Journal of Engineering Mathematics (2006) 55: 151–166
DOI 10.1007/s10665-005-9024-z

Primal-dual sensitivity analysis of active sets for mixed boundary-value contact problems

VICTOR A. KOVTUNENKO
Lavrent'ev Institute of Hydrodynamics, 630090 Novosibirsk, Russia (e-mail: kovtunenko@hydro.nsc.ru)

Received 21 March 2005; accepted in revised form 28 October 2005 / Published online: 3 January 2006

Abstract. The constrained minimization problem of contact mechanics is investigated as a mixed boundary-value problem determined on the active (contact) set of the solution. Using primal-dual methods of the shape sensitivity analysis, asymptotic expansions of the primal and dual state variables and the cost functional of energy are obtained with respect to a perturbation of the active set in the direction of an arbitrary velocity vector field.

Key words: contact problem, constrained optimization, primal-dual methods, shape sensitivity analysis

1. Introduction

Problems involving contact have a wide range of applications in engineering sciences. Its classical representation is named after A. Signorini and considers the contact of an elastic solid with a rigid obstacle, which we deal with here. Contact problems are nonlinear; their inherent speciality concerns the fact that the contact set is unknown *a priori*. Moreover, at this contact set, reaction (contact) forces are singular (unbounded) in nature.

Early progress in the investigation of contact problems was motivated by the development of variational methods for free-boundary and unilaterally constrained problems. While there are many works on this topic, we give only a few selected references [1–3].

Recently, the fast development of computing techniques has increased the interest in this field. Efficient iterative methods are being developed for the numerical solution of contact problems within the framework of discrete (finite-dimensional) constrained optimization. However, discrete formulations lose the singular character of the reaction (contact) forces, thus resulting in a decrease of the convergence rate of iterations as the dimension of a finite basis of discretization increases. These observations motivate our turning to a continuous (infinite-dimensional) analysis of contact problems.

One of the most efficient numerical strategies involves a split of the geometric set where contact is unknown, into active and inactive complementary sets; see [4–6]. Following the arguments of complementarity problems in optimization, we regard contact sets as the active ones. To give a mathematical foundation of active-set strategies, one has to endow the active set at the solution with proper measures, which distinguish it uniquely from all admissible (variable) active sets.

In this paper we start with an active set found *a posteriori* at the solution of the contact problem, and we study its sensitivity with respect to geometric perturbations of the active (contact) set. For this reason we apply a primal-dual technique of the shape-sensitivity analysis, which is based on the results of [7–10]. In fact, once the active set is given, we restate the contact problem via a mixed-boundary-value formulation, which is linear. Using the primal-dual setting of the problem, we overcome difficulties of the classical approach connected with curving of the boundary of a contacting body. In this way we derive expansion terms of the stress and the energy characteristics of a solution of the contact problem, for an arbitrary order of the expansion. For a specific 2-dimensional case, a method of singular perturbations was applied to the mixed-boundary-value contact problem in [11].

2. Mathematical backgrounds

We investigate the constrained minimization problem of contact mechanics, which is presented in the following form: Find the primal state variable u^0 (displacements) such that $\nu^\top u^0 \le \psi$ at Γ_C (contact conditions) and

$$\Pi(u^0) \le \Pi(u) \quad \text{for all} \quad u : \nu^\top u \le \psi \quad \text{on } \Gamma_C, \tag{1}$$

with a positive-definite quadratic cost functional Π of the potential energy, an obstacle function ψ and the normal vector ν referenced to a geometric set Γ_C.

To reformulate the contact problem (1) in an equivalent primal-dual form, a dual state variable λ^0 (the contact force) can be introduced such that the pair (u^0, λ^0) satisfies the relations:

$$L(u^0, \lambda^0) \le L(u, \lambda^0) := \Pi(u) - \langle \lambda^0, \nu^\top u - \psi \rangle_{\Gamma_C} \quad \text{for all } u, \tag{2a}$$

$$\nu^\top u^0 \le \psi, \quad \lambda^0 \le 0, \quad \langle \lambda^0, \nu^\top u^0 - \psi \rangle_{\Gamma_C} = 0 \quad \text{on } \Gamma_C, \tag{2b}$$

with u^0 obtained from (1).

Due to the complementarity conditions (2b), the geometric set Γ_C can be split into the active set A^0 (where $\nu^\top u^0 = \psi$) and its complement, the inactive set I^0 yielding

$$\nu^\top u^0 = \psi \quad \text{on } A^0, \quad \lambda^0 = 0 \quad \text{on } I^0, \tag{3a}$$

$$\nu^\top u^0 < \psi \quad \text{on } I^0, \quad \lambda^0 \le 0 \quad \text{on } A^0. \tag{3b}$$

Once A^0 is given, relations (2a) and (3a) result in the minimax problem: Find (u^0, λ^0) such that $\lambda^0 = 0$ at I^0 and

$$L(u^0, \lambda) = L(u^0, \lambda^0) \le L(u, \lambda^0) \quad \text{for all } u \quad \text{and } \lambda : \lambda = 0 \text{ on } I^0. \tag{4}$$

For an arbitrary given set A^t and its complement I^t in Γ_C, we have the corresponding problem: Find (u^t, λ^t) such that $\lambda^t = 0$ at I^t and

$$L(u^t, \lambda) = L(u^t, \lambda^t) \le L(u, \lambda^t) \quad \text{for all } u \quad \text{and } \lambda : \lambda = 0 \text{ on } I^t.$$

It is well-posed in the sense that its solution can be derived from the following primal-dual formulation of a mixed-boundary-value problem: Find (u^t, λ^t) such that

$$\begin{aligned} &L(u^t, \lambda^t) \le L(u, \lambda^t) \quad \text{for all } u, \\ &\nu^\top u^t = \psi \quad \text{on } A^t, \quad \lambda^t = 0 \quad \text{on } I^t. \end{aligned} \tag{5}$$

However, it does not guarantee the fulfillment of inequalities like (3b) as long as $A^t \ne A^0$.

From a constrained optimization viewpoint, the mixed-boundary-value problem (5) corresponds to an iteration of the solution of (2) by active-set strategies: Find $(u^{(n)}, \lambda^{(n)})$ such that

$$\begin{aligned} &L(u^{(n)}, \lambda^{(n)}) \le L(u, \lambda^{(n)}) \quad \text{for all } u, \\ &\nu^\top u^{(n)} = \psi \quad \text{on } A^{(n-1)}, \quad \lambda^{(n)} = 0 \quad \text{on } I^{(n-1)}. \end{aligned}$$

The principal question is a proper determination of iterations $A^{(n-1)}$ of the active set providing a convergence $(u^{(n)}, \lambda^{(n)}, A^{(n)}) \to (u^0, \lambda^0, A^0)$ as $n \to \infty$. Based on the property of generalized Newton differentiability, the super-linear convergence of a primal-dual active-set strategy is obtained in [4–6] with

$$A^{(n-1)} = \{x \in \Gamma_C : (\nu^\top u^{(n-1)} - \psi - c\lambda^{(n-1)})(x) \geq 0\} \quad (c > 0).$$

However, the difficulty of this strategy concerns a fortuitous regularity of $\lambda^{(n)}$ in the mixed-boundary-value problem of contact mechanics.

Motivated by this consideration, in the present paper we study the sensitivity of the contact problem with respect to perturbations of the active set at the solution.

From a physical point of view, the active set A^0 implies the contact zone, the inactive set I^0 characterizes a zone where no contact occurs, and the dual state variable λ^0 describes the contact force at A^0. For fixed external data (load and geometry) of the contact problem, these characteristics can be uniquely obtained from the solution of (1) due to its uniqueness. Relations (5) imply a fictitious contact force λ^t found *a posteriori* at a prescribed active set A^t. In this light, the mixed-boundary-value formulation (4) provides a tool to describe the variation of the true contact force λ^0 just varying the active set from A^0 to A^t without changes in the external data of the contact problem.

Considering A^t as a perturbation of A^0 in dependence of a parameter t, we get an asymptotic expansion of the solution (u^t, λ^t) and the cost functional $\Pi(u^t)$ with respect to $t \to 0$. We prove that the shape derivative $\Pi'_V(u^0)$ in an arbitrary direction V of the perturbation is zero.

3. Perturbation problem

3.1. Formulation of a contact problem

Let $\Omega \subset \mathbb{R}^N$, where $N = 2$ or $N = 3$, be a bounded domain with the boundary $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_C$ such that Γ_N and Γ_C are disjoint by Γ_D, as illustrated in Figure 1. We assume an *outward* normal vector $\nu = (\nu_1, \ldots, \nu_N)^\top$ at $\partial\Omega$ being sufficiently smooth. The standard notation of linear elasticity is used for a displacement vector $u = (u_1, \ldots, u_N)^\top(x)$ with the spatial variable $x = (x_1, \ldots, x_N)^\top \in \mathbb{R}^N$, for the linear strain tensor $\varepsilon_{ij}(u) = 0.5(u_{i,j} + u_{j,i})$ with $i, j = 1, \ldots, N$, and for the symmetric stress tensor $\sigma_{ij}(u) = c_{ijkl}\varepsilon_{kl}(u)$ with a positive-definite $N \times N \times N \times N$-tensor of elasticity coefficients $c_{ijkl}(x)$. The convention of summation over repeated indices $i, j, k, l, s = 1, \ldots, N$ and differentiation with respect to a variable with the index following after a comma is utilized.

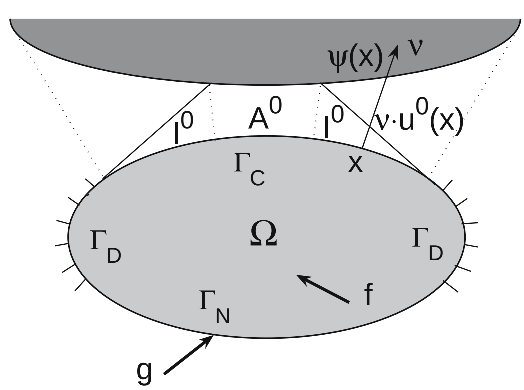

Figure 1. The geometry and load for the contact problem.

Supposing a clamping at Γ_D of a solid occupying the domain Ω, we apply a volume load field $f=(f_1,\dots,f_N)^\top(x)$ in Ω and a boundary traction force $g=(g_1,\dots,g_N)^\top(x)$ at Γ_N. The solid is assumed to be constrained at Γ_C by an obstacle, which we express with the help of a regular scalar function $\psi(x)$ such that $\psi>0$ at the boundary of Γ_C. These constructions are illustrated in Figure 1. Thus, the following equations and inequalities are considered:

$$-\sigma_{ij,j}(u)=f_i \quad i=1,\dots,N \quad \text{in } \Omega, \tag{6a}$$

$$u=0 \quad \text{on } \Gamma_D, \tag{6b}$$

$$\sigma_{ij}(u)\nu_j=g_i \quad i=1,\dots,N \quad \text{on } \Gamma_N, \tag{6c}$$

$$\sigma_\tau(u)=0 \quad \text{on } \Gamma_C, \tag{6d}$$

$$\nu^\top u\le\psi, \quad \sigma_\nu(u)\le 0, \quad \sigma_\nu(u)\big(\nu^\top u-\psi\big)=0 \quad \text{on } \Gamma_C, \tag{6e}$$

where a decomposition into normal and tangential components at Γ_C is applied according to

$$\begin{aligned}&\sigma_{ij}(u)\nu_j=\sigma_\nu(u)\nu_i+\sigma_\tau(u)_i \quad i=1,\dots,N,\\ &\sigma_\nu(u):=\sigma_{ij}(u)\nu_j\nu_i, \quad \sigma_\tau(u)_i:=\sigma_{ij}(u)\nu_j-\sigma_\nu(u)\nu_i.\end{aligned} \tag{7}$$

Let us denote the set of admissible displacements accounting (6b) by

$$H:=\{u\in H^1(\Omega)^N: \quad u=0 \quad \text{on } \Gamma_D\}.$$

For given $f\in L^2(\Omega)^N$ and $g\in L^2(\Gamma_N)^N$ we introduce a quadratic functional of the potential energy of the solid as

$$\Pi(u)=\frac{1}{2}\int_\Omega \sigma_{ij}(u)\varepsilon_{ij}(u)\,\mathrm{d}x-\int_\Omega f_iu_i\,\mathrm{d}x-\int_{\Gamma_N} g^\top u\,\mathrm{d}s. \tag{8}$$

The weak solution to the boundary-value contact problem (6) can be defined from the following constrained minimization problem: Find $u^0\in H$ such that $\nu^\top u^0\le\psi$ almost everywhere Γ_C and

$$\Pi(u^0)\le\Pi(u) \quad \text{for all} \quad u\in H: \nu^\top u\le\psi \ \text{ on } \Gamma_C. \tag{9}$$

Minimization problem (9) is equivalent to the variational inequality

$$\begin{aligned}&\int_\Omega \sigma_{ij}(u^0)\varepsilon_{ij}(u-u^0)\,\mathrm{d}x\ge\int_\Omega f_i(u-u^0)_i\,\mathrm{d}x+\int_{\Gamma_N} g^\top(u-u^0)\,\mathrm{d}s\\ &\quad\text{for all } u\in H: \quad \nu^\top u\le\psi \ \text{ on } \Gamma_C.\end{aligned} \tag{10}$$

3.2. Mixed formulation of the contact problem

The contact force $\sigma_\nu(u^0)$ is defined as a distribution in $H^{-1/2}(\Gamma_C)$ from (10) and Green's formula

$$\begin{aligned}\int_\Omega \sigma_{ij}(u^0)\varepsilon_{ij}(u)\,\mathrm{d}x=&-\int_\Omega \sigma_{ij,j}(u^0)u_i\,\mathrm{d}x+\int_{\Gamma_N}\sigma_{ij}(u^0)\nu_ju_i\,\mathrm{d}s\\ &+\langle\sigma_\nu(u^0),\nu^\top u\rangle_{\Gamma_C}+\langle\sigma_\tau(u^0)_i,u_{\tau i}\rangle_{\Gamma_C} \quad \text{for } u\in H,\end{aligned} \tag{11}$$

where decomposition (7) is applied, and $\langle\cdot,\cdot\rangle_{\Gamma_C}$ denotes a duality pairing at Γ_C between $H_{00}^{1/2}(\Gamma_C)$ and its dual space $H^{-1/2}(\Gamma_C)$; see [9]. Therefore, conditions (6e) are fulfilled in the generalized sense that

$$\begin{aligned} &\nu^\top u^0 \le \psi \quad \text{almost everywhere } \Gamma_C,\\ &\langle \sigma_\nu(u^0), \eta + \nu^\top u^0 - \psi\rangle_{\Gamma_C} \le 0 \quad \text{for all } 0 \le \eta \in H_{00}^{1/2}(\Gamma_C). \end{aligned} \tag{12}$$

We define a dual variable as

$$\lambda^0 = \sigma_\nu(u^0). \tag{13}$$

Due to (6a), (6c), (6d), it follows from (11) that the primal variable u^0 and the dual variable in (13) are connected by the relation for all $u \in H$:

$$\int_\Omega \sigma_{ij}(u^0)\varepsilon_{ij}(u)\,\mathrm{d}x - \langle \lambda^0, \nu^\top u\rangle_{\Gamma_C} = \int_\Omega f_i u_i\,\mathrm{d}x + \int_{\Gamma_N} g^\top u\,\mathrm{d}s. \tag{14}$$

Note that (14) can also be obtained as an optimality condition with respect to the primal variable u of the Lagrangian

$$L(u,\lambda) := \Pi(u) - \langle \lambda, \nu^\top u - \psi\rangle_{\Gamma_C}. \tag{15}$$

For problem (9) we define active/inactive sets, respectively as

$$A^0 = \{x \in \Gamma_C : \nu^\top u^0(x) = \psi(x)\}, \quad I^0 = \Gamma_C \setminus A^0; \tag{16}$$

see Figure 1 for an illustration. Let us look for boundary conditions fulfilled at A^0 and I^0. Obviously, $\nu^\top u^0 - \psi = 0$ on A^0. If λ^0 is a point-wise function, then $\lambda^0 = 0$ at I^0 due to (6e), thus fulfilling a strict complementarity condition which is formulated later in (17). In the general case, we suppose that the support of A^0 is compact in Γ_C. Henceforth, there exists $0 \le \chi \in C_0^\infty(\Gamma_C)$ such that $\chi = 1$ at A^0. Assuming that $\nu^\top u^0$ is continuous at $\overline{\Gamma}_C$, for an arbitrary fixed $\delta > 0$ and $\xi \in H_{00}^{1/2}(\Gamma_C) \cap C_0(\Gamma_C)$ with $\xi = 0$ at A^0, a constant $c > 0$ exists such that $\eta = \psi - \nu^\top u^0 + c(\delta\chi \pm \xi) \ge 0$ at Γ_C. The substitution of such a test function η in (12) follows

$$|\langle \lambda^0, \xi\rangle_{\Gamma_C}| \le -\delta \langle \lambda^0, \chi\rangle_{\Gamma_C}.$$

Letting $\delta \to 0$ in this inequality and using density arguments (see [12, Theorem 1.4.2.2, p.24]), we derive

$$\langle \lambda^0, \xi\rangle_{\Gamma_C} = 0 \quad \text{for all } \xi \in H_{00}^{1/2}(\Gamma_C): \quad \xi = 0 \text{ on } A^0. \tag{17}$$

Alternatively to the assumption of the continuity of $\nu^\top u^0$, we can suppose that a tangent cone

$$T(u^0) := cl\,\{\xi \in H_{00}^{1/2}(\Gamma_C): \quad c > 0 \quad \text{exists such that } \psi - \nu^\top u^0 + c\xi \ge 0 \quad \text{on } \Gamma_C\} \tag{18}$$

coincides with the following closed convex set

$$T(u^0) = \{\xi \in H_{00}^{1/2}(\Gamma_C): \quad \xi \ge 0 \quad \text{on } A^0\} \tag{19}$$

according to the definition and the results on tangent cones given in [7]. In the case of equivalence of (18) and (19), the equality stated in (17) holds also true. To prove this fact, we observe that, for any $\xi \in H_{00}^{1/2}(\Gamma_C)$ with $\xi = 0$ at A^0, the inclusion $\pm\xi \in T(u^0)$ holds due to (19). On the other hand, in view of (18), two sequences $\xi_\pm^n \in H_{00}^{1/2}(\Gamma_C)$ exist such that

$\xi_{\pm}^n \to \pm\xi$ strongly in $H_{00}^{1/2}(\Gamma_C)$ as $n \to \infty$, and constants $c_{\pm}^n > 0$ exist such that $\eta = \psi - \nu^\top u^0 + c_{\pm}^n \xi_{\pm}^n \geq 0$ at Γ_C. The substitution of such a test function η in (12) leads to

$$\langle \lambda^0, \xi_{\pm}^n \rangle_{\Gamma_C} \leq 0.$$

Letting $n \to \infty$ in this inequality we arrive at (17).

We denote the dual cone corresponding to (17) by

$$M_0 = \{\lambda \in H^{-1/2}(\Gamma_C): \quad \langle \lambda, \xi \rangle_{\Gamma_C} = 0 \quad \text{for all } \xi = 0 \text{ on } A^0\}.$$

From (14) and (17) it follows that the pair (u^0, λ^0) obtained in (9) and (13) satisfies a minimax problem with the Lagrangian (15): Find $(u^0, \lambda^0) \in H \times M_0$ such that

$$L(u^0, \lambda) = L(u^0, \lambda^0) \leq L(u, \lambda^0) \quad \text{for all } (u, \lambda) \in H \times M_0. \tag{20}$$

The minimax problem (20) is well-posed, as will be proved in the following section. The first-order optimality condition for (20) yields the variational equation (14) and the relation

$$\langle \lambda, \nu^\top u^0 - \psi \rangle_{\Gamma_C} = 0 \quad \text{for all } \lambda \in M_0 \tag{21}$$

with respect to the dual variable λ.

In order to obtain the uniqueness of the solution to the linear equations (14) and (21) (thus the uniqueness to (20)), it is sufficient to prove that the corresponding homogeneous equations

$$\int_\Omega \sigma_{ij}(\bar{u}) \varepsilon_{ij}(u)\, \mathrm{d}x - \langle \bar{\lambda}, \nu^\top u \rangle_{\Gamma_C} = 0 \quad \text{for all } u \in H, \tag{22a}$$

$$\langle \lambda, \nu^\top \bar{u} \rangle_{\Gamma_C} = 0 \quad \text{for all } \lambda \in M_0 \tag{22b}$$

have only the trivial solution $(\bar{u}, \bar{\lambda}) \in H \times M_0$. Indeed, substituting a smooth test function λ in (22b) such that $\lambda = 0$ at I^0, we derive $\nu^\top \bar{u} = 0$ at A^0. Therefore $\langle \bar{\lambda}, \nu^\top \bar{u} \rangle_{\Gamma_C} = 0$, and the substitution of $u = \bar{u}$ in (22a) follows $\bar{u} = 0$, hence $\bar{\lambda} = 0$.

3.3. Perturbation of the active set

For a perturbation parameter $0 \leq t \leq T$ with fixed $T > 0$, let $V(t, x) \in C([0, T]; W^{1,\infty}(\mathbb{R}^N))^N$ be a given velocity vector field. We suppose that for all t

$$V(t) = 0 \quad \text{on } \Gamma_D \cup \Gamma_N, \quad \nu^\top V(t) = 0 \quad \text{on } \Gamma_C, \tag{23}$$

i.e., the velocity is tangential to Γ_C. As an example of such a function consider the velocity vector field $V = \chi \Lambda$ with a vector Λ tangential to the boundary $\partial\Omega$, which is multiplied by a scalar cut-off function χ supported in a neighborhood of the boundary Γ_C. Now we define a map $\Phi \in C^1([0, T]; W^{1,\infty}(\mathbb{R}^N))^N$ as the classical solution to the nonlinear ODE

$$\frac{\mathrm{d}\Phi}{\mathrm{d}t} = V(t, \Phi) \quad \text{for } t \geq 0, \quad \Phi(0) = x. \tag{24}$$

The inverse map $\Phi^{-1} \in W^{1,\infty}((0, T) \times \mathbb{R}^N)^N$ exists, and is unique. The corresponding one-to-one coordinate transformation is defined as

$$y = \Phi(t, x): (\Omega, \Gamma_D, \Gamma_N, \Gamma_C) \to (\Omega, \Gamma_D, \Gamma_N, \Gamma_C) \quad \text{for } t \in [0, T]. \tag{25}$$

For fixed $t \in (0,T)$ consider a perturbation of the active set in (16)

$$A^t := A^0 \circ \Phi^{-1}(t) \quad (\subset \Gamma_C \text{ according to (25)}).$$

On the perturbed dual cone

$$M_t = \{\mu \in H^{-1/2}(\Gamma_C): \quad \langle \mu, \eta \rangle_{\Gamma_C} = 0 \quad \text{for all } \eta = 0 \text{ on } A^t\}$$

we define the following perturbed problem: Find $(u^t, \lambda^t) \in H \times M_t$ such that

$$L(u^t, \mu) = L(u^t, \lambda^t) \le L(u, \lambda^t) \quad \text{for all } (u, \mu) \in H \times M_t. \tag{26}$$

The solution of the minimax problem (26) can be obtained by using the following equivalent relations:

$$u^t \in H \quad \text{such that } \nu^\top u^t = \psi \quad \text{on } A^t, \tag{27a}$$

$$\Pi(u^t) \le \Pi(u) \quad \text{for all } u \in H: \nu^\top u = \psi \quad \text{on } A^t, \tag{27b}$$

$$\lambda^t = \sigma_\nu(u^t), \tag{27c}$$

which define a weak solution to the mixed-boundary-value problem with respect to u^t (compare with (6)):

$$\begin{aligned}
&-\sigma_{ij,j}(u^t) = f_i \quad i = 1, \dots, N \quad \text{in } \Omega,\\
&u^t = 0 \quad \text{on } \Gamma_D,\\
&\sigma_{ij}(u^t)\nu_j = g_i \quad i = 1, \dots, N \quad \text{on } \Gamma_N,\\
&\sigma_\tau(u^t) = 0 \quad \text{on } \Gamma_C,\\
&\nu^\top u^t = \psi \quad \text{on } A^t, \quad \sigma_\nu(u^t) = 0 \quad \text{on } I^t.
\end{aligned} \tag{28}$$

In the following, we establish the equivalence of the formulations (26) and (27). Let (26) hold true. The substitution of a test function $\mu = \lambda^t \pm \eta$ in (26) with smooth η such that $\eta = 0$ at I^t leads to (27a). Therefore, $\langle \lambda^t, \nu^\top u^t - \psi \rangle_{\Gamma_C} = 0$, and taking test functions $u \in H$ in (26) such that $\nu^\top u = \psi$ at A^t results in (27b). The Euler equation for (26) with respect to the primal state variable u^t reads

$$\int_\Omega \sigma_{ij}(u^t)\varepsilon_{ij}(u)\,dy - \langle \lambda^t, \nu^\top u \rangle_{\Gamma_C} = \int_\Omega f_i u_i \,dy + \int_{\Gamma_N} g^\top u \,ds \quad \text{for all } u \in H. \tag{29}$$

Applying Green's formula similar to (11) with u^t instead of u^0 in the standard way from (29), we arrive at (27c).

Conversely, let (27) hold true. In view of (27a) we get

$$\langle \mu, \nu^\top u^t - \psi \rangle_{\Gamma_C} = 0 \quad \text{for all } \mu \in M_t. \tag{30}$$

The minimization problem: Find $u^t \in H$ such that $\nu^\top u^t = \psi$ at A^t fulfilling (27b) is equivalent to the variational inequality

$$\begin{aligned}
&\int_\Omega \sigma_{ij}(u^t)\varepsilon_{ij}(u - u^t)\,dy - \int_\Omega f_i(u - u^t)_i\,dy - \int_{\Gamma_N} g^\top (u - u^t)\,ds \ge 0\\
&\quad \text{for all } u \in H: \nu^\top u = \psi \quad \text{on } A^t.
\end{aligned} \tag{31}$$

Applying Green's formula to the left-hand side of (31), due to the equilibrium equation and boundary conditions fulfilled in (28), we derive the inequality

$$\langle \sigma_\nu(u^t), \nu^\top (u - u^t) \rangle_{\Gamma_C} \ge 0 \quad \text{for all } u \in H: \nu^\top u = \psi \quad \text{on } A^t. \tag{32}$$

Substituting $u=u^t\pm\xi$ in (32) with $\xi\in H$ such that $\xi=0$ at A^t and using (27c), we conclude that $\lambda^t\in M_t$. Hence, (30) gets

$$L(u^t,\mu)=L(u^t,\lambda^t)\quad\text{for all}\ \ \mu\in M_t.$$

Green's formula provides us with the equality (29), which is equivalent to

$$L(u^t,\lambda^t)\le L(u,\lambda^t)\quad\text{for all}\ \ u\in H.$$

Thus we obtain the equation and the inequality in (26).

In view of the unique solvability of the minimization problem fulfilling (27a) and (27b), the solution $(u^t,\lambda^t)\in H\times M_t$ to (26) exists, is unique, and satisfies the optimality conditions

$$\int_\Omega \sigma_{ij}(u^t)\varepsilon_{ij}(u)\,\mathrm{d}y-\langle\lambda^t,\nu^\top u\rangle_{\Gamma_C}=\int_\Omega f_iu_i\,\mathrm{d}y+\int_{\Gamma_N} g^\top u\,\mathrm{d}s \quad \text{for all}\ \ u\in H, \tag{33a}$$

$$\langle\mu,\nu^\top u^t-\psi\rangle_{\Gamma_C}=0\quad\text{for all}\ \ \mu\in M_t. \tag{33b}$$

Our aim is to expand (33) with respect to $t\to 0$. To this purpose we employ the coordinate transformation (25). Obviously, $A^t\circ\Phi=A^0$. The following one-to-one correspondence property holds true:

$$\begin{aligned}&(u,\lambda)\in H\times M_0\Rightarrow(u\circ\Phi^{-1},\lambda\circ\Phi^{-1})\in H\times M_t,\\&(u,\mu)\in H\times M_t\Rightarrow(u\circ\Phi,\mu\circ\Phi)\in H\times M_0,\end{aligned} \tag{34}$$

where the transformation of distributions λ and μ in (34) is defined in the generalized sense:

$$\begin{aligned}&\langle\lambda\circ\Phi^{-1},\xi\rangle_{\Gamma_C}:=\langle\lambda,\omega(\xi\circ\Phi)\rangle_{\Gamma_C}\quad\text{for}\ \ \xi\in H_{00}^{1/2}(\Gamma_C),\\&\langle\mu\circ\Phi,\xi\rangle_{\Gamma_C}:=\langle\mu,(\omega^{-1}\xi)\circ\Phi^{-1}\rangle_{\Gamma_C}\quad\text{for}\ \ \xi\in H_{00}^{1/2}(\Gamma_C),\end{aligned} \tag{35}$$

with the Jacobian at Γ_C

$$\omega=\det(\Phi_{,x})\big|(\Phi_{,x}^{-1})^\top\nu\big|. \tag{36}$$

It will be shown later in (38) that the Jacobian ω is strictly positive for small t.

4. Sensitivity analysis

4.1. Expansion of the operator of the problem

We start with expansions of the used functions as $t\to 0$. For this purpose we assume the sufficient smoothness of data involved later. From (24) it follows that

$$\begin{aligned}&\Phi=x+tV+\tfrac{t^2}{2}W+\cdots,\quad W:=V_{,t}+V_{,x}V,\\&\Phi_{,x}=I+tV_{,x}+\tfrac{t^2}{2}W_{,x}+\cdots,\\&\Phi_{,x}^{-1}=I-tV_{,x}+\tfrac{t^2}{2}\big(2V_{,x}V_{,x}-W_{,x}\big)+\cdots,\\&\det(\Phi_{,x})=1+t\,\mathrm{div}V+\tfrac{t^2}{2}\big(2\det(V_{,x})-\mathrm{div}W\big)+\cdots,\end{aligned} \tag{37}$$

where I means the identity operator, and the following notation is used:

$$\xi_{,x}:=(\xi_{,j})_{j=1}^N=(\nabla\xi)^\top\quad\text{for}\,\xi:\mathbb{R}^N\to\mathbb{R},$$

$$\xi_{,x}:=(\xi_{i,j})_{i,j=1}^N,\quad\mathrm{div}\xi:=\xi_{i,i}\quad\text{for}\,\xi:\mathbb{R}^N\to\mathbb{R}^N.$$

From (36) and (37) we derive

$$\omega = 1 + t\,\mathrm{div}_\tau V + \tfrac{t^2}{2}\omega^{(2)} + \cdots,$$
$$\omega^{(2)} = 2\big(\det(V_{,x}) + \nu^\top V_{,x} V_{,x}\nu\big) + |V_{,x}\nu|^2 - \mathrm{div}_\tau V(\nu^\top V_{,x}\nu), \tag{38}$$

with the standard notation of tangential derivatives at Γ_C as

$$\nabla_\tau \xi \ := \nabla\xi - (\nu^\top \nabla\xi)\nu \quad \text{for} \ \xi : \mathbb{R}^N \to \mathbb{R},$$
$$\mathrm{div}_\tau \xi := \mathrm{div}\xi - \nu^\top \xi_{,x}\nu \quad \text{for} \ \xi : \mathbb{R}^N \to \mathbb{R}^N. \tag{39}$$

Taylor expansion of a smooth function $\xi : \mathbb{R}^N \to \mathbb{R}$ provides

$$\xi \circ \Phi = \xi + tV^\top \nabla\xi + \frac{t^2}{2}\big(V^\top \nabla\xi_{,x} V + W^\top \nabla\xi\big) + \cdots. \tag{40}$$

Since $u_{,y} = (u \circ \Phi)_{,x}\Phi_{,x}^{-1}$ we arrive at the generalized strain tensor

$$E_{ij}(\Phi_{,x}^{-1}; u) := 0.5\big(u_{i,k}\Phi_{k,j}^{-1} + u_{j,k}\Phi_{k,i}^{-1}\big) \quad i, j = 1, \cdots, N, \tag{41}$$

which admits a decomposition as $t \to 0$, in view of (37), as

$$E_{ij}(\Phi_{,x}^{-1}; u) = \varepsilon_{ij}(u) - tE_{ij}(V_{,x}; u) + \frac{t^2}{2}E_{ij}(2V_{,x}V_{,x} - W_{,x}; u) + \cdots \tag{42}$$

Note that the coordinate transformation (25) applied to (33), with account taken of (34), (35), and (41), results in an equivalent problem with respect to $(u^t \circ \Phi, \lambda^t \circ \Phi) \in H \times M_0$:

$$\int_\Omega \det(\Phi_{,x})(c_{ijkl} \circ \Phi)E_{kl}(\Phi_{,x}^{-1}; u^t \circ \Phi)E_{ij}(\Phi_{,x}^{-1}; u)\,\mathrm{d}x$$
$$-\langle \lambda^t \circ \Phi, \omega(\nu \circ \Phi)^\top u\rangle_{\Gamma_C} = \int_\Omega \det(\Phi_{,x})(f_i \circ \Phi)u_i\,\mathrm{d}x + \int_{\Gamma_N} g^\top u\,\mathrm{d}s \quad \text{for all} \ u \in H, \tag{43a}$$

$$\langle \lambda, \omega\big((\nu \circ \Phi)^\top (u^t \circ \Phi) - \psi \circ \Phi\big)\rangle_{\Gamma_C} = 0 \quad \text{for all} \ \lambda \in M_0. \tag{43b}$$

With the help of expansions (37), (38), (40), and (42) we can expand the terms in (43) as

$$\int_\Omega \det(\Phi_{,x})(c_{ijkl} \circ \Phi)E_{kl}(\Phi_{,x}^{-1}; u)E_{ij}(\Phi_{,x}^{-1}; u)\,\mathrm{d}x$$
$$= \int_\Omega \Big(\sigma_{ij}(u)\varepsilon_{ij}(u) + ta^{(1)}(V; u, u) + \frac{t^2}{2}a^{(2)}(V, W; u, u) + \cdots\Big)\,\mathrm{d}x,$$
$$\langle \lambda, \omega(\nu \circ \Phi)^\top u\rangle_{\Gamma_C} = \langle \lambda, \nu^\top u + tb^{(1)}(V; \nu_i)u_i + \frac{t^2}{2}b^{(2)}(V, W; \nu_i)u_i + \cdots\rangle_{\Gamma_C},$$
$$\int_\Omega \det(\Phi_{,x})(f_i \circ \Phi)u_i\,\mathrm{d}x = \int_\Omega \Big(f_i u_i + t\,\mathrm{div}(Vf_i)u_i + \frac{t^2}{2}c^{(2)}(V, W; f_i)u_i + \cdots\Big)\,\mathrm{d}x, \tag{44}$$
$$\langle \lambda, \omega\big((\nu \circ \Phi)^\top (u^t \circ \Phi) - \psi \circ \Phi\big)\rangle_{\Gamma_C} = \langle \lambda, \nu^\top u - \psi + t\big(b^{(1)}(V; \nu_i)u_i - b^{(1)}(V; \psi)\big)$$
$$+ \frac{t^2}{2}\big(b^{(2)}(V, W; \nu_i)u_i - b^{(2)}(V, W; \psi)\big) + \cdots\rangle_{\Gamma_C},$$

where

$$a^{(1)}(V; u, u) \ := \mathrm{div}(Vc_{ijkl})\varepsilon_{kl}(u)\varepsilon_{ij}(u) - 2\sigma_{ij}(u)E_{ij}(V_{,x}; u),$$
$$b^{(1)}(V; \psi) := \mathrm{div}_\tau V\psi + V^\top \nabla\psi, \ b^{(1)}(V; \nu_i) := \mathrm{div}_\tau V\nu_i + (\nu_{,x}V)_i, \tag{45a}$$

$$
\begin{aligned}
&a^{(2)}(V,W;u,u) := \big(2\det(V_{,x}) - \operatorname{div} W\big)\sigma_{ij}(u)\varepsilon_{ij}(u)\\
&\quad +\big(2\operatorname{div} V(V^\top \nabla c_{ijkl}) + V^\top \nabla c_{ijkl,x} V + W^\top \nabla c_{ijkl}\big)\varepsilon_{kl}(u)\varepsilon_{ij}(u)\\
&\quad -4\operatorname{div}(V c_{ijkl})\varepsilon_{kl}(u)E_{ij}(V_{,x};u) + 2c_{ijkl}E_{kl}(V_{,x};u)E_{ij}(V_{,x};u)\\
&\quad +2\sigma_{ij}(u)E_{ij}(2V_{,x}V_{,x} - W_{,x};u),\\
&b^{(2)}(V,W;\psi) := 2\operatorname{div}_\tau V(V^\top \nabla\psi) + V^\top \nabla\psi_{,x} V + W^\top \nabla\psi + \omega^{(2)}\psi,\\
&b^{(2)}(V,W;\nu_i) := 2\operatorname{div}_\tau V(V^\top \nabla\nu_i) + V^\top \nabla\nu_{i,x} V + W^\top \nabla\nu_i + \omega^{(2)}\nu_i,\\
&c^{(2)}(V,W;f_i) := \big(2\det(V_{,x}) - \operatorname{div} W\big) f_i\\
&\quad +2\operatorname{div} V(V^\top \nabla f_i) + V^\top \nabla f_{i,x} V + W^\top \nabla f_i \quad i=1,\dots,N.
\end{aligned}
\tag{45b}
$$

Note that $\nu_{,x}V$ is a vector tangential at Γ_C since $\nu^\top \nu_{,x}V=0$ due to $\nu^\top\nu=1$.

4.2. Material derivatives of the solution

We look for a global expansion as $t\to 0$ of the primal and the dual variables in the form

$$
\begin{aligned}
u^t\circ\Phi &= u^0 + t\dot u_V + \frac{t^2}{2}\ddot u_V + \cdots \quad \text{in } H,\\
\lambda^t\circ\Phi &= \lambda^0 + t\dot\lambda_V + \frac{t^2}{2}\ddot\lambda_V + \cdots \quad \text{in } M_0,
\end{aligned}
\tag{46}
$$

where the dot and the subscript V stand for the directional (material) derivative of a function in direction of the velocity vector V. The substitution of (46) in (43) together with (44) provide formal equations for the expansion terms of the same powers of t. The equations for the zero-power terms coincides with (14) and (21). To obtain zero terms at the first-power of t in the expansion of (43), we should determine $(\dot u_V, \dot\lambda_V)\in H\times M_0$ satisfying the following system

$$
\begin{aligned}
\int_\Omega \sigma_{ij}(\dot u_V)\varepsilon_{ij}(u)\,\mathrm{d}x - \langle\dot\lambda_V, \nu^\top u\rangle_{\Gamma_C} = \int_\Omega \big(\operatorname{div}(Vf_i)u_i\\
-a^{(1)}(V;u^0,u)\big)\,\mathrm{d}x + \langle\lambda^0, b^{(1)}(V;\nu_i)u_i\rangle_{\Gamma_C} \quad \text{for all } u\in H,
\end{aligned}
\tag{47a}
$$

$$
\langle\lambda, \nu^\top\dot u_V + b^{(1)}(V;\nu_i)u_i^0 - b^{(1)}(V;\psi)\rangle_{\Gamma_C} = 0 \quad \text{for all } \lambda\in M_0.
\tag{47b}
$$

Relations (47) can be obtained as optimality conditions for the minimax problem: Find $(\dot u_V, \dot\lambda_V)\in H\times M_0$ such that

$$
L^1(\dot u_V,\lambda) = L^1(\dot u_V,\dot\lambda_V) \le L^1(u,\dot\lambda_V) \quad \text{for all } (u,\lambda)\in H\times M_0,
\tag{48}
$$

where

$$
\begin{aligned}
L^1(u,\lambda) := \int_\Omega \left(\frac{1}{2}\sigma_{ij}(u)\varepsilon_{ij}(u) + a^{(1)}(V;u^0,u) - \operatorname{div}(Vf_i)u_i\right)\mathrm{d}x\\
-\langle\lambda, \nu^\top u + b^{(1)}(V;\nu_i)u_i^0 - b^{(1)}(V;\psi)\rangle_{\Gamma_C} - \langle\lambda^0, b^{(1)}(V;\nu_i)u_i\rangle_{\Gamma_C}.
\end{aligned}
\tag{49}
$$

Problem (48) (hence (47)) is well-posed, similarly to (26), due to the fact that the quadratic functionals L^1 in (49) and L in (15) coincide in the second-order terms, and only their linear terms are different.

We apply to (47a) formally Green's formula and derive with the help of (45a), (6), and (23) the following identity

$$\int_\Omega \big(\mathrm{div}(Vf_i)u_i - a^{(1)}(V;u^0,u)\big)\,\mathrm{d}x + \int_{\Gamma_C} \lambda^0 b^{(1)}(V;\nu_i)u_i\,\mathrm{d}s = -\int_\Omega \sigma_{ij,j}(u^0_{,x}V)u_i\,\mathrm{d}x \\ +\int_{\Gamma_C}\Big(d_\nu(V;u^0)(\nu^\top u) + \big(d_\tau(V;u_0)+\lambda^0(\nu_{,x}V)\big)^\top u_\tau\Big)\,\mathrm{d}s, \tag{50}$$

where $u_\tau = u-(\nu^\top u)\nu$, with the notation

$$d_\nu(V;u^0) := \big(-V^\top\nabla c_{ijkl}\varepsilon_{kl}(u^0) + c_{ijkl}E_{kl}(V_{,x};u^0)\big)\nu_j\nu_i, \\ d_\tau(V;u^0)_i := \big(-V^\top\nabla c_{ijkl}\varepsilon_{kl}(u^0) + c_{ijkl}E_{kl}(V_{,x};u^0)\big)\nu_j \\ -d_\nu(V;u^0)\nu_i + \sigma_{ij}(u^0)\nu_k V_{k,j} - \lambda^0(\nu^\top V_{,x}\nu)\nu_i \quad i=1,\dots,N. \tag{51}$$

Relations (11) and (50) lead to a mixed-boundary-value formulation of the variational problem (47) with respect to the primal variable $\dot u_V$ as follows:

$$\begin{aligned} -\sigma_{ij,j}(\dot u_V) &= -\sigma_{ij,j}(u^0_{,x}V) \quad i=1,\dots,N && \text{in } \Omega,\\ \dot u_V &= 0 && \text{on } \Gamma_D,\\ \sigma_{ij}(\dot u_V)\nu_j &= 0 \quad i=1,\dots,N && \text{on } \Gamma_N,\\ \sigma_\tau(\dot u_V) &= d_\tau(V;u_0)+\lambda^0(\nu_{,x}V) && \text{on } \Gamma_C,\\ \sigma_\nu(\dot u_V) &= d_\nu(V;u_0) && \text{on } I^0,\\ \nu^\top\dot u_V &= b^{(1)}(V;\psi) - (\nu_{,x}V)^\top u^0_\tau && \text{on } A^0, \end{aligned} \tag{52}$$

and $\dot\lambda_V = \sigma_\nu(\dot u_V) - d_\nu(V;u_0)$. Note that (52) differs from (28) (with $t=0$) only in the right-hand sides.

To obtain that the terms of the second power of t are zero in the expansion of (43), we should determine the second-order material derivatives $(\ddot u_V, \ddot\lambda_V)\in H\times M_0$ from the equations

$$\int_\Omega \sigma_{ij}(\ddot u_V)\varepsilon_{ij}(u)\,\mathrm{d}x - \langle\ddot\lambda_V, \nu^\top u\rangle_{\Gamma_C} \\ = \int_\Omega\big(c^{(2)}(V,W;f_i)u_i - 2a^{(1)}(V;\dot u_V,u) - a^{(2)}(V,W;u^0,u)\big)\,\mathrm{d}x \\ +2\langle\dot\lambda_V, b^{(1)}(V;\nu_i)u_i\rangle_{\Gamma_C} + \langle\lambda^0, b^{(2)}(V,W;\nu_i)u_i\rangle_{\Gamma_C} \quad \text{for } u\in H, \tag{53a}$$

$$\langle\lambda, \nu^\top\ddot u_V + 2b^{(1)}(V;\nu_i)(\dot u_V)_i + b^{(2)}(V,W;\nu_i)u^0_i \\ -b^{(2)}(V,W;\psi)\rangle_{\Gamma_C} = 0 \quad \text{for all } \lambda\in M_0. \tag{53b}$$

The unique solvability of (53) can be obtained similarly to (47), and this system implies the optimality conditions for the minimax problem: Find $(\ddot u_V, \ddot\lambda_V)\in H\times M_0$ such that

$$L^2(\ddot u_V,\lambda) = L^2(\ddot u_V,\ddot\lambda_V) \le L^2(u,\ddot\lambda_V) \quad \text{for all } (u,\lambda)\in H\times M_0, \tag{54}$$

with the Lagrangian

$$L^2(u,\lambda) := \int_\Omega\left(\frac12\sigma_{ij}(u)\varepsilon_{ij}(u) + 2a^{(1)}(V;\dot u_V,u) + a^{(2)}(V,W;u^0,u) - c^{(2)}(V,W;f_i)u_i\right)\mathrm{d}x \\ -\langle\lambda, \nu^\top u + 2b^{(1)}(V;\nu_i)(\dot u_V)_i + b^{(2)}(V,W;\nu_i)u^0_i - b^{(2)}(V,W;\psi)\rangle_{\Gamma_C} \\ -2\langle\dot\lambda_V, b^{(1)}(V;\nu_i)u_i\rangle_{\Gamma_C} - \langle\lambda^0, b^{(2)}(V,W;\nu_i)u_i\rangle_{\Gamma_C}. \tag{55}$$

Also higher-order derivatives can be determined in the same way. Justification of the global asymptotic expansion will be given in the Appendix.

5. Shape differentiability

5.1. Asymptotic expansion of the potential energy

Let us consider a reduced function of the potential energy for the perturbed problem (33) depending on the parameter t as follows

$$P(t) := \Pi(u^t) = L(u^t, \lambda^t) = \frac{1}{2}\int_\Omega \sigma_{ij}(u^t)\varepsilon_{ij}(u^t)\,\mathrm{d}x - \int_\Omega f_i u_i^t\,\mathrm{d}x - \int_{\Gamma_N} g^\top u^t\,\mathrm{d}s. \tag{56}$$

Respectively, for the unperturbed problem (14), (21) we have according to (8) and (56) that at $t=0$

$$P(0) = \Pi(u^0) = L(u^0, \lambda^0). \tag{57}$$

Now we give an expansion of (56) with respect to $t \to 0$ with the help of (46).

The coordinate transformation (25) applied to (56) provides its equivalent representation

$$\begin{aligned} P(t) = \int_\Omega \Big(&\frac{1}{2}\det(\Phi_{,x})(c_{ijkl}\circ\Phi)E_{kl}(\Phi_{,x}^{-1}; u^t\circ\Phi)E_{ij}(\Phi_{,x}^{-1}; u^t\circ\Phi) \\ &-\det(\Phi_{,x})(f_i\circ\Phi)(u^t\circ\Phi)_i\Big)\,\mathrm{d}x + \int_{\Gamma_N} g^\top(u^t\circ\Phi)\,\mathrm{d}s. \end{aligned} \tag{58}$$

An asymptotic expansion of (58) as $t \to 0$ can be obtained by using (44), (46), and (A8) in the form

$$P(t) = P(0) + tP_V'(0) + \frac{t^2}{2}P_V''(0) + o(t^2), \tag{59}$$

where

$$P_V'(0) = \int_\Omega \Big(\sigma_{ij}(u^0)\varepsilon_{ij}(\dot u_V) + \frac{1}{2}a^{(1)}(V; u^0, u^0) - \operatorname{div}(Vf_i)u_i^0 - f_i(\dot u_V)_i\Big)\,\mathrm{d}x - \int_{\Gamma_N} g^\top \dot u_V\,\mathrm{d}s, \tag{60a}$$

$$\begin{aligned} P_V''(0) = \int_\Omega \big(&\sigma_{ij}(u^0)\varepsilon_{ij}(\ddot u_V) + \sigma_{ij}(\dot u_V)\varepsilon_{ij}(\dot u_V) + 2a^{(1)}(V; u^0, \dot u_V) + \frac{1}{2}a^{(2)}(V, W; u^0, u^0) \\ &-c^{(2)}(V, W; f_i)u_i^0 - 2\operatorname{div}(Vf_i)(\dot u_V)_i - f_i(\ddot u_V)_i\big)\,\mathrm{d}x - \int_{\Gamma_N} g^\top \ddot u_V\,\mathrm{d}s. \end{aligned} \tag{60b}$$

The substitution of $u = \dot u_V$ in (14) and $\lambda = \lambda^0$ in (47b) provides the equality

$$\int_\Omega \sigma_{ij}(u^0)\varepsilon_{ij}(\dot u_V)\,\mathrm{d}x + \langle\lambda^0, b^{(1)}(V; \nu_i)u_i^0 - b^{(1)}(V;\psi)\rangle_{\Gamma_C} = \int_\Omega f_i(\dot u_V)_i\,\mathrm{d}x + \int_{\Gamma_N} g^\top \dot u_V\,\mathrm{d}s,$$

and the following representation of the first derivative in (60a) is obtained as

$$P_V'(0) = \int_\Omega \Big(\frac{1}{2}a^{(1)}(V; u^0, u^0) - \operatorname{div}(Vf_i)u_i^0\Big)\,\mathrm{d}x - \langle\lambda^0, b^{(1)}(V;\nu_i)u_i^0 - b^{(1)}(V;\psi)\rangle_{\Gamma_C}, \tag{61}$$

which is independent of the material derivatives of the solution. We recall the definition of $b^{(1)}$ in (45a) and note that

$$\langle\lambda^0, \operatorname{div}_\tau V(\nu^\top u^0 - \psi)\rangle_{\Gamma_C} = 0, \tag{62}$$

due to the fact that $\nu^\top u^0-\psi=0$ at A^0 and $\lambda^0=0$ at I^0. Therefore, accounting for (62), from (61) we arrive at the final formula

$$P'_V(0)=\int_\Omega\left(\frac{1}{2}a^{(1)}(V;u^0,u^0)-\mathrm{div}(Vf_i)u_i^0\right)\mathrm{d}x-\langle\lambda^0,\,V^\top(\nu_{,x}^\top u^0-\nabla\psi)\rangle_{\Gamma_C}. \tag{63}$$

Similarly, the substitution of $u=\ddot{u}_V$ in (14), $\lambda=\lambda^0$ in (53b), and $u=\dot{u}_V$ in (47a) yields

$$\int_\Omega\sigma_{ij}(u^0)\varepsilon_{ij}(\ddot{u}_V)\,\mathrm{d}x+\langle\lambda^0,2b^{(1)}(V;\nu_i)(\dot{u}_V)_i+b^{(2)}(V,W;\nu_i)u_i^0$$
$$-b^{(2)}(V,W;\psi)\rangle_{\Gamma_C}=\int_\Omega f_i(\ddot{u}_V)_i\,\mathrm{d}x+\int_{\Gamma_N}g^\top\ddot{u}_V\,\mathrm{d}s,$$
$$\int_\Omega\sigma_{ij}(\dot{u}_V)\varepsilon_{ij}(\dot{u}_V)\,\mathrm{d}x=\int_\Omega\big(\mathrm{div}(Vf_i)(\dot{u}_V)_i-a^{(1)}(V;u^0,\dot{u}_V)\big)\,\mathrm{d}x$$
$$+\langle\lambda^0,b^{(1)}(V;\nu_i)(\dot{u}_V)_i\rangle_{\Gamma_C}$$

and the representation of the second derivative in (60b) as

$$P''_V(0)=\int_\Omega\left(\frac{1}{2}a^{(2)}(V,W;u^0,u^0)-\sigma_{ij}(\dot{u}_V)\varepsilon_{ij}(\dot{u}_V)\right.$$
$$\left.-c^{(2)}(V,W;f_i)u_i^0\right)\mathrm{d}x-\langle\lambda^0,b^{(2)}(V,W;\nu_i)u_i^0-b^{(2)}(V,W;\psi)\rangle_{\Gamma_C}, \tag{64}$$

which is dependent only on the first material derivatives of the solution. Higher-order derivatives of P can be derived in a similar way.

5.2. The case of a smooth solution

In this section we assume that the solution (u^0,λ^0) to (14), (21) possesses an additional $H^2\times L^2$-regularity on the support of V in Ω. This assumption holds true for smooth data.

Integration by parts applied to the integral in (61) gives

$$\begin{aligned}\int_\Omega\left(\frac{1}{2}a^{(1)}(V;u^0,u^0)-\mathrm{div}(Vf_i)u_i^0\right)\mathrm{d}x&=\int_\Omega\big(\sigma_{ij,j}(u^0)+f_i\big)V^\top\nabla u_i^0\,\mathrm{d}x\\&-\int_{\partial\Omega}\big(\sigma_{ij}(u^0)\nu_j(V^\top\nabla u_i^0)+(\nu^\top V)f_iu_i^0\big)\,\mathrm{d}s.\end{aligned} \tag{65}$$

Due to the regularity of u^0, we can represent the boundary term in (63) with the help of (39) and the following identity

$$\begin{aligned}V^\top(\nu_{,x}^\top u^0-\nabla\psi)&=V^\top\big(\nabla_\tau(\nu^\top u^0-\psi)-(u_{,x}^0)^\top\nu\big)\\&+(\nu^\top V)\big(\nu^\top\nu_{,x}^\top u^0+\nu^\top(u_{,x}^0)^\top\nu-\nu^\top\nabla\psi\big).\end{aligned} \tag{66}$$

Using (23), decomposition (7), and relations (6), it follows that

$$\sigma_{ij}(u^0)\nu_j(V^\top\nabla u_i^0)=\lambda_0(V^\top(u_{,x}^0)^\top\nu)\quad\text{on }\Gamma_C,$$

and from (63), (65), and (66) we derive the equality

$$P'_V(0)=-\int_{\Gamma_C}\lambda^0V^\top\nabla_\tau(\nu^\top u^0-\psi)\,\mathrm{d}s.$$

In view of the smoothness of the solution and the complementarity conditions (6e) at Γ_C, $\nu^\top u^0-\psi=0$ is fulfilled and, additionally, $\nabla_\tau(\nu^\top u^0-\psi)=0$ on the active set A^0. On the other hand, $\lambda^0=0$ on the inactive set I^0. Thus $P'_V(0)=0$ in this case.

6. Concluding remarks

Restating the contact problem (6) as a mixed-boundary-value contact problem (28) (with $t=0$), we avoid the nonlinearity feature of the contact problem. However, without employing dual arguments, we would encounter the following difficulty. Note that the following two sets are different

$$\{u \in H: \quad \nu^\top u = \psi \quad \text{on } A^0\}$$
$$\neq \{u \circ \Phi \in H: \quad (\nu \circ \Phi)^\top u \circ \Phi = \psi \circ \Phi \quad \text{on } A^0 = A^t \circ \Phi\}$$

when considering the curvilinear boundary in contact. Consequently, there is no one-to-one correspondence between

$$\{u \in H: \nu^\top u = \psi \text{ on } A^0\} \quad \text{and} \quad \{u \in H: \nu^\top u = \psi \text{ on } A^t\}.$$

This feature renders the sensitivity analysis difficult within a primal formulation of the contact problem. Employing the dual variable (contact force) in the minimax problem (26), which is equivalent to (28), we provide the required property of one-to-one correspondence stated in (34). Thus, relaxing on the primal-dual formulation of the mixed-boundary-value contact problem provides the treatment of curvilinear boundaries in contact.

The other principal point of our approach concerns the equivalence of the contact problem (6) and the mixed-boundary-value contact problem (28) (with $t=0$). Generally speaking, these two problems are different. Of course, they are the same in the case of smooth solutions and in the finite-dimensional (discrete) setting of the problems. Nevertheless, in (18) and (19) we get a sufficient property for the equivalence in the general setting of the contact problem.

One of the findings of our study is that the derivative of the potential-energy functional with respect to perturbations of the active (contact) set is zero for the contact problem. However, we do not have its converse assertion. Generally speaking, only the inequalities in (3b) guarantee that the solution obtained in (4) is also a solution to the contact problem (1).

Finally, we stress that the obtained asymptotic formulas are useful for applications, since they provide approximations of the solution to the contact problem, which is nonlinear, by employing mixed-boundary-value problems only, which are linear.

Acknowledgement

The research results are obtained with the support of the Russian Foundation for Basic Research (grant 03-01-00124) and the INTAS Project 03-51-6046.

Appendix

Let us justify rigorously expansion (46) for the solutions of (20), (26), (48), and (54).

From (43a) we can derive that there exists a small constant $t_0 > 0$ such that the following estimation is uniform for all $0 \le t \le t_0$:

$$\|u^t \circ \Phi\|_H + \|\lambda^t \circ \Phi\|_{M_0} \le \text{const.} \tag{A1}$$

Due to $\lambda^0, \lambda^t \circ \Phi \in M_0$, the substitution of $\lambda^t \circ \Phi - \lambda^0$ in (21) and (43b) provides in view of (44) that

$$\langle \lambda^t \circ \Phi - \lambda^0, \nu^\top (u^t \circ \Phi - u^0) \rangle_{\Gamma_C} = -t \langle \lambda^t \circ \Phi - \lambda^0, b^{(1)}(V; \nu_i)(u^t \circ \Phi)_i - b^{(1)}(V; \psi) \rangle_{\Gamma_C} + o(t).$$

Therefore, substituting $u^t \circ \Phi - u^0$ in (14) and (43a) yields the decomposition

$$\int_\Omega \sigma_{ij}(u^t \circ \Phi - u^0)\varepsilon_{ij}(u^t \circ \Phi - u^0)\,\mathrm{d}x = t\int_\Omega \big(\mathrm{div}(Vf_i)(u^t \circ \Phi - u^0)_i - a^{(1)}(V; u^0, u^t \circ \Phi - u^0)\big)\,\mathrm{d}x - t\langle \lambda^t \circ \Phi, b^{(1)}(V;\nu_i)u_i^0 - b^{(1)}(V;\psi)\rangle_{\Gamma_C} + t\langle \lambda^0, b^{(1)}(V;\nu_i)(u^t \circ \Phi)_i - b^{(1)}(V;\psi)\rangle_{\Gamma_C} + o(t),$$

and due to (A1) it follows the uniform estimation

$$\|u^t \circ \Phi - u^0\|_H \le \mathrm{c}t. \tag{A2}$$

Now from (14) and (43a) we derive that for $u \in H$

$$\langle \lambda^t \circ \Phi - \lambda^0, \nu^\top u\rangle_{\Gamma_C} = \int_\Omega \sigma_{ij}(u^t \circ \Phi - u^0)\varepsilon_{ij}(u)\,\mathrm{d}x - t\int_\Omega \big(\mathrm{div}(Vf_i)u_i - a^{(1)}(V; u^t \circ \Phi, u)\big)\,\mathrm{d}x - t\langle \lambda^t \circ \Phi, b^{(1)}(V;\nu_i)u_i\rangle_{\Gamma_C} + o(t),$$

and in view of (A1) and (A2) we conclude with the next estimation

$$\|u^t \circ \Phi - u^0\|_H + \|\lambda^t \circ \Phi - \lambda^0\|_{M_0} \le \mathrm{c}t. \tag{A3}$$

Similarly, from (14), (43a), and (47a), which is multiplied by t, it follows that

$$\langle \lambda^t \circ \Phi - \lambda^0 - t\dot{\lambda}_V, \nu^\top u\rangle_{\Gamma_C} = \int_\Omega \Big(\sigma_{ij}(u^t \circ \Phi - u^0 - t\dot{u}_V)\varepsilon_{ij}(u) + t a^{(1)}(V; u^t \circ \Phi - u^0, u) + \frac{t^2}{2}a^{(2)}(V, W; u^t \circ \Phi, u) - \frac{t^2}{2}c^{(2)}(V, W; f_i)u_i\Big)\,\mathrm{d}x - \frac{t^2}{2}\langle \lambda^t \circ \Phi, b^{(2)}(V, W;\nu_i)u_i\rangle_{\Gamma_C} + o(t^2). \tag{A4}$$

The substitution of $\lambda = \lambda^t \circ \Phi - \lambda^0 - t\dot{\lambda}_V$ in (21), (43b), and (47b), which is multiplied by t, provides the decomposition

$$\langle \lambda^t \circ \Phi - \lambda^0 - t\dot{\lambda}_V, \nu^\top(u^t \circ \Phi - u^0 - t\dot{u}_V)\rangle_{\Gamma_C} = -\langle \lambda^t \circ \Phi - \lambda^0 - t\dot{\lambda}_V, t b^{(1)}(V;\nu_i)(u^t \circ \Phi - u^0)_i + \frac{t^2}{2}b^{(2)}(V, W;\nu_i)(u^t \circ \Phi)_i - \frac{t^2}{2}b^{(2)}(V, W;\psi)\rangle_{\Gamma_C} + o(t^2). \tag{A5}$$

Taking $u = u^t \circ \Phi - u^0 - t\dot{u}_V$ as a test function in (A4) and subtracting it from (A5), we have the identity

$$\begin{aligned}
&\int_\Omega \sigma_{ij}(u^t \circ \Phi - u^0 - t\dot{u}_V)\varepsilon_{ij}(u^t \circ \Phi - u^0 - t\dot{u}_V)\,\mathrm{d}x\\
&= -\int_\Omega \Big(t a^{(1)}(V; u^t \circ \Phi - u^0, u^t \circ \Phi - u^0 - t\dot{u}_V) + \frac{t^2}{2}a^{(2)}(V, W; u^t \circ \Phi, u^t \circ \Phi - u^0 - t\dot{u}_V)\\
&\quad - \frac{t^2}{2}c^{(2)}(V, W; f_i)(u^t \circ \Phi - u^0 - t\dot{u}_V)_i\Big)\,\mathrm{d}x\\
&\quad - \langle \lambda^t \circ \Phi - \lambda^0 - t\dot{\lambda}_V, t b^{(1)}(V;\nu_i)(u^t \circ \Phi - u^0)_i - \frac{t^2}{2}b^{(2)}(V, W;\psi)\rangle_{\Gamma_C}\\
&\quad + t\langle \lambda^0, b^{(1)}(V;\nu_i)(u^t \circ \Phi)_i - \frac{t^2}{2}\langle \lambda^0 + t\dot{\lambda}_V, b^{(2)}(V, W;\nu_i)(u^t \circ \Phi)_i\rangle_{\Gamma_C}\\
&\quad - \frac{t^2}{2}\langle \lambda^t \circ \Phi, b^{(2)}(V, W;\nu_i)(u^0 + t\dot{u}_V)_i\rangle_{\Gamma_C} + o(t^2).
\end{aligned}$$

Hence, in view of (A1) and (A3), this implies the uniform estimate

$$\|u^t \circ \Phi - u^0 - t\dot{u}_V\|_H \leq \mathrm{c}t^2. \tag{A6}$$

Relations (A4) and (A6) then result in the final estimation

$$\|u^t \circ \Phi - u^0 - t\dot{u}_V\|_H + \|\lambda^t \circ \Phi - \lambda^0 - t\dot{\lambda}_V\|_{M_0} \leq \mathrm{c}t^2. \tag{A7}$$

A rigorous justification of the second-order expansion in (46) with

$$\|u^t \circ \Phi - u^0 - t\dot{u}_V - \frac{t^2}{2}\ddot{u}_V\|_H + \|\lambda^t \circ \Phi - \lambda^0 - t\dot{\lambda}_V - \frac{t^2}{2}\ddot{\lambda}_V\|_{M_0} \leq \mathrm{c}t^3 \tag{A8}$$

can be obtained in the same manner as (A7). To derive higher-order asymptotic terms in (46), one needs to repeat the procedure described above.

References

1. G. Duvaut and J.L. Lions, *Inequalities in Mechanics and Physics*. Berlin, New York: Springer-Verlag (1976) 397 pp.
2. N. Kikuchi and J.T. Oden, *Contact Problems in Elasticity: Study of Variational Inequalities and Finite Element Methods*. Philadelphia: SIAM (1988) 495 pp.
3. I.I. Argatov and N.N. Dmitriev, *Fundamentals of the Theory of Elastic Discrete Contact*. St. Petersburg: Polytechnics (2003) 233 pp. (in Russian)
4. M. Hintermüller, K. Ito and K. Kunisch, The primal-dual active set strategy as a semismooth Newton method. *SIAM J. Optim.* 13 (2003) 865–888.
5. K. Ito and K. Kunisch, Semi-smooth Newton methods for the variational inequalities of the first kind. *ESAIM Math. Modelling Numer. Anal.* 37 (2003) 41–62.
6. M. Hintermüller, V.A. Kovtunenko and K. Kunisch, Semismooth Newton methods for a class of unilaterally constrained variational problems. *Adv. Math. Sci. Appl.* 14 (2004) 513–535.
7. J. Sokolowski and J.-P. Zolesio, *Introduction to Shape Optimization. Shape Sensitivity Analysis*. Berlin, Heidelberg: Springer-Verlag (1992) 250 pp.
8. A.M. Khludnev and J. Sokolowski, *Modelling and Control in Solid Mechanics*. Basel, Boston, Berlin: Birkhäuser (1997) 366 pp.
9. A.M. Khludnev and V.A. Kovtunenko, *Analysis of Cracks in Solids*. Southampton, Boston: WIT-Press (2000) 408 pp.
10. M.C. Delfour and J.-P. Zolesio, *Shapes and Geometries: Analysis, Differential Calculus and Optimization*. Philadelphia: SIAM (2001) 461 pp.
11. C. Eck, S.A. Nazarov and W.L. Wendland, Asymptotic analysis for a mixed boundary-value contact problem. *Arch. Rational Mech. Anal.* 156 (2001) 275–316.
12. P. Grisvard, *Elliptic Problems in Nonsmooth Domains*. Boston: Pitman (1985) 410 pp.