PENETRATION

M. Hintermüller[1], V.A. Kovtunenko[1,2] and K. Kunisch[1]

[1] Institute of Mathematics, University of Graz, 8010 Graz, Austria
[2] Lavrent'ev Institute of Hydrodynamics, 630090 Novosibirsk, Russia

Abstract. The Lamé problem in a 2D-domain with a crack under a non-penetration condition is considered as a variational inequality. A primal-dual active set method is proposed as efficient numerical solution technique and compared to a previously employed iterative method for a penalized formulation. Sufficient conditions for monotone convergence of a discretized version of the proposed algorithm are given and numerical experiments are presented.

Mathematics Subject Classification. 49J40, 49Q10, 49Q12, 73M25

Keywords and phrases: crack, non-penetration, variational inequality, active set algorithm, numerical simulation.

1. Introduction

Problems with cracks belong to an area of common interests of mathematicians and mechanical engineers and are of great importance in application in fracture mechanics. From a mathematical point of view one principal difficulty of crack problems lies in the non-regular character of boundaries caused by the presence of a crack within a domain. This fact leads to a reduced regularity of the solution in the domain with a crack.

Classical crack problems are formulated as linear problems. This allows interpenetration between crack faces which is unacceptable from a physical point of view. In the present work we avoid such an inconsistency by the use of a non-penetration condition that is imposed at the crack faces. This results in a model based on a variational inequality that was already suggested in e.g. (Khludnev and Sokolowski 1999), (Khludnev and Kovtunenko 2000). On the discrete level the variational inequality can be reformulated as a classical linear complementarity problem (Cottle, Pang and Stone 1992).

In (Kovtunenko 2003) the numerical realization of the nonlinear crack problem with non-penetration was realized with the help of an iteration method applied to a penalized formulation of the variational inequality. Based on a variational (weak) formulation of the problem and a particular finite element discretization, in the present paper we propose and test a primal-dual active set method which turns out to significantly improve upon the earlier method. In fact, numerical tests show that the primal-dual active set strategy determines the exact solution of the discretized model in only a few iterations. Decreasing the mesh-size results in a moderate increase of the required number of iterations. Our weak formulation takes into account singularities which appear near crack tips. In the examples presented here we consider regular as well as singular solutions when the opening and shifting of the crack faces occur near its tips.

While several authors considered numerical methods for linear crack problems, see (Kuhn 1988), (Hsiao, Schnack and Wendland 1999), (Bach, Nazarov and Wendland 2000) and other works, the literature on numerical methods for nonlinear models is quite scarce (Guz and Zozulya 2001). We tested the method that we propose for the cases of symmetric as well as non-symmetric body forces, and for a wide range of different Lamé constants. For general results on variational inequalities, we refer to (Glowinski 1984), (Glowinski, Lions and Tremolieres 1981), (Hlavaček, Haslinger and Nečas 1984), for example. The primal-dual active set method is closely related to semi-smooth Newton methods, see (Hintermüller, Ito and Kunisch 2002), (Ito and Kunisch 2000), (Ito and Kunisch 2002).

The general idea of *primal-dual* methods is related to the fact that the primal and dual variables are used in an independent fashion. In fact, starting with some primal and dual initial guesses, both variables are updated independently in the course of an iterative process. The advantage of this update procedure can be argued as follows: As noted earlier one way of recasting the variational inequality formulation of the crack problem on the discrete level is given by a transformation into a linear complementarity problem. The latter problem class allows to introduce the active (or coincidence) set at the solution of the problem and its complement, the inactive set. In the context of crack problems, we consider the jump of the displacements across the crack as a condition depending on the primal variable, i.e., the displacement, and we consider the stress at the crack as the dual variable. This duality relation becomes evident by studying the weak formulation of the crack problem (12) (see (21) for the discretized version). The active set at the solution is defined as the set of points where the jump in the displacement is zero across the crack. The inactive set is its complement along the crack. While on the active set the stresses are non-negative, we have that the jump is positive on the inactive set. This behavior again reflects the duality between the primal and dual variables and makes visible that both quantities (primal and dual) influence the location of the active and inactive sets at the solution. The advantage of a primal-dual procedure lies in the fact that, according to the latter observation, it makes use of the primal and the dual variables independently to find the active and inactive sets at the solution. Moreover, in degenerate cases, e.g. where the jump is close to zero on the inactive set, the dual variable (the stresses) can help to accurately locate the active and inactive sets and, hence, the solution. In this situation, it is known that pure primal methods (like e.g. penalty methods; see Section 5) may start to chatter for large penalty parameters. This chattering is typically influenced by the limited accuracy in computer calculations.

The structure of the paper is as follows. In Section 2 we state the 2D-Lamé problem for a domain with a crack and non-penetration condition. This model is discretized in Section 3 and the active set algorithm is proposed. Section 4 is devoted to the convergence analysis of the method. In Section 5 we briefly explain the iterative penalty method which is used for comparison to the proposed method. Finally Section 6 is devoted to a description of the numerical tests.

2. The crack problem with non-penetration

Let $\Omega \subset \mathbf{R}^2$ be a bounded domain with the Lipschitz continuous boundary Γ, which consists of disjoint nonempty sets Γ_D, Γ_N, and Γ_S. We assume that the rectilinear crack Γ_l of length $l > 0$ is located on the x_1-axis and either lies inside the domain Ω or that it meets the boundary with one of its endpoints. In the latter case it is assumed that the angles between Γ and Γ_l are non-zero, and that $\Gamma_N \cap \Gamma_l = \emptyset$. The positive Γ_l^+ and negative Γ_l^- faces of the crack are the limit of points $x = (x_1, x_2) \in \mathbf{R}^2$ with $x_2 > 0$ and $x_2 < 0$ as $x_2 \to 0$, respectively. We consider $\Omega_l = \Omega \setminus \overline{\Gamma}_l$ as the domain with a crack.

As model we employ the plane-stress Lamé equation of an isotropic solid occupying the domain Ω_l in every cross-section $x_3 = const$. Henceforth the standard tensor notation common in solid mechanics and the summation convention for repeated indices $i, j \in \{1, 2\}$ are used.

For the two-component displacement vector $u = (u_1(x), u_2(x))$, with $x \in \mathbf{R}^2$, the symmetric tensor of stresses is given as follows:

$$\sigma_{11}(u) = 2\mu\, u_{1,1} + \lambda \operatorname{div} u, \quad \sigma_{22}(u) = 2\mu\, u_{2,2} + \lambda \operatorname{div} u, \tag{1a}$$

$$\sigma_{12}(u) = \sigma_{21}(u) = \mu(u_{1,2} + u_{2,1}), \quad \operatorname{div} u = u_{1,1} + u_{2,2}, \tag{1b}$$

with the Lamé constants

$$\mu = \frac{E}{2(1+\nu)}, \quad \lambda = \frac{2\nu\mu}{1-2\nu}, \tag{2}$$

where $E > 0$ and $\nu \in (0, 0.5)$. For a given load $g = (g_1, g_2) \in L^2(\Gamma_N)^2$, we first recall the following linear elasticity model consisting of the Lamé equations:

$$-\mu\Delta u_i - (\lambda+\mu)(\operatorname{div} u)_{,i} = 0, \quad i = 1,2, \quad \text{in } \Omega_l, \tag{3}$$

with Dirichlet boundary conditions:

$$u_1 = u_2 = 0 \quad \text{on } \Gamma_D, \tag{4}$$

and Neumann-type boundary conditions:

$$\sigma_{ij}(u)\nu_j = 0, \quad i = 1,2, \quad \text{on } \Gamma_S, \tag{5a}$$

$$\sigma_{ij}(u)\nu_j = g_i, \quad i = 1,2, \quad \text{on } \Gamma_N, \tag{5b}$$

where $\nu = (\nu_1, \nu_2)$ denotes the outward normal vector at Γ.

Following the classical fracture mechanics concept, we have to state the linear boundary conditions of the stress-free crack faces, i.e.

$$\mp\sigma_{12}(u) = \mp\sigma_{22}(u) = 0 \quad \text{on } \Gamma_l^{\pm}. \tag{6}$$

The weak formulation of the linear crack problem (3)–(6) is given by:

$$u \in \widetilde{H}^1(\Omega_l), \quad \int_{\Omega_l} \sigma_{ij}(u) v_{i,j} = \int_{\Gamma_N} g_i v_i \quad \text{for all } v \in \widetilde{H}^1(\Omega_l), \tag{7}$$

where

$$\widetilde{H}^1(\Omega_l) = \{u = (u_1, u_2) \in H^1(\Omega_l)^2 : \quad u_1 = u_2 = 0 \quad \text{on } \Gamma_D\}. \tag{8}$$

This linear model does *not* exclude interpenetration between the crack faces $\Gamma_l^{\pm}$, which is unacceptable from the physical point of view. To correct the model, (6) is replaced by non-penetration conditions between the crack faces, see (Khludnev and Kovtunenko 2000), as follows:

$$\mp\, \sigma_{12}(u) = 0 \quad \text{on } \Gamma_l^{\pm}, \tag{9a}$$

$$[\![\sigma_{22}(u)]\!] = 0,\ \sigma_{22}(u) \le 0,\ [\![u_2]\!] \ge 0,\ \sigma_{22}(u)[\![u_2]\!] = 0 \quad \text{on } \Gamma_l. \tag{9b}$$

Here the doubled brackets $[\![\,\cdot\,]\!]$ designate the jump across the crack Γ_l, i.e. $[\![u_2]\!] = u_2|_{\Gamma_l^+} - u_2|_{\Gamma_l^-}$ and $[\![\sigma_{22}(u)]\!] = \sigma_{22}(u)|_{\Gamma_l^+} - \sigma_{22}(u)|_{\Gamma_l^-}$.
To express the resulting model in a function space formulation we define the convex closed set of admissible displacements with non-penetration by

$$K_l = \{u = (u_1, u_2) \in \widetilde{H}^1(\Omega_l) : \quad [\![u_2]\!] \geq 0 \quad \text{on } \Gamma_l\}. \tag{10}$$

The variational formulation of the nonlinear crack problem (3)–(5), (9) is then given by:

$$u \in K_l, \quad \int\limits_{\Omega_l} \sigma_{ij}(u)(v-u)_{i,j} \geq \int\limits_{\Gamma_N} g_i(v-u)_i \quad \text{for all } v \in K_l. \tag{11}$$

Due to the Korn inequality and the assumption that a Dirichlet condition (4) holds on part of the boundary the quadratic form on the left-hand side of (11) is uniformly positive. Therefore, there exists a unique solution u of the variational inequality (11). We can rewrite (11) also as the following complementarity system where we use $\langle \cdot, \cdot \rangle_{00} = \langle \cdot, \cdot \rangle_{H_{00}^{1/2}(\Gamma_l)^\star, H_{00}^{1/2}(\Gamma_l)}$:

$$u \in K_l, \quad \sigma \in [H_{00}^{1/2}(\Gamma_l)^\star]^2, \tag{12a}$$

$$\int\limits_{\Omega_l} \sigma_{ij}(u) v_{i,j} + \langle \sigma_i, [\![v_i]\!] \rangle_{00} = \int\limits_{\Gamma_N} g_i v_i \quad \text{for all } v \in \widetilde{H}^1(\Omega_l), \tag{12b}$$

$$\sigma_1 = 0, \tag{12c}$$

$$\langle \sigma_2, \xi - [\![u_2]\!] \rangle_{00} \quad \leq 0 \quad \text{for all } \xi \in H_{00}^{1/2}(\Gamma_l),\ \xi \geq 0, \tag{12d}$$

where, with some abuse of notation, the Lagrange multiplier σ denotes the stress at the crack:

$$\sigma = (\sigma_1, \sigma_2) = (\sigma_{12}(u), \sigma_{22}(u)) \in [H_{00}^{1/2}(\Gamma_l)^\star]^2. \tag{13}$$

Here $H_{00}^{1/2}(\Gamma_l)^\star$ is the dual space to the space $H_{00}^{1/2}(\Gamma_l)$ of functions from the $H^{1/2}$-class on the crack Γ_l, which admit the continuation by zero onto any closed curve. Problem (12) gives us a complete system of boundary conditions which are fulfilled at Γ_l for $[\![u_2]\!] \in H_{00}^{1/2}(\Gamma_l)$ and $\sigma_2 \in H_{00}^{1/2}(\Gamma_l)^\star$ in the sense of these dual spaces. If the regularity property $u \in H^2(\Omega_l)^2$ holds, then $\sigma_2 \in H^{1/2}(\Gamma_l)$ and the statements in (9) are satisfied in the almost everywhere sense. For an analysis of variational inequalities of the types (11) and (12) in crack mechanics, see (Khludnev and Kovtunenko 2000).

3. Discretization and primal-dual algorithm

To realize problems (7), respectively (11) or (12), numerically we introduce basis functions $\{e_k\}_{k=1}^N$ in $H^1(\Omega_l)$ with $e_k = 0$ on Γ_D and define

$$H_l^N = \{u = ((U_1)_k e_k, (U_2)_s e_s) : \ U \in \mathbf{R}^{2N}, \ 1 \le k, s \le N\}, \tag{14}$$

$H_l^N \subset \widetilde{H}^1(\Omega_l)$, where $N \in \mathbb{N}$ depends on the mesh-size of discretization and where we used the summation convention over repeated indices $1 \le k, s \le N$. Restriction of (7) onto H_l^N results in the finite-dimensional linear problem:

$$u \in H_l^N, \tag{15a}$$

$$\int\limits_{\Omega_l} \sigma_{ij}(u)(e_k)_{,j} = \int\limits_{\Gamma_N} g_i e_k, \quad i = 1, 2, \quad \text{for } k \in \{1, ..., N\}. \tag{15b}$$

To guarantee existence of a solution to (15) we assume the positive definiteness of the stiffness matrix with respect to the basis $\{e_k\}_{k=1}^N$:

$$\int\limits_{\Omega_l} \sigma_{ij}(u) u_{i,j} > 0 \quad \text{for all } 0 \ne u = ((U_1)_k e_k, (U_2)_s e_s) \in H_l^N. \tag{16}$$

Let us discretize (11), or equivalently (12), next. In order to express the jump condition $[\![u_2]\!] \ge 0$ in an efficient manner in terms of the coefficients U_2 we assume that the basis functions with $[\![e_k]\!] \ne 0$ on Γ_l can be separated uniquely into pairs (e_{k^+}, e_{k^-}), with $(k^+, k^-) \in C$, where

$$C = \{(k^+, k^-) : \, k^\pm \in \{1, ..., N\}, e_{k^+} \ne 0 \text{ on } \Gamma_l^+, e_{k^-} \ne 0 \text{ on } \Gamma_l^-\}, \tag{17}$$

$\operatorname{supp} e_{k^\pm} \cap \Omega^\mp = \emptyset$ with $\Omega^\mp = \{(x_1, x_2) \in \Omega : \mp x_2 > 0\}$, and that the following property which allows to characterize the jump condition in terms of the coefficients is satisfied:

$$U \in \mathbf{R}^N, \ [\![U_k e_k]\!] \ge 0 \iff U_{k^+} - U_{k^-} \ge 0 \quad \text{for all } (k^+, k^-) \in C. \tag{18}$$

By the uniqueness of the pairs (k^+, k^-) we mean that every index k^+ meets only one index k^- and vice versa. Moreover, we assume that $\Gamma_N \cap e_{k^\pm} = \emptyset$ for $(k^+, k^-) \in C$. Subsequently we will frequently use the notation $\{1, \ldots, N\} \setminus C$ indicating indices which are in $\{1, \ldots, N\}$ but do not occur as first or second component index of any pair in C.

A finite element space for which (18) is satisfied is specified in Section 7. Based on (18) the variational inequality (11) can be expressed as

(19a) $\quad u \in H_l^N, \quad (U_2)_{k^+} - (U_2)_{k^-} \geq 0 \quad \text{for } (k^+, k^-) \in C,$

(19b) $$\int\limits_{\Omega_l} \sigma_{ij}(u)(v-u)_{i,j} \geq \int\limits_{\Gamma_N} g_i(v-u)_i$$

for all $v = ((V_1)_k e_k, (V_2)_s e_s) \in H_l^N$ with $(V_2)_{k^+} - (V_2)_{k^-} \geq 0$.

In the finite-dimensional case, the stress σ at the crack Γ_l can be defined by setting

(20a) $$\langle \sigma_i, e_{k^\pm} \rangle = (\Sigma_i)_{k^\pm}, \quad i = 1, 2,$$

(20b) $$(\Sigma_i)_{k^\pm} = \mp \int\limits_{\Omega_l} \sigma_{ij}(u)(e_{k^\pm})_{,j} \quad \text{for } (k^+, k^-) \in C.$$

In view of (18) and (20) problem (12) together with relations (9) restricted onto H_l^N imply that

(21a) $\quad u \in H_l^N,$

(21b) $$\int\limits_{\Omega_l} \sigma_{ij}(u)(e_k)_{,j} = \int\limits_{\Gamma_N} g_i e_k, \quad i = 1, 2, \quad \text{for } k \in \{1, ..., N\} \setminus C,$$

(21c) $$\int\limits_{\Omega_l} \sigma_{ij}(u)(e_{k^\pm})_{,j} \pm (\Sigma_i)_{k^\pm} = 0, \quad i = 1, 2, \quad \text{for } (k^+, k^-) \in C,$$

(21d) $\quad (\Sigma_1)_{k^\pm} = 0, \quad (\Sigma_2)_{k^+} - (\Sigma_2)_{k^-} = 0,$

(21e) $\quad (\Sigma_2)_{k^\pm} \leq 0, \quad (U_2)_{k^+} - (U_2)_{k^-} \geq 0, \quad \text{for } (k^+, k^-) \in C.$

(21f) $\quad ((U_2)_{k^+} - (U_2)_{k^-})(\Sigma_2)_{k^\pm} = 0$

The unique solvability of (19) or equivalently (21) follows from (16).

Let us note that u is the solution of problem (11) if and only if u is the solution to the minimization problem

(22) $$\min_{u \in K_l} \Big\{ \frac{1}{2} \int\limits_{\Omega_l} \sigma_{ij}(u) u_{i,j} - \int\limits_{\Gamma_N} g_i u_i \Big\}.$$

Moreover, σ_2 in (12) can be interpreted as the Lagrange multiplier associated to the constraint $[\![u_2]\!] \geq 0$ on Γ_l. It is instructive to establish the relationship between the discrete stresses on Γ_l and the Lagrange multiplier associated to $[\![U_k e_k]\!] \geq 0$ for the discretized problem. For this purpose we consider (22) with u restricted to $K_l \cap H_l^N$ and realize the inequality constraint by utilizing a Lagrangian multiplier $\Lambda \in \mathbf{R}^{|C|}$, where $|C|$ denotes the cardinality of pairs in C. This leads to the Lagrangian

$$\begin{aligned}\mathcal{L}(u,\Lambda) &= \frac{1}{2}\int_{\Omega_l} \sigma_{ij}(u)u_{i,j} - \int_{\Gamma_N} g_i u_i \\ &\quad + \sum_{(k^+,k^-)\in C} \Lambda_{s((k^+,k^-))}((U_2)_{k^+} - (U_2)_{k^-}),\end{aligned} \tag{23}$$

with $(u,\Lambda) \in H_l^N \times \mathbf{R}^{|C|}$ and $s((k^+,k^-))$ the component of the multiplier vector associated with $(U_2)_{k^+} - (U_2)_{k^-} \geq 0$. Stationarity of the Lagrangian implies system (21), and the relationship between the discrete stress Σ_2 and the Lagrange parameter Λ is given by

$$\Lambda_{s((k^+,k^-))} = (\Sigma_2)_{k^\pm} = \mp \int_{\Omega_l} \sigma_{2j}(u)(e_{k^\pm})_{,j} \quad \text{for } (k^+,k^-) \in C. \tag{24}$$

To prepare the description of the algorithm we introduce the active and inactive sets related to the constraint $[\![u_2]\!] \geq 0$ at the solution $u \in H_l^N$ to (21) with corresponding Lagrange multiplier Σ_2 (cf. (20)). Let $\alpha > 0$ be an arbitrarily fixed constant, and define the subsets of active and inactive indices in C according to

$$A = \{(k^+,k^-) \in C : \quad (U_2)_{k^+} - (U_2)_{k^-} + \alpha(\Sigma_2)_{k^\pm} < 0\}, \tag{25a}$$

$$I = \{(k^+,k^-) \in C : \quad (U_2)_{k^+} - (U_2)_{k^-} + \alpha(\Sigma_2)_{k^\pm} \geq 0\}. \tag{25b}$$

Then the complementarity system (21) can be equivalently expressed by

$$u \in H_l^N, \tag{26a}$$

$$\int_{\Omega_l} \sigma_{ij}(u)(e_k)_{,j} = \int_{\Gamma_N} g_i e_k, \quad i = 1,2, \quad \text{for } k \in \{1,...,N\} \setminus C, \tag{26b}$$

$$\int_{\Omega_l} \sigma_{ij}(u)(e_{k^\pm})_{,j} \pm (\Sigma_i)_{k^\pm} = 0, \quad i = 1,2, \quad \text{for } (k^+,k^-) \in C, \tag{26c}$$

$$(\Sigma_1)_{k^\pm} = 0 \quad \text{for } (k^+,k^-) \in C, \tag{26d}$$

$$(\Sigma_2)_{k^+} - (\Sigma_2)_{k^-} = 0, \quad (\Sigma_2)_{k^\pm} < 0 \quad \text{for } (k^+,k^-) \in A, \tag{26e}$$

$$(U_2)_{k^+} - (U_2)_{k^-} \geq 0, \quad (\Sigma_2)_{k^\pm} = 0 \quad \text{for } (k^+,k^-) \in I. \tag{26f}$$

The primal-dual active set strategy is an iterative algorithm based on (26). Starting from an initialization u^0, Σ^0 the algorithm consists of a prediction step for the active/inactive set structure of C and an equation solving step for a linear auxiliary problem.

Algorithm A (non-symmetric case)

(0) *Choose* u^0, Σ^0*; set* $n = 1$.
(1) *The discrete crack indices* C *are decomposed according to*

$$A_{n-1} = \{(k^+, k^-) \in C : (U_2^{n-1})_{k^+} - (U_2^{n-1})_{k^-} + \alpha(\Sigma_2^{n-1})_{k^\pm} < 0\}, \tag{27}$$

$$I_{n-1} = \{(k^+, k^-) \in C : (U_2^{n-1})_{k^+} - (U_2^{n-1})_{k^-} + \alpha(\Sigma_2^{n-1})_{k^\pm} \geq 0\}. \tag{28}$$

(2) *If* $n \geq 2$ *and* $A_{n-1} = A_{n-2}$ *then STOP; else go to step 3.*
(3) *Solve for* $u^n \in H_l^N$*:*

$$\int_{\Omega_l} \sigma_{ij}(u^n)(e_k)_{,j} = \int_{\Gamma_N} g_i e_k,\ i = 1, 2,\ \textit{for}\ k \in \{1, ..., N\} \setminus C, \tag{29a}$$

$$\int_{\Omega_l} \sigma_{ij}(u^n)(e_{k^\pm})_{,j} \pm (\Sigma_i^n)_{k^\pm} = 0,\ i = 1, 2,\ \textit{for}\ (k^+, k^-) \in C, \tag{29b}$$

$$(\Sigma_1^n)_{k^\pm} = 0 \quad \textit{for}\ (k^+, k^-) \in C, \tag{29c}$$

$$(U_2^n)_{k^+} - (U_2^n)_{k^-} = 0 \quad \textit{for}\ (k^+, k^-) \in A_{n-1} \tag{29d}$$

$$(\Sigma_2^n)_{k^+} - (\Sigma_2^n)_{k^-} = 0 \quad \textit{for}\ (k^+, k^-) \in A_{n-1}, \tag{29e}$$

$$(\Sigma_2^n)_{k^\pm} = 0 \quad \textit{for}\ (k^+, k^-) \in I_{n-1}. \tag{29f}$$

(4) *Set* $n = n + 1$ *and go to step 1.*

For our calculations we used $\Sigma^0 = 0$ and u^0 as the coordinate vector representing the solution to the linear crack problem (15).

Note that system (29) is equivalent to the first order optimality conditions for the strongly convex minimization problem

$$\min_{v \in E_l^N} \left\{ \frac{1}{2} \int_{\Omega_l} \sigma_{ij}(u) u_{i,j} - \int_{\Gamma_N} g_i u_i \right\}, \tag{30}$$

with

$$E_l^N := \{v \in H_l^N : V_{k^+} - V_{k^-} = 0 \text{ for all } (k^+, k^-) \in A_{n-1}\}. \tag{31}$$

Since (30) admits a unique solution, system (29) is uniquely solvable. Numerically, the following technique may be used when solving (30).

One can combine the basis functions across Γ_l according to

$$e_k^{n-1} = \begin{cases} e_{k^+} & \text{in } \Omega_l^+ \\ e_{k^-} & \text{in } \Omega_l^- \end{cases} \quad \text{for } (k^+, k^-) \in A_{n-1} \tag{32}$$

to determine the unknown parameters $(U_2^n)_k = (U_2^n)_{k^+} = (U_2^n)_{k^-}$ and $(\Sigma_2^n)_k = (\Sigma_2^n)_{k^+} = (\Sigma_2^n)_{k^-}$ on the active set A_{n-1}. Hence, whenever the stiffness matrix obtained from this modification is positive definite, then the corresponding modification of (29) with (32) admits a unique solution.

The stopping rule in step 2 of Algorithm A is motivated by the following considerations. For $(k^+, k^-) \in A_{n-2}$ we have $(U_2^{n-1})_{k^+} - (U_2^{n-1})_{k-} = 0$, and for $(k^+, k^-) \in I_{n-2}$ we obtain $(\Sigma_2^{n-1})_{k^\pm} = 0$. Hence, if we assume that $A_{n-1} = A_{n-2}$, then, by $(U_2^{n-1})_{k^+} - (U_2^{n-1})_{k-} = 0$, we infer $(\Sigma_2^{n-1})_{k^\pm} < 0$ for all $(k^+, k^-) \in A_{n-2}$. Analogously, for $(k^+, k^-) \in I_{n-2}$ we obtain $(U_2^{n-1})_{k^+} - (U_2^{n-1})_{k-} \geq 0$. Combining this with the system in step 3 yields that the iterate upon termination of the algorithm satisfies (26), i.e. it is the solution of the discrete crack problem.

These considerations concerning the stopping rule immediately imply that whenever the primal iterates $\{u^n\}$ converge, then–by step 3–$\{\Sigma^n\}$ converge. Moreover, due to the fact that there are only a finite number of pairs of active and inactive sets (A_n, I_n), there exists an iteration $n^* < +\infty$ with $A_{n^*-1} = A_{n^*}$ and u^{n^*}, Σ^{n^*} satisfying the optimality system (26). Hence, the algorithm terminates finitely at the solution of the problem.

Finally, let us comment on the choice of α when determining the active/inactive sets. First note that $\alpha > 0$ is fixed for all iterations. Our convergence result, Theorem 4.2, in the next section contains no restriction on the choice of $\alpha > 0$. Numerically, however, we observe that Algorithm A performs best when α is chosen rather small, i.e. $\alpha \in [10^{-4}, 10^{-2}] \times (\max U^0 / \max \Sigma^0)$.

4. Analysis of the active set method

In Section 6 our numerical results will demonstrate an extremely high efficiency of the proposed method to solve the crack problem with non-penetration condition. In all cases that we tested we obtained convergence in a small number of steps. Nevertheless, as common for active set methods, it is difficult to provide a stringent convergence proof. In (Hintermüller et al. 2002) we related active set methods to semi-smooth Newton methods which in turn allows to argue superlinear convergence if the initialization is sufficiently close to the solution of (26). This result can be applied in the present situation.

Theorem 4.1. *Let* (u, Σ) *denote the solution of* (26). *If* (u^0, Σ^0) *is sufficiently close to* (u, Σ), *then the sequence* $\{(u^n, \Sigma^n)\}$ *generated by Algorithm A converges to* (u, Σ) *at a locally superlinear rate.*

For the proof we refer to (Hintermüller et al. 2002, Theorem 1.2). Here we shall analyze another aspect, too. In the numerical tests we observed that for a wide choice of different initializations the first iteration provides a feasible iterate, and that the iterates remain feasible thereafter. Moreover the convergence is monotone in the sense that $A_0 \supset A_1 \supset \dots \supset A_n = A$ with A the active set defined in (25) corresponding to the solution u of (26). We henceforth aim for providing sufficient conditions which guarantee this monotone behavior.

Let the coordinates of u be ordered such that

$$U = ((U_1)_1, (U_2)_1, (U_1)_2, (U_2)_2, \dots, (U_1)_N, (U_2)_N) \tag{33}$$

and denote by L the $(2N \times 2N)$ system matrix of problem (29), consisting of the following (2×2) submatrices:

$$L_{ks} = \begin{pmatrix} \int\limits_{\Omega_l} (\kappa e_{k,1} e_{s,1} + \mu e_{k,2} e_{s,2}) & \int\limits_{\Omega_l} (\lambda e_{k,2} e_{s,1} + \mu e_{k,1} e_{s,2}) \\ \int\limits_{\Omega_l} (\lambda e_{k,1} e_{s,2} + \mu e_{k,2} e_{s,1}) & \int\limits_{\Omega_l} (\mu e_{k,1} e_{s,1} + \kappa e_{k,2} e_{s,2}) \end{pmatrix} \tag{34}$$

for $k, s = 1, ..., N$, where $\kappa = 2\mu + \lambda$. We split L into block matrices according to basis functions which intersect with the crack (indicated by subscripts B) and the others which do not (with subscripts D), i.e. we introduce:

$$\{(L_{DD})_{ks} = L_{ks} : k, s \in \{1, ..., N\} \setminus C\}, \tag{35a}$$
$$\{(L_{DB})_{ks} = L_{ks} : k \in \{1, ..., N\} \setminus C,\ s = s^{\pm} \text{ for } (s^+, s^-) \in C\}, \tag{35b}$$
$$\{(L_{BD})_{ks} = L_{ks} : k = k^{\pm} \text{ for } (k^+, k^-) \in C,\ s \in \{1, ..., N\} \setminus C\}, \tag{35c}$$
$$\{(L_{BB})_{ks} = L_{ks} : k = k^{\pm},\ s = s^{\pm} \text{ for } (k^+, k^-), (s^+, s^-) \in C\}. \tag{35d}$$

Then equations (29a) and (29b) can be expressed as

$$\begin{pmatrix} L_{DD} & L_{DB} \\ L_{BD} & L_{BB} \end{pmatrix} \begin{pmatrix} U_D^n \\ U_B^n \end{pmatrix} + \begin{pmatrix} 0 \\ S_B^n \end{pmatrix} = \begin{pmatrix} G_D \\ 0 \end{pmatrix} \tag{36}$$

with

$$S_B^n = (S_1^n, S_2^n)_B = \{\pm((\Sigma_1^n)_{k^\pm}, (\Sigma_2^n)_{k^\pm}) \text{ for } (k^+, k^-) \in C\}, \tag{37a}$$

$$G_D = (G_1, G_2)_D, \tag{37b}$$

$$(G_i)_k = \int\limits_{\Gamma_N} g_i e_k, \; i = 1, 2, \text{ for } k \in \{1, \ldots, N\} \setminus C. \tag{37c}$$

Computing the Schur complement for (36) we obtain an equation for variables on the boundary Γ_l only:

$$(L_{BB} - L_{BD} L_{DD}^{-1} L_{DB}) U_B^n + S_B^n = -L_{BD} L_{DD}^{-1} G_D. \tag{38}$$

It consists of $4|C|$ equations.

Let us introduce the notation $dU_B^n = U_B^n - U_B^{n-1}$ and $dS_B^n = S_B^n - S_B^{n-1}$ for the difference of displacements and stresses at iteration levels n and $n-1$. From equation (38) we obtain

$$dU_B^n = -(L_{BB} - L_{BD} L_{DD}^{-1} L_{DB})^{-1} dS_B^n. \tag{39}$$

We recall that $(\Sigma_1^n)_{k^\pm} = (\Sigma_1^{n-1})_{k^\pm} = 0$ for all $(k^+, k^-) \in C$. Therefore, the even equations in system (39) give us $2|C|$ relations between the second components $(dU_2^n)_B$ and $(dS_2^n)_B$. In matrix form this can be expressed as

$$(dU_2^n)_B = -R\,(dS_2^n)_B, \tag{40a}$$

$$R = \{\big((L_{BB} - L_{BD} L_{DD}^{-1} L_{DB})^{-1}\big)_{ks} : \; k, s \text{ are even}\}. \tag{40b}$$

Finally, we split $(dU_2^n)_B = ((dU_2^n)_{B^+}, (dU_2^n)_{B^-})$, where

$$(dU_2^n)_{B^\pm} = \{(U_2^n - U_2^{n-1})_k : \quad k = k^\pm \quad \text{for } (k^+, k^-) \in C\}. \tag{41}$$

The continuity of stresses across the crack implies that $(dS_2^n)_{B^+} = (dS_2^n)_{B^-} = d\Sigma_2^n$, where

$$d\Sigma_2^n = \{(\Sigma_2^n - \Sigma_2^{n-1})_k : \quad k = k^\pm \quad \text{for } (k^+, k^-) \in C\}. \tag{42}$$

Therefore, equation (40) can be rewritten as

$$\begin{pmatrix} (dU_2^n)_{B^+} \\ (dU_2^n)_{B^-} \end{pmatrix} = -\begin{pmatrix} R_{B^+B^+} & R_{B^+B^-} \\ R_{B^-B^+} & R_{B^-B^-} \end{pmatrix} \begin{pmatrix} d\Sigma_2^n \\ -d\Sigma_2^n \end{pmatrix}, \tag{43}$$

and we obtain $|C|$ equations for the jump:

$$[\![dU_2^n]\!] = (dU_2^n)_{B^+} - (dU_2^n)_{B^-} = -M\, d\Sigma_2^n, \tag{44a}$$

$$M = R_{B^+B^+} - R_{B^+B^-} - R_{B^-B^+} + R_{B^-B^-}. \tag{44b}$$

Next the matrix M is split into blocks, which correspond to active A_{n-1} and inactive I_{n-1} sets on the boundary Γ_l as

$$\{(M_{A_{n-1}A_{n-1}})_{ks} = M_{ks} : k = k^{\pm}, s = s^{\pm}, (k^+, k^-), (s^+, s^-) \in A_{n-1}\},$$
$$\{(M_{A_{n-1}I_{n-1}})_{ks} = M_{ks} : k = k^{\pm}, s = s^{\pm}, (k^+, k^-) \in A_{n-1},\ (s^+, s^-) \in I_{n-1}\},$$
$$\{(M_{I_{n-1}A_{n-1}})_{ks} = M_{ks} : k = k^{\pm}, s = s^{\pm}, (k^+, k^-) \in I_{n-1},\ (s^+, s^-) \in A_{n-1}\},$$
$$\{(M_{I_{n-1}I_{n-1}})_{ks} = M_{ks} : k = k^{\pm}, s = s^{\pm}, (k^+, k^-), (s^+, s^-) \in I_{n-1}\}.$$

With this notation equation (44) is equivalent to the following system:

$$\begin{pmatrix} [\![dU_2^n]\!]_{A_{n-1}} \\ [\![dU_2^n]\!]_{I_{n-1}} \end{pmatrix} = -\begin{pmatrix} M_{A_{n-1}A_{n-1}} & M_{A_{n-1}I_{n-1}} \\ M_{I_{n-1}A_{n-1}} & M_{I_{n-1}I_{n-1}} \end{pmatrix} \begin{pmatrix} (d\Sigma_2^n)_{A_{n-1}} \\ (d\Sigma_2^n)_{I_{n-1}} \end{pmatrix}, \tag{45}$$

which can be expressed as

$$(d\Sigma_2^n)_{A_{n-1}} = M^{-1}_{A_{n-1}A_{n-1}} [\![dU_2^n]\!]_{A_{n-1}} - M^{-1}_{A_{n-1}A_{n-1}} M_{A_{n-1}I_{n-1}} (d\Sigma_2^n)_{I_{n-1}} \tag{46}$$

and

$$[\![dU_2^n]\!]_{I_{n-1}} = M_1^{n-1} [\![dU_2^n]\!]_{A_{n-1}} - M_2^{n-1} (d\Sigma_2^n)_{I_{n-1}}, \tag{47}$$

where

$$M_1^{n-1} = M_{I_{n-1}A_{n-1}} M^{-1}_{A_{n-1}A_{n-1}}, \tag{48}$$

$$M_2^{n-1} = M_{I_{n-1}I_{n-1}} - M_{I_{n-1}A_{n-1}} M^{-1}_{A_{n-1}A_{n-1}} M_{A_{n-1}I_{n-1}}. \tag{49}$$

Assumption A. *The elements of the Schur complements M_2^{n-1} are nonnegative for the partitioning of Γ_l into the active A_{n-1} and inactive I_{n-1} sets for every iteration n.*

We call the solution u^n of problem (29) feasible if $(U_2^n)_{k^+} - (U_2^n)_{k^-} \geq 0$ for all $(k^+, k^-) \in C$.

Theorem 4.2. *If Assumption A holds and the active set algorithm determines a feasible solution u^{n-1} at some iteration $n-1$, then all subsequent iterations are feasible and the whole sequence converges monotonically to the solution of (26) in a finite number of steps.*

Admittedly, these assumptions are restrictive. However, let us mention that the nonnegativity of M_2^{n-1} is obtained for e.g. the Shortly-Weller discretization for rather general geometries. We observed numerically that our assumptions are satisfied and they describe the behavior of the algorithm in practice.

Proof. Assume that u^{n-1} is feasible, i.e. $(U_2^{n-1})_{k^+} - (U_2^{n-1})_{k^-} \geq 0$ for all $(k^+, k^-) \in C$. Then from the definition of active and inactive sets we find that

$$A_{n-1} = \{(U_2^{n-1})_{k^+} - (U_2^{n-1})_{k^-} = 0,\ (\Sigma_2^{n-1})_{k^+} - (\Sigma_2^{n-1})_{k^-} = 0,\ (\Sigma_2^{n-1})_{k^\pm} < 0\},$$

$$I_{n-1} = \{(U_2^{n-1})_{k^+} - (U_2^{n-1})_{k^-} \geq 0,\ (\Sigma_2^{n-1})_{k^+} - (\Sigma_2^{n-1})_{k^-} = 0,\ (\Sigma_2^{n-1})_{k^\pm} \geq 0\}.$$

For the solution u^n of (29) we have

$$(U_2^n)_{k^+} - (U_2^n)_{k^-} = 0 \quad \text{for } (k^+, k^-) \in A_{n-1},$$

$$(\Sigma_2^n)_{k^\pm} = 0 \quad \text{for } (k^+, k^-) \in I_{n-1}.$$

Therefore, $[\![dU_2^n]\!]_{A_{n-1}} = 0$, $(d\Sigma_2^n)_{I_{n-1}} \leq 0$. From Assumption A and (47) we conclude $[\![dU_2^n]\!]_{I_{n-1}} \geq 0$. In view of $[\![U_2^{n-1}]\!]_{I_{n-1}} \geq 0$ we have $[\![U_2^n]\!]_{I_{n-1}} \geq 0$, and hence u^n and all further iterates are feasible. Monotonicity now easily follows:

$$A_n = \{(U_2^n)_{k^+} - (U_2^n)_{k^-} = 0,\ (\Sigma_2^{n-1})_{k^+} - (\Sigma_2^{n-1})_{k^-} = 0,\ (\Sigma_2^n)_{k^\pm} < 0\}$$

$$\subseteq A_{n-1},$$

$$I_n = \{(U_2^n)_{k^+} - (U_2^n)_{k^-} = 0,\ (\Sigma_2^{n-1})_{k^+} - (\Sigma_2^{n-1})_{k^-} = 0,\ (\Sigma_2^n)_{k^\pm} \geq 0\}$$

$$\cup \{(U_2^n)_{k^+} - (U_2^n)_{k^-} \geq 0,\ (\Sigma_2^n)_{k^\pm} = 0\}\} \supseteq I_{n-1}.$$

Convergence in a finite number of iterations is a consequence of set-theoretic monotonicity of the active sets and finite-dimensionality of H_l^N. This completes the proof. □

An analogous result holds true in the case of symmetric crack problems. By exploiting the symmetry the determination of A_{n-1} and I_{n-1} in every iteration of Algorithm A can be simplified. In Appendix A we provide a brief discussion of the symmetric case and introduce the primal-dual active set method for the symmetric crack problem. The resulting algorithm is analogous to Algorithm A.

We end this section by briefly addressing the differences between Algorithm A, resp. its symmetric analogue in Appendix A, and the complementarity pivoting method of Lemke. The latter method is similar to the simplex algorithm well-known from linear programming and works with primal and dual variables. A good account for Lemke's method can be found in (Cottle, Pang and Stone 1992). It is well-established as a direct solution method for contact problems; see e.g. (Klarbring 1987) and (Raous, Chabrand, and Lebon 1988). It essentially operates on the Schur complement formulation (38). While Lemke's method can be carried over to the symmetric crack problem in a straight forward manner, one has to be careful in the non-symmetric case. In the latter situation we do not have inequality constraints on the displacement U_2 directly rather on the jump across the crack. Typical convergence assertions for Lemke's method state that, under suitable assumptions (like non-degeneracy), the method successfully terminates after a finite number of steps (Cottle, Pang and Stone 1992, Section 4.4). This iteration number depends on the number of constrained unknowns. However, this convergence assertion includes no rate of convergence result as it is the case with our method. Further it is known that for large problems Lemke's method requires a large number of iterations. This can be attributed to the fact that a typical cycle of Lemke's method activates and inactivates one component of the vectors of primal and dual unknowns. Our active set method on the other hand has the ability to activate and inactivate whole sets of unknowns from one iteration to the next. This behavior is responsible for the rather small number of iterations required by our primal-dual active set method for finding the exact solution of the discretized crack problem.

5. Approximations by the penalty method

In the numerical section we compare the primal-dual active set algorithm to a well-known iteration method based on a penalty formulation. To recall this method consider for $\delta > 0$ the penalty equations

$$\int_{\Omega_l} \sigma_{ij}(u^\delta) v_{i,j} - \frac{1}{\delta} \int_{\Gamma_l} [\![u_2^\delta]\!]^- [\![v_2]\!] = \int_{\Gamma_N} g_i v_i \quad \text{for all } v \in \widetilde{H}^1(\Omega_l). \tag{50}$$

Here $[\![\cdot]\!]^-$ means the negative part of the value, i.e. $[\![u_2^\delta]\!]^- = \max(0, -[\![u_2^\delta]\!])$. The solutions $u^\delta \in \widetilde{H}^1(\Omega_l)$ of (50) converge to the solution u of problem (11) in the H^1-norm as $\delta \to 0$ (Glowinski et al. 1981). Following (Khludnev and Kovtunenko 2000), (Kovtunenko 2003), we approximate equation (50) by the iteration penalty (IP) scheme:

$$\int_{\Omega_l} \sigma_{ij}(u^n) v_{i,j} + \frac{1}{\delta} \int_{\Gamma_l} [\![u_2^n - u_2^{n-1}]\!] [\![v_2]\!] = \int_{\Gamma_N} g_i v_i + \frac{1}{\delta} \int_{\Gamma_l} [\![u_2^{n-1}]\!]^- [\![v_2]\!]. \tag{51}$$

Convergence of the iterates u^n to u^δ in the H^1-norm was established in (Kovtunenko 1997).

To relate the penalized problem (50) to the active set method note that its solutions u^δ satisfy

$$\sigma_2^\delta = \sigma_{22}(u^\delta) = -\frac{1}{\delta}[\![u_2^\delta]\!]^-. \tag{52}$$

Referring to (25) the active set should be defined as the sub-set of Γ_l when $[\![u_2^\delta]\!] + \alpha\sigma_2^\delta < 0$. Utilizing (52) the active and inactive sets for the penalty formulation can therefore be defined according to

$$A^\delta = \{[\![u_2^\delta]\!] < 0 \text{ on } \Gamma_l\}, \quad I^\delta = \{[\![u_2^\delta]\!] \geq 0 \text{ on } \Gamma_l\}, \tag{53}$$

which implies the relation $-[\![u_2^\delta]\!]^- = \chi(A^\delta)[\![u_2^\delta]\!]$ for the indicator function χ of the active set A^δ.

6. Numerical examples

We commence with a symmetric example and choose $\Omega \subset \mathbf{R}^2$ as the unit square,

$$\Omega = \{x = (x_1, x_2) \in \mathbf{R}^2,\ 0 < x_1 < 1,\ |x_2| < 0.5\}, \tag{54}$$

and the axis of symmetry will be the interface

$$\Sigma = \{0 < x_1 < 1,\ x_2 = 0\}. \tag{55}$$

The crack Γ_l is a part of the interface Σ i.e.

$$\Gamma_l = \{0 < x_1 < l,\ x_2 = 0\}, \quad 0 < l < 1, \tag{56}$$

and the domain with crack is $\Omega_l = \Omega \setminus \overline{\Gamma}_l$. The boundary of the domain Ω_l is assumed to consist of the following symmetric parts:

$$\Gamma_D = \Gamma_D^+ \cup \Gamma_D^-, \tag{57a}$$

$$\Gamma_D^\pm = \{x_1 = 0, 0.45 < \pm x_2 < 0.5\} \cup \{0 \leq x_1 < 0.05, x_2 = \pm 0.5\} \tag{57b}$$

under the Dirichlet boundary condition,

$$\Gamma_S = \Gamma_{S1}^+ \cup \Gamma_{S1}^- \cup \Gamma_{S2}^+ \cup \Gamma_{S2}^-, \tag{58a}$$

$$\Gamma_{S1}^\pm = \{x_1 = 0, 0 < \pm x_2 < 0.45\}, \tag{58b}$$

$$\Gamma_{S2}^\pm = \{0.05 < x_1 < 1, x_2 = \pm 0.5\} \tag{58c}$$

under the homogeneous Neumann-type boundary condition,

$$\Gamma_N = \{x_1 = 1,\ |x_2| < 0.5\} \tag{59}$$

under the loading by traction forces, and the crack faces

$$\Gamma_l^\pm = \{0 < x_1 < l,\ x_2 = \pm 0\} \tag{60}$$

as illustrated in Fig. 1.

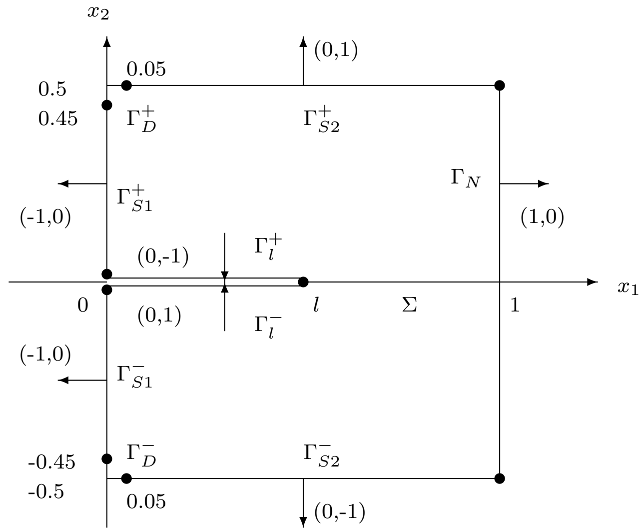

FIGURE 1. The domain Ω_l with the crack Γ_l.

The loading applied to the solid is characterized by the piecewise-linear function g_1 given by formula:

$$g_1(x_2) = -t_0\mu(1 - 2|x_2|), \quad t_0 = 5.85 \cdot 10^{-3}, \tag{61}$$

with $\max|g_1| \approx 160\,(mPa)$, and is illustrated in Fig. 2. To define the Lamé constants μ and λ, the following values of the material parameters are taken: $\nu = 0.34$, $E = 7.3 \cdot 10^4\,(mPa)$.

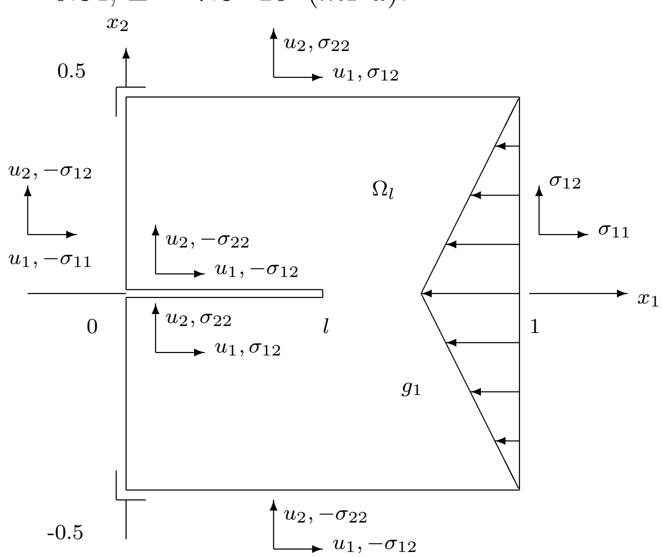

FIGURE 2. The loading model applied on $\overline{\Omega}_l$.

For our case the boundary conditions (5) take the form:

(62a) $$-\sigma_{11}(u) = -\sigma_{12}(u) = 0 \quad \text{on } \Gamma^{\pm}_{S1},$$

(62b) $$\pm\sigma_{12}(u) = \pm\sigma_{22}(u) = 0 \quad \text{on } \Gamma^{\pm}_{S2},$$

(62c) $$\sigma_{11}(u) = g_1, \quad \sigma_{12}(u) = 0 \quad \text{on } \Gamma_N.$$

Before giving the numerical specifications let us present some of the results with comments on the physical nature of the linear as well as the nonlinear model in terms of stress intensity factors. For the linear crack model (3)–(6), the numerical values of the jump $[\![u_2]\!] = u_2|_{\Sigma^+} - u_2|_{\Sigma^-}$ across the interface Σ are depicted in Fig. 3 for the crack length $l = 0.35$. Here, negative values $[\![u_2]\!] < 0$ imply penetration between the crack faces $\Gamma^{\pm}_l$. For the nonlinear crack model (3)–(5) including the condition (7), the corresponding jump $[\![u_2]\!] \geq 0$ at the interface Σ is presented in the same Fig. 3. This jump determines two zones: opening $[\![u_2]\!] > 0$, and contact $[\![u_2]\!] = 0$ between the crack faces. The different zones are separated by the point $x_1 = 0.175$ at the crack Γ_l. On the other hand, in Fig. 4 we present the stress intensity factor K_I for the linear crack problem, calculated numerically for various crack lengths $l = \frac{D}{40}$ with $D = 2, ..., 38$. The second stress intensity factor K_{II}, which belongs to the nonlinear model, satisfies $K_{II} = 0$. In both cases the corresponding calculations were made with the help of singular functions by the perturbation method, which is described in (Kovtunenko 2003). This figure shows two intervals which are characterized by $K_I > 0$ and $K_I < 0$, respectively. The intervals are separated by the point $l^* \approx 0.166$. Comparing the numerical results depicted in Fig. 3 and Fig. 4, we conclude that the point $x_1 = 0.175$ separating the open (inactive) and contact (active) zones for the nonlinear crack model in Fig. 3 is the point on the grid considered in Fig. 4 which is closest to the point l^* where $K_I = 0$. Similar results are valid for all crack lengths $l \geq l^*$ tested.

Let us turn to a description of the discretization. We chose a uniform triangular mesh T^l_h of mesh-size h in the domain Ω_l. For the choices $h = 0.25$ and $l = 0.5$ this is depicted in Fig. 5. This construction incorporates the radial structure of a possible singularity of the solution at the crack tip (Grisvard 1991). The crack length is always chosen as a multiple of the mesh size, i.e. $l = Dh$ for some integer D such that $0 < l < 1$. This results in double nodes along the crack Γ_l, as presented in Fig. 5 for $D = 2$.

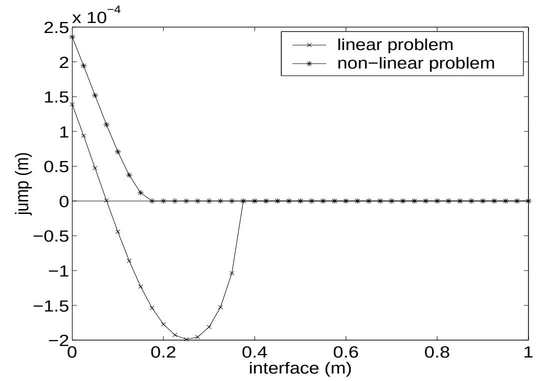

FIGURE 3. Jump $[\![u_2]\!]$ across the interface Σ for the linear crack problem.

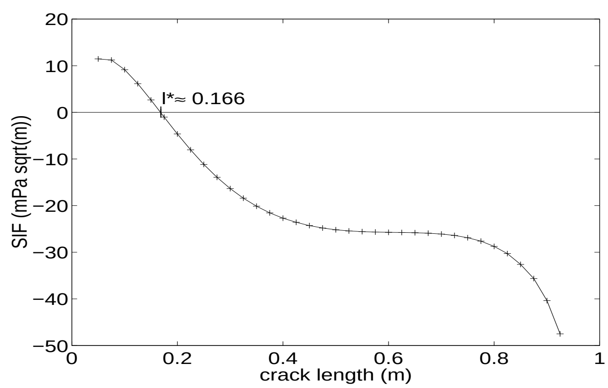

FIGURE 4. Jump $[\![u_2]\!]$ across the interface Σ for the non-linear crack problem.

With respect to this triangulation the basis of piecewise-linear functions $\{e_k\}_{k=1}^N$ supported on the mesh T_h^l, with $e_k = 0$ on $\Gamma_D^{\pm}$ is constructed. The non-linear crack models were solved by the primal-dual active set (AS) method with $\alpha = 10^{-3}$. In all cases that we tested the algorithm terminated after finitely many iterations by producing the same active/inactive set structure in two consecutive iterations and thus found the solution of the discretized problem.

To present some of the numerical findings we define the potential energy of the solution of problems (11) or (12) by

$$P(u) = \frac{1}{2}\int_{\Omega_l} \sigma_{ij}(u)u_{i,j} - \int_{\Gamma_N} g_i u_i, \tag{63}$$

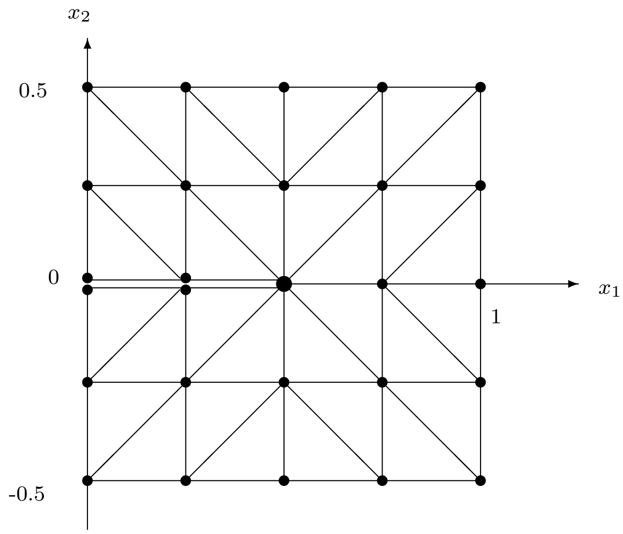

FIGURE 5. Triangular mesh T_h^l for $l = 0.5$ and $h = 0.25$.

which is equivalent to the square of the $H^1(\Omega_l)^2$-norm of u. In Fig. 6 the energy introduced above is presented for the mesh-sizes $h_0 = 0.05$, $h_1 = 0.025$, $h_2 = 0.0125$, and $h_3 = 0.00625$, for the fixed crack length $l = 0.35$. The results indicate a linear rate of convergence of the energy as $h \to 0$. The required number of iterations of the primal-dual active set algorithm increases moderately as h decreases: the number of iterations until successful termination is 3 for h_0, 4 for h_1, 5 for h_2, and 7 for h_3.

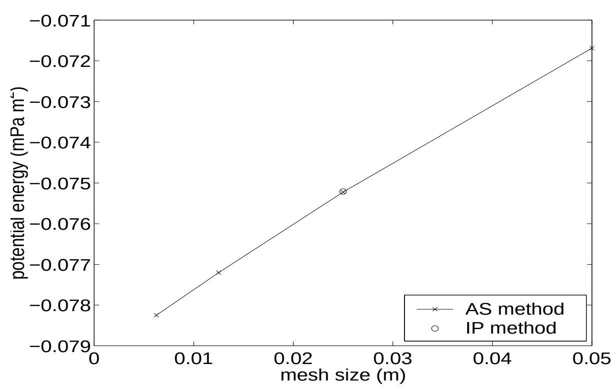

FIGURE 6. Convergence of the potential energy $P(u)$.

We compared the numerical results for AS with the IP method, described in formula (51). In Fig. 6 we see coincidence of the energies obtained by these two methods for h_1. The IP method requires significantly more iterations than the AS strategy. For the result in Fig. 6, for example, IP took about 50, while AS needed only 4 iterations. Moreover, AS terminated at the solution of the discretized problem. The computational work required by IP and AS per iteration, respectively, is comparable.

For this symmetric case the AS method does not use the basis functions on the active set at the crack. This may further decrease the number of iterations, however, as we report on below, for the non-symmetric case the number of iterations required by AS is very small as well.

In Fig. 7 and Fig. 8 we present the values of the iterates of AS for the jump $[\![u_2^n]\!]$ and the generalized stress $\Sigma_2^n = (\Sigma_2^n)_k e_k$ at the interface Σ, for $l = 0.35$ and $h = 0.025$, respectively. We also compare the results for AS and IP and observe that the two methods produce the same active and inactive sets A and I. The IP method was realized with the stopping error $\|u^0\|_{C(\Omega_l)^2} \cdot 10^{-5}$. Requiring further iterations of IP yields no additional progress for $[\![u_2]\!]$.

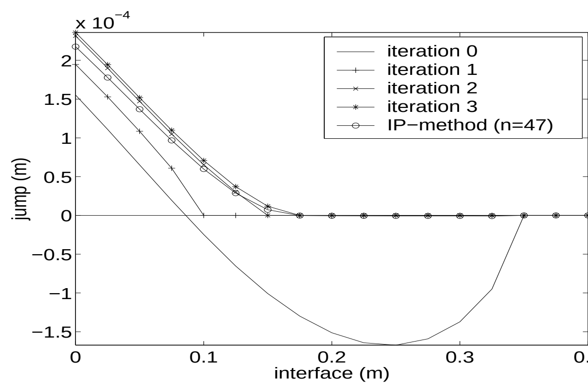

FIGURE 7. The jump $[\![u_2^n]\!]$ as $l = 0.35$ under the g_1 loading.

From our numerical tests we can report on the following features of AS.

- The convergence is always monotone, i.e. $A_0 \supset A_1 \supset ... \supset A_n = A$ and $I_0 \subset I_1 \subset ... \subset I_n = I$.
- Referring to the assumptions made in Section 4, we found that in the examples $M \geq 0$ and $M_2^{n-1} \geq 0$, $n = 1, 2, ...$
- We tested various feasible as well as infeasible initializations u^0, and found that the first iteration u^1 was always feasible. Thus, the assumption of Theorem 4.2 is satisfied numerically for the tests that we performed.

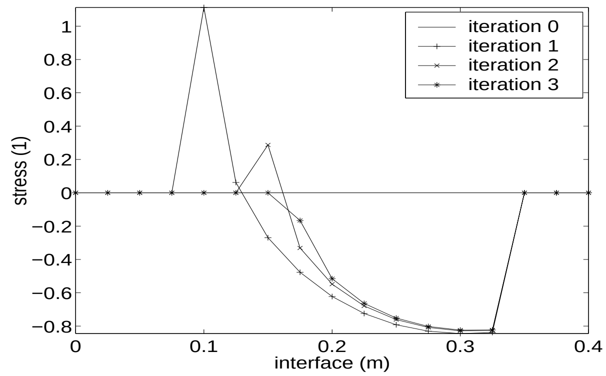

FIGURE 8. The stress Σ_2^n as $l = 0.35$ under the g_1 loading.

- As can be seen from Tab. 1, the number of iterations for AS (until successful termination) grows only moderately for decreasing mesh-size h.

h	0.05	0.025	0.0125	0.00625
#it	3	4	5	7

TABLE 1. Number of iterations #it of AS for different mesh-sizes h.

- We further tested Assumption A concerning matrix M_2 for arbitrary splittings and found that it is not valid in general. Negative elements can occur in M_2 in cases which correspond to a rapid oscillation of the sets A and I along the crack Γ_l.
- We carried out further experiments with the loading described above but different Lamé constants λ and μ for the model. Even for very large values of $\frac{\lambda+\mu}{\mu}$, which strongly emphasize the problematic $(\operatorname{div} u)_{,i}$ part in the Lamé equation, the monotonicity property remained valid. In Tab. 2 we report on the number of iterations required by AS for various values for $\frac{\lambda+\mu}{\mu}$. The results indicate that AS is rather insensitive with respect to $\frac{\lambda+\mu}{\mu}$.

$\frac{\lambda+\mu}{\mu}$	10^0	10^1	10^2	10^3	10^4
#it	5	4	5	6	6

TABLE 2. Number of iterations #it of AS for different parameter values $\frac{\lambda+\mu}{\mu}$.

- We tested a non-symmetric problem by choosing a non-symmetric loading

$$g_1 = \begin{cases} g_1 & \text{at } \Gamma_N \cap \{x_2 \geq 0\}, \\ 0 & \text{at } \Gamma_N \cap \{x_2 < 0\}. \end{cases} \tag{64}$$

  Again monotone convergence of the AS method was observed. In Fig. 7 one can see a closing of the crack faces $\Gamma_l^{\pm}$ in a region containing the crack tip $(l, 0)$. From the fracture mechanics standpoint, the stress intensity factor is $K_I = 0$. To simulate $K_I \neq 0$, we tested the crack problem with the loading $-g_1$, which is applied in the opposite direction to the case presented in Fig. 2. Then an opening of the crack faces $\Gamma_l^{\pm}$ occurs near the crack tip as presented in Fig. 9. In this case, the AS method converges in the same number of steps as for $K_I = 0$. The corresponding iterates are depicted in Fig. 9 and Fig. 10.

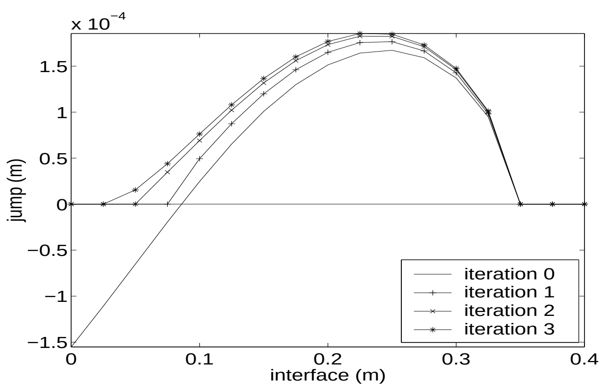

FIGURE 9. The jump $[\![u_2^n]\!]$ as $l = 0.35$ under the $-g_1$ loading.

- We also considered the case of a non-homogeneous solid, by bonding two isotropic materials across the interface Σ, with different Lamé constants μ^+, λ^+ and μ^-, λ^- in the corresponding upper Ω_l^+ and lower Ω_l^- domains, where $\Omega_l^{\pm} = \Omega_l \cap \{\pm x_2 > 0\}$. For simplicity we took proportional constants

$$\mu^{\pm} = (1 \pm b)\mu, \quad \lambda^{\pm} = (1 \pm b)\lambda, \tag{65}$$

  which implies a one-parametric dependence

$$\mu^+/\mu^- = \lambda^+/\lambda^- = (1 + b)/(1 - b) = \text{bond} \tag{66}$$

  in the parameter *bond* of bonding. Note that *bond* $= 1$ describes the homogeneous, isotropic solid considered before. The case *bond* $\neq 1$ in our example implies that both stress intensity

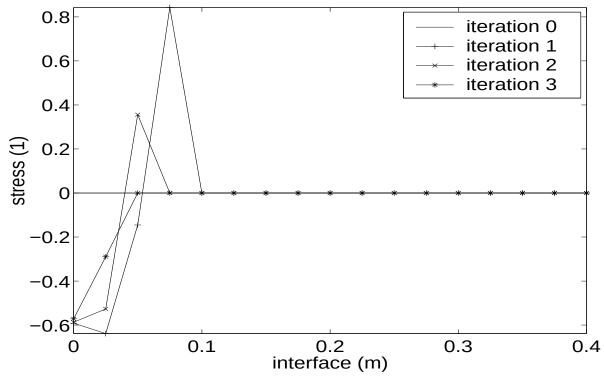

FIGURE 10. The stress Σ_2^n as $l = 0.35$ under the $-g_1$ loading.

factors $K_I \neq 0$ and $K_{II} \neq 0$. For the various values of the parameter *bond* tested, the monotone convergence of the non-symmetric AS algorithm remains valid, too.

In Fig. 11 and 12 we show the displacements u_1 and u_2 for both crack faces $\Gamma_l^{\pm}$ with $l = 0.35$. Here we chose *bond*=2. Both components of the displacements clearly reflect the non-symmetry of the problem. In contrast to the present situation, note that in the symmetric case we always had $[\![u_1]\!] = 0$.

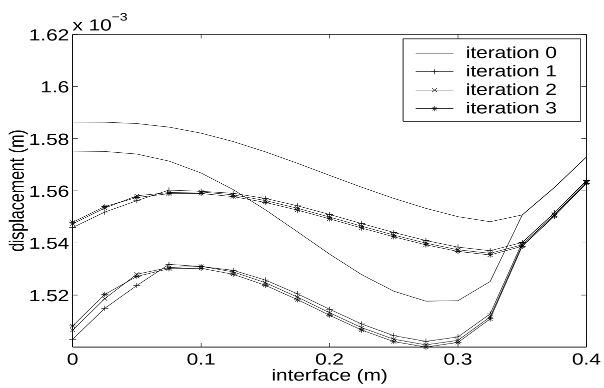

FIGURE 11. Displacements $(u_1^n)_{k^\pm}$ for *bond* = 2.

7. CONCLUSION

The primal-dual active set algorithm for both, symmetric and non-symmetric crack problems with non-penetration is formulated and shown

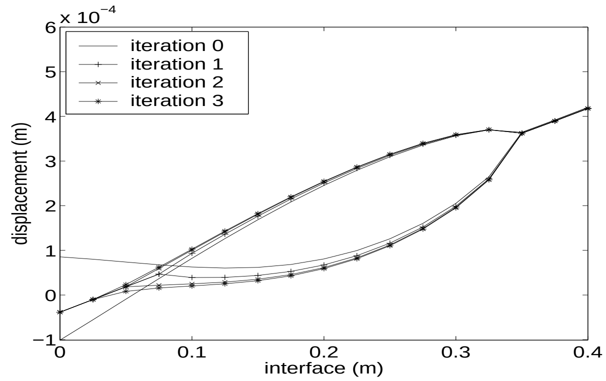

FIGURE 12. Displacements $(u_2^n)_{k^\pm}$ for $bond = 2$.

to be efficient numerically. In the finite-dimensional case, superlinear local convergence is proved and and global convergence is obtained under the positiveness assumption made on some matrix connecting the jump of the traces and stress at the crack by the active set iteration. This assumption implies monotonicity of the estimates of the active set.

Our numerical tests indicate the following. In comparison with a regularization method, the active set method requires a significantly smaller number of iterations. The number of iterations required depends only moderately on the mesh-size of the discretization.

The active sets converge monotonically independently of the initialization. These assertions were tested for the closed and opened crack faces, for the symmetric and non-symmetric loading, for the homogeneous and bonded isotropic materials, and for various Lamé constants.

Acknowledgments. The research results were obtained with support of the Austrian Science Fund (FWF) in framework of the SFB project F 003 "Optimierung und Kontrolle" and the Lise Meitner project M 622/ M 737 "Variational methods in application to crack problems".

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Appendix A. The symmetric problem

In fracture mechanics it is common to consider the symmetric crack problem when investigating the mode-1 model of a crack. Therefore, we formulate the primal-dual active set algorithm for this specific case.

Let the domain Ω_l with its boundary and the loading g applied at Γ_N be symmetric with respect to the x_1-axis. It implies the following structure of the solution of problem (11):

$$u = (u_1, u_2) = \begin{cases} (u_1^+, u_2^+)(x_1, x_2) & \text{for } x_2 > 0, \\ (u_1^+, -u_2^+)(x_1, x_2) & \text{for } x_2 < 0. \end{cases} \tag{67}$$

Then $[\![u_2]\!] = 2u_2|_{\Gamma_l^+} = -2u_2|_{\Gamma_l^-}$, and the non-penetration conditions (9) at the crack implies

$$\mp \sigma_{12}(u) = 0 \quad \text{on } \Gamma_l^{\pm}, \tag{68a}$$

$$\sigma_{22}(u) \leq 0, \quad u_2 \geq 0, \quad \sigma_{22}(u) u_2 = 0 \quad \text{on } \Gamma_l^+, \tag{68b}$$

$$u_2|_{\Gamma_l^-} = -u_2|_{\Gamma_l^+}, \quad \sigma_{22}(u)|_{\Gamma_l^-} = \sigma_{22}(u)|_{\Gamma_l^+}. \tag{68c}$$

Problem (3)–(5), (9) on Ω_l can be reduced onto the half-domain $\Omega_l^+ = \Omega_l \cap \{x_2 > 0\}$ by setting the additional boundary conditions

$$u_2 = 0, \quad \sigma_{12}(u) = 0 \quad \text{on } \{x_2 = 0\} \cap \Omega_l. \tag{69}$$

Next we consider the consequences for the active set algorithm. In the finite-dimensional case we define the active and inactive sets as

$$A = \{k^+ \in C : \ (U_2 + \alpha \Sigma_2)_{k^+} < 0\}, \tag{70a}$$

$$I = \{k^+ \in C : \ (U_2 + \alpha \Sigma_2)_{k^+} \geq 0\}. \tag{70b}$$

Then (26) results in

$$u \in H_l^N, \tag{71a}$$

$$\int\limits_{\Omega_l} \sigma_{ij}(u)(e_k)_{,j} = \int\limits_{\Gamma_N} g_i e_k, \quad i = 1, 2, \quad \text{for } k \in \{1, ..., N\} \setminus C, \tag{71b}$$

$$\int\limits_{\Omega_l} \sigma_{ij}(u)(e_{k^{\pm}})_{,j} \pm (\Sigma_i)_{k^{\pm}} = 0, \quad i = 1, 2, \quad \text{for } (k^+, k^-) \in C, \tag{71c}$$

$$(\Sigma_1)_{k^+} = 0, \ (U_2)_{k^+} = 0, \ (\Sigma_2)_{k^+} < 0 \quad \text{for } k^+ \in A, \tag{71d}$$

$$(\Sigma_1)_{k^+} = 0, \ (U_2)_{k^+} \geq 0, \ (\Sigma_2)_{k^+} = 0 \quad \text{for } k^+ \in I, \tag{71e}$$

$$(\Sigma_i)_{k^-} = (\Sigma_i)_{k^+}, \quad i = 1, 2, \quad \text{for all } (k^+, k^-) \in C, \tag{71f}$$

$$(U_1)_{k^-} = (U_1)_{k^+}, \quad (U_2)_{k^-} = -(U_2)_{k^+} \quad \text{for all } (k^+, k^-) \in C, \tag{71g}$$

and the steps of the active set algorithm reduced to:

Algorithm B (symmetric case)

(0) *Choose* u^0, Σ^0*; set* $n = 1$.

(1) *The discrete crack indices C are decomposed according to*

(72a) $$A_{n-1} = \{k^+ \in C : \quad (U_2^{n-1} + \alpha \Sigma_2^{n-1})_{k^+} < 0\},$$

(72b) $$I_{n-1} = \{k^+ \in C : \quad (U_2^{n-1} + \alpha \Sigma_2^{n-1})_{k^+} \geq 0\}.$$

(2) *If $n \geq 2$ and $A_{n-1} = A_{n-2}$ then STOP; else go to step 3.*
(3) *Solve for $u^n \in H_l^N$ the mixed problem:*

(73a) $$\int\limits_{\Omega_l} \sigma_{ij}(u^n)(e_k)_{,j} = \int\limits_{\Gamma_N} g_i e_k, \quad i = 1,2, \quad \textit{for } k \in \{1, ..., N\} \setminus C,$$

(73b) $$\int\limits_{\Omega_l} \sigma_{ij}(u^n)(e_{k^\pm})_{,j} \pm (\Sigma_i^n)_{k^\pm} = 0, \quad i = 1,2, \quad \textit{for } (k^+, k^-) \in C,$$

(73c) $$(\Sigma_1^n)_{k^\pm} = 0 \quad \textit{for } (k^+, k^-) \in C,$$

(73d) $$(U_2^n)_{k^+} = 0 \quad \textit{for } k^+ \in A_{n-1},$$

(73e) $$(\Sigma_2^n)_{k^+} = 0 \quad \textit{for } k^+ \in I_{n-1},$$

(73f) $$(U_2^n)_{k^-} = 0 \quad \textit{on } A_{n-1}, \quad (\Sigma_2^n)_{k^-} = 0 \quad \textit{on } I_{n-1}.$$

(4) *Set $n = n + 1$ and go to 1.*

Theorem 4.1 also applies in the present situation. Further, Theorem 4.2 can easily be adapted to the symmetric case. Formula (44), for example, simplifies to

(74a) $$(dU_2^n)_{B^+} = -M\, d\Sigma_2^n, \text{ with}$$

(74b) $$M = R_{B^+B^+} - R_{B^+B^-} = -R_{B^-B^+} + R_{B^-B^-}.$$