Time derivatives of integrals and functionals defined on varying volume and surface domains

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THE EXPRESSIONS are derived for the first and second time derivatives of integrals and functionals whose volume or surface domains of integration vary in time. As an example, the time derivative of the potential energy in non-linear elasticity in the case of varying body domain is determined. A moving strain and stress discontinuity surface is also considered and the associated energy derivatives are obtained. The derivatives of functionals with additional constraint conditions are finally discussed by using the primary and adjoint state fields.

Wyprowadzono wzory na pierwsze i drugie pochodne czasowe całek i funkcjonałów, których dziedzina całkowania stanowi zmienny w czasie obszar objętościowy lub powierzchniowy. Jako przykład, określono pochodną czasową energii potencjalnej dla ciała nieliniowo sprężystego w przypadku zmiennego obszaru ciała. Rozpatrzono także ruchomą powierzchnię nieciągłości odkształceń i naprężeń oraz otrzymano odpowiednie wyrażenia na pochodne energii. Badano także pochodne funkcjonałów przy dodatkowych warunkach ograniczających, wykorzystując pola zmiennych pierwotnych i sprzężonych.

Выведены формулы для первой и второй временных производных интегралов и функциогалов, которых область интегрирования составляют переменные во времени объемная или поверхностная области. Как пример определена временная производная потенциальной энергии для нелинейно упругого тела в случае переменной области тела. Рассмотрена тоже подвижная поверхность разрыва деформаций и напряжений, получены соответствующие выражения для производных энергии. Исследованы производные функционалов при дополнительных ограничивающих условиях, используя поля первичных и сопряженных переменных.

1. Introduction

THE PRESENT paper is concerned with derivation of the expressions for first and second time derivatives of integrals and functionals defined on volume or surface domains which vary in time. Such derivatives are essential in sensitivity analysis associated with shape variation, cf. [1–7], when the variations of stress, strain and displacement fields or of integral functionals with respect to the shape transformation field are needed. The derivatives of integral functionals defined on varying domains are of importance in studying stability conditions for damaged structures, cf. DEMS and MRÓZ [4], in the analysis of phase-transformation processes or propagation of discontinuity surfaces, cf. ESHELBY [8], ABEYRATNE [9], etc. However, our analysis is intended to be sufficiently general to be applicable in various contexts of continuum or structural mechanics and applied mathematics.

Whereas the expression for the first derivative of volume integral is well known in the context of continuum mechanics, cf. for instance PRAGER [10] or MALVERN [11], this is not the case for the surface (or line) integrals, especially when the surface is composed

of several smooth sections intersecting along edge lines. A derivation of the expression for the first derivative of the surface integral defined over a regular moving surface can be found e.g. in the book by KOSIŃSKI [12]. However, the result presented in this paper is somewhat more general as it pertains to piecewise regular surfaces and contains the edge terms. The second time derivatives of volume or surface integrals or functionals defined on varying domains do not seem to be studied in the literature, to the authors' knowledge. They are essential in generating stability conditions in phase transformation [13, 14] or damage [4] problems and also in deriving strong optimality condition in optimal shape design of structures [1, 2].

In Sect 2 the expressions for first and second time derivatives of volume and surface integrals will be derived, while in Sect. 3 the derivatives of integral functionals will be considered. Some applications related to continuum mechanics will be presented in Sect. 4. In Sect. 5 the derivative of a functional with an additional constraint condition will be examined by using the concept of an adjoint system.

2. Time derivatives of volume, surface and line integrals

2.1. Fundamental definitions and relations

Consider a domain V_t in three-dimensional Euclidean space E_3 bounded by a closed surface $\hat{S}_t$, which is composed of a finite number or regular surface sections S_t intersecting along piecewise smooth edges $\hat{L}_t$, Fig. 1. It is assumed that the angle of intersection of
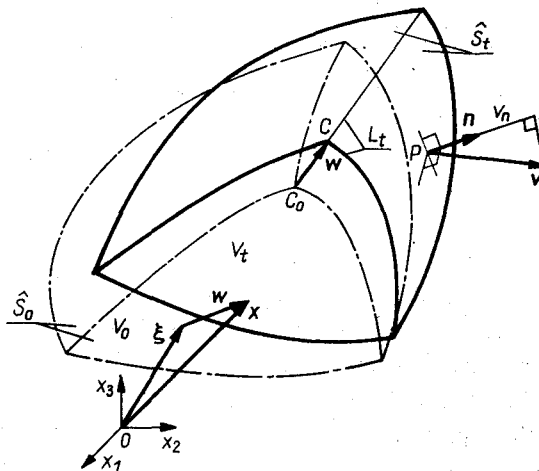

FIG. 1. Varying volume domain with piecewise regular boundary surface.

the surface sections or edges tends nowhere to zero. The subscript t indicates that the shape of the corresponding domain varies with a time-like parameter t, called time for simplicity. The reference shape corresponds to $t = 0$ and is indicated by the subscript 0. The shape transformation can be defined by specifying the transformation vector field $w = x - \xi$, where x and ξ denote the position vector of a typical point of the domain after

the shape transformation and at $t = 0$, respectively. Let the indices i, j, k ranging from 1 to 3 denote the vector or tensor components in a fixed rectangular Cartesian coordinate system in E_3. We assume that the fields $w_i = w_i(\xi_j, t)$ are functions of class C^3 specified on the product Ω_0 of an open region in E_3 containing the closure $\overline{V}_0$ of V_0 and of an open time interval $\mathcal{T}$ containing 0 and that for each t from $\mathcal{T}$ the mapping $\xi \to x = \xi + w$ of V_0 onto V_t is one-to-one with non-vanishing Jacobian. The scalar function $f = f(x_i, t)$ considered below is assumed to be of class C^2 on a four-dimensional neighbourhood Ω_t of $\overline{V}_t \times \{t\}$ for arbitrary $t \in \mathcal{T}^{(1)}$.

The shape transformation can naturally be defined by specifying the transformation vector field on the reference surface $\hat{S}_0$ only. Let each of the regular surface sections S_0 be parametrized by curvilinear coordinates y^α, $\alpha, \beta, \gamma = 1, 2,$ such that the pairs (y^1, y^2) belong to the corresponding (fixed) open subset Σ_0 of R^2. A surface point of coordinates (y^α) has the spatial coordinates $\tilde{\xi}_i(y^\alpha)$ at $t = 0$ and the spatial coordinates

$$(2.1) \qquad x_i = \tilde{x}_i(y^\alpha, t) = \tilde{\xi}_i(y^\alpha) + w_i\big(\tilde{\xi}_j(y^\alpha), t\big)$$

at a typical instant $t \in \mathcal{T}$ during the shape transformation process. The functions $\tilde{x}_i(y^\alpha, t)$ describing geometry of a regular transformed surface section S_t are assumed to be of class C^3 and such that the matrix $(\partial \tilde{x}_i/\partial y^\alpha)$ has always rank two.

A surface function of the variables (y^α, t) and generated by a spatial field (i.e. being the restriction of a spatial field to the surface S_t) is distinguished by a tilda, for instance $\tilde{f}(y^\alpha, t) = f(\tilde{x}_i(y^\alpha, t), t)$. The partial differentiation with respect to the curvilinear surface coordinates y^α or Cartesian spatial coordinates x_i is denoted by the corresponding index preceded by a comma, viz.

$$(2.2) \qquad (\cdot)_{,\alpha} = \frac{\partial(\cdot)}{\partial y^\alpha}, \qquad (\cdot)_{,i} = \frac{\partial(\cdot)}{\partial x_i}.$$

The usual summation convention for repeated indices is used throughout the paper. It is convenient to introduce the following notation: for any unit spatial vector $\boldsymbol{\eta}$, the directional derivative of any spatial field f and the component of any spatial vector $\mathbf{v}$, both in the direction of $\boldsymbol{\eta}$, are written respectively as

$$(2.3) \qquad f_{,\eta} = f_{,i}\eta_i, \qquad v_\eta = v_i\eta_i.$$

We recall some standard formulae of differential geometry of surfaces. Consider a regular oriented surface parametrized by y^α. Covariant components of the metric tensor $\mathbf{g}$ of the surface (i.e. coefficients of the first fundamental surface form) are specified as follows:

$$(2.4) \qquad g_{\alpha\beta} = \tilde{x}_{i,\alpha}\tilde{x}_{i,\beta}.$$

The contravariant components $g^{\alpha\beta}$ of $\mathbf{g}$ are defined by

$$(2.5) \qquad g_{\alpha\beta}g^{\beta\gamma} = \delta_\alpha^\gamma,$$

where $\delta_\alpha^\gamma \equiv \delta_{\alpha\gamma}$ is the Kronecker symbol, and satisfy the relationship

$$(2.6) \qquad g^{\alpha\beta}\tilde{x}_{i,\alpha}\tilde{x}_{j,\beta} = \delta_{ij} - n_i n_j,$$

(^{1}) When calculating the first time derivatives of integrals, the assumed order of differentiability of all functions considered may by reduced by one.

where $\mathbf{n}$ is the unit normal to the surface. The surface covariant derivative is denoted by $(\cdot)_{;\alpha}$. For instance, we have the formula

(2.7)
$$c^\alpha_{;\beta} = c^\alpha_{,\beta} + c^\gamma \Gamma^\alpha_{\gamma\beta},$$

where c^α are contravariant components of a surface vector $\mathbf{c}$ and $\Gamma^\alpha_{\gamma\beta}$ are the Christoffel symbols of second kind determined by the metric on the surface. Also, there is

(2.8)
$$g_{\alpha\beta;\gamma} = 0.$$

The components of the second fundamental surface form are defined by

(2.9)
$$b_{\alpha\beta} = \tilde{x}_{i,\alpha\beta} n_i$$

and satisfy the formulae of Gauss and Weingarten:

(2.10)
$$\tilde{x}_{i,\alpha;\beta} \equiv x_{i;\alpha\beta} = b_{\alpha\beta} n_i,$$

(2.11)
$$n_{i,\alpha} = -g^{\beta\gamma} b_{\alpha\beta} \tilde{x}_{i,\gamma}.$$

The mean curvature K_m and the Gauss curvature K_g of the surface are defined by

(2.12)
$$K_m = \frac{1}{2} b_{\alpha\beta} g^{\alpha\beta} = \frac{1}{2} b^\alpha_\alpha,$$

(2.13)
$$K_g = \frac{\det(b_{\alpha\beta})}{\det(g_{\alpha\beta})} = \det(b^\alpha_\beta).$$

Any spatial vector $\mathbf{c}$ can be decomposed at a point on the surface as follows:

(2.14)
$$c_i = c_n n_i + c^\alpha \tilde{x}_{i,\alpha},$$

where

(2.15)
$$c_n = c_i n_i \quad \text{and} \quad c^\alpha = g^{\alpha\beta} c_\beta = g^{\alpha\beta} c_i \tilde{x}_{i,\beta}.$$

For any unit vector τ tangential to the surface we may write

(2.16)
$$\varphi_{,\tau} = \varphi_{,\alpha} \tau^\alpha,$$

where φ is any function specified over the surface. If a surface vector field $\tilde{\mathbf{c}}$ is generated by a differentiable spatial vector field $\mathbf{c}$, then, by using Eqs. (2.15), (2.10), (2.6) and (2.12), we obtain

(2.17)
$$\tilde{c}^\alpha_{;\alpha} = c_{i,j}(\delta_{ij} - n_i n_j) + 2c_n K_m.$$

The area of a surface element is expressed as follows:

(2.18)
$$da = \sqrt{\bar{g}}\, dy^1 dy^2, \quad \bar{g} = \det(g_{\alpha\beta}).$$

The Green theorem for a continuous and continuously differentiable surface vector field $\mathbf{c}$ specified on a regular surface S bounded by a piecewise smooth closed curve $\hat{L}$ reads

(2.19)
$$\int_S c^\alpha_{;\alpha}\, da = \oint_{\hat{L}} c^\alpha \mu_\alpha\, dl = \oint_{\hat{L}} c_\mu\, dl,$$

where the line integral is taken with respect to the arc length l, and μ denotes the unit vector normal to $\hat{L}$ and tangent to S and pointed towards the outside of S.

Now, consider the moving regular surface S_t during the shape transformation process described by a field $\mathbf{w}(\boldsymbol{\xi}, t)$. Define the transformation velocity $\mathbf{v}$ and the normal velocity v_n of the transformed surface as follows:

$$(2.20) \qquad v_i = \frac{\partial w_i}{\partial t}\bigg|_{\boldsymbol{\xi}=\mathrm{const}} \equiv \frac{D w_i}{Dt}, \qquad v_n = v_i n_i.$$

In general, the tangential components v^α of $\mathbf{v}$ do not vanish. The derivative

$$(2.21) \qquad \frac{D}{Dt}(\cdot) = \frac{\partial(\cdot)}{\partial t}\bigg|_{\boldsymbol{\xi}=\mathrm{const}} = \frac{\partial(\cdot)}{\partial t}\bigg|_{\mathbf{x}=\mathrm{const}} + (\cdot)_{,i} v_i,$$

also when evaluated at a point on the surface, is thus dependent (though v_n is not) on the choice of the particular field $\mathbf{w}$ used to describe a geometrically given shape transformation process. To construct an invariant time derivative relative to the moving regular surface S_t, introduce on S_t the *convected coordinate system* (z^α) such that the trajectory in space of a surface point with constant coordinates z^α is normal to S_t at each t, that is,

$$(2.22) \qquad \frac{\partial x_i}{\partial t}\bigg|_{z^\alpha=\mathrm{const}} = v_n n_i.$$

Any scalar, vector or tensor field $\boldsymbol{\Psi}$ specified on the moving surface S_t can be expressed as a function $\overline{\boldsymbol{\Psi}}(z^\alpha, t)$. *The transformation derivative* $\delta/\delta t$ is defined as the time derivative following the normal trajectory of the moving surface, viz.

$$(2.23) \qquad \frac{\delta\boldsymbol{\Psi}}{\delta t} = \frac{\partial\overline{\boldsymbol{\Psi}}}{\partial t}\bigg|_{z^\alpha=\mathrm{const}}.$$

The transformation derivative is thus the usual partial derivative but for the special choice of independent variables. This derivative was used by Thomas [15, 16] and called by him "δ time derivative" though the form (2.23) was given explicitly later by Bowen and Wang [17] (who employed the term "total displacement derivative"). The transformation derivative of a spatial field $f(x_i, t)$ is given by (cf. Thomas [15, 16])

$$(2.24) \qquad \frac{\delta f}{\delta t} = \frac{\partial f}{\partial t} + f_{,n} v_n, \qquad f_{,n} = \frac{\partial f}{\partial x_i} n_i.$$

More generally, the transformation derivative defined by Eq. (2.23) of any scalar, vector or (mixed) tensor field $\boldsymbol{\Psi}(x_i, y^\alpha, t)$ is expressed by the formula (cf. Bowen and Wang [17])

$$(2.25) \qquad \frac{\delta\boldsymbol{\Psi}}{\delta t} = \frac{\partial\boldsymbol{\Psi}}{\partial t} + \frac{\partial\boldsymbol{\Psi}}{\partial x_i} n_i v_n - \frac{\partial\boldsymbol{\Psi}}{\partial y^\alpha} v^\alpha.$$

The transformation derivative defined above in general differs from the "displacement derivative" defined by Truesdell and Toupin [18] but coincides with it if $\boldsymbol{\Psi}$ is any scalar field or a *spatial* vector field (cf. Bowen and Wang [17]).

It can be shown that (cf. Thomas [15, 16])

$$(2.26) \qquad \frac{\delta n_i}{\delta t} = -g^{\alpha\beta} v_{n,\alpha} \tilde{x}_{i,\beta},$$

and (cf. Truesdell and Toupin [18])

$$(2.27) \qquad \frac{\delta K_m}{\delta t} = \frac{1}{2} v_{n;\,\alpha\beta} g^{\alpha\beta} + (2K_m^2 - K_g)v_n.$$

For further relations holding on moving surfaces or interfaces, we refer the reader to the book by Kosiński [12].

2.2. First derivative of volume and surface integrals

Consider the volume integral

$$(2.28) \qquad I_V = \int\limits_{V_t} f d\mathscr{V}$$

over the variable domain V_t. The time derivative of I_V is given by the classical Reynolds formula expressed in three equivalent forms, cf. for instance Prager [10] or Malvern [11],

$$(2.29) \qquad \frac{d}{dt} I_V = \int\limits_{V_t} \left(\frac{Df}{Dt} + f v_{i,\,i} \right) d\mathscr{V} = \int\limits_{V_t} \left\{ \frac{\partial f}{\partial t} + (f v_i)_{,\,i} \right\} d\mathscr{V} = \int\limits_{V_t} \frac{\partial f}{\partial t} d\mathscr{V} + \int\limits_{S_t} f v_n da.$$

This can be proved by reducing first the integral (2.28) over the variable domain to an integral over a fixed domain through an appropriate change of variables, then performing differentiation in the standard manner and finally returning to the original integration domain. Such a procedure will be applied below to surface and line integrals.

Consider the surface integral

$$(2.30) \qquad I_S = \int\limits_{S_t} f da$$

over the moving regular surface S_t. By using the relations (2.1) and (2.18), the integral I_S can be equivalently written as an integral over the fixed plane domain Σ_0, viz.

$$(2.31) \qquad I_S = \int\int\limits_{\Sigma_0} f(\tilde{x}_i(y^\alpha, t), t) \sqrt{\overline{g(y^\alpha, t)}} dy^1 dy^2.$$

By performing standard calculations and substituting Eq. (2.6), we obtain

$$(2.32) \qquad \frac{D}{Dt} \sqrt{\overline{g}} = \frac{1}{2} \sqrt{\overline{g}} g^{\alpha\beta} \frac{D}{Dt} g_{\alpha\beta} = \sqrt{\overline{g}} v_{i,\,j} (\delta_{ij} - n_i n_j).$$

By differentiating the right hand side of Eq. (2.31) with respect to t, using Eq. (2.32) and returning to the actual area measure, we arrive at the result

$$(2.33) \qquad \frac{d}{dt} I_S = \int\limits_{S_t} \left\{ \frac{Df}{Dt} + f v_{i,\,j} (\delta_{ij} - n_i n_j) \right\} da.$$

This can be written equivalently as (cf. e.g. Kosiński [12])

$$(2.34) \qquad \frac{d}{dt} I_S = \int\limits_{S_t} \left\{ \frac{Df}{Dt} + f(v^\alpha_{;\,\alpha} - 2v_n K_m) \right\} da = \int\limits_{S_t} \left\{ \frac{\delta f}{\delta t} + (\tilde{f} v^\alpha_{\scriptscriptstyle{a}})_{;\,\alpha} - 2f v_n K_m \right\} da.$$

The former expression in Eq. (2.34) follows from Eq. (2.17), while the latter results from the identity (cf. Eq. (2.25))

$$(2.35) \qquad \frac{Df}{Dt} = \frac{\delta f}{\delta t} + f_{,j} v_i (\delta_{ij} - n_i n_j) = \frac{\delta f}{\delta t} + \tilde{f}_{,\alpha} v^\alpha.$$

Now, by using the Green theorem (2.19), we finally obtain

$$(2.36) \qquad \frac{d}{dt} I_S = \int_{S_t} \frac{\delta f}{\delta t} da - 2 \int_{S_t} f v_n K_m da + \oint_{\hat{L}_t} f v_\mu dl,$$

where $\hat{L}_t$ is (the piecewise smooth) closed boundary line of S_t and $v_\mu = v^\alpha \mu_\alpha = v_i \mu_i$ is the component of the transformation velocity vector $\mathbf{v}$ in the direction of the unit vector $\boldsymbol{\mu}$ which is normal to $\hat{L}_t$ and tangent to S_t and is pointed towards the outside of S_t.

To calculate the time derivative of the surface integral over a piecewise regular moving surface, we may directly apply the formula (2.36) to each of the regular surface sections and add the results. In particular, the time derivative of the integral over the *closed* piecewise regular surface $\hat{S}_t$ takes the form

$$(2.37) \qquad \frac{d}{dt} \int_{\hat{S}_t} f da = \int_{\hat{S}_t} \frac{\delta f}{\delta t} da - 2 \int_{\hat{S}_t} f v_n K_m da + \sum \int_{L_t} (f^+ v_\mu^+ + f^- v_\mu^-) dl,$$

where the sum of the line integrals is taken over all edges of the surface S_t. The $(+)$ and $(-)$ signs refer to the quantities evaluated on the two regular surface sections intersecting along an edge L_t. The result (2.37) pertains to the cases where the function f is defined for each regular surface section S_t separately so that in Eq. (2.37) we may have $f^+ \neq f^-$. Note that the pair (v_μ^+, v_μ^-) of the "tangential surface velocities" at an edge point is, by simple geometry, uniquely defined by the pair (v_n^+, v_n^-) of the normal surface velocities at that point, provided that the intersection angle is not equal to π nor to 0 (Fig. 2). Hence the expression (2.37) involves, in effect, only the normal component of the transformation velocity vector (as it could be expected from a geometric argument).
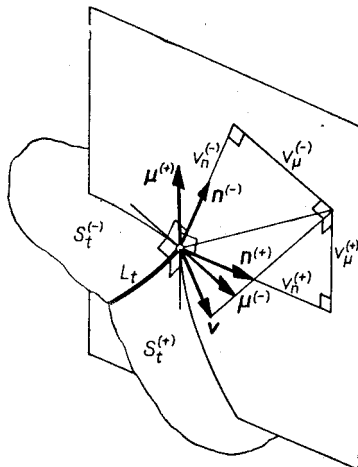

FIG. 2. Decomposition of transformation velocity vector at the edge of intersection of two regular surfaces.

2.3. First derivative of line integral

Consider a line integral with respect to the arc length l,

(2.38)
$$I_L = \int_{L_t} f\,dl,$$

taken along a smooth curve L_t moving in space with varying t and contained in Ω_t. The motion is described by the transformation vector field $\mathbf{w}(\xi_i, t)$ as above. The curve can be parametrized by a scalar variable y such that a line point has the space coordinates $\tilde{\xi}_i(y)$ at $t = 0$ and the space coordinates

(2.39)
$$x_i = \tilde{x}_i(y, t) = \tilde{\xi}_i(y) + w_i((\tilde{\xi}_j(y), t)$$

at an instant $t \in \mathscr{T}$. The line integral (2.38) can be equivalently written down as an integral over the fixed interval (y^A, y^B),

(2.40)
$$I_L = \int_{y^A}^{y^B} f(\tilde{x}_i(y, t), t)s(y, t)\,dy,$$

where y^A and y^B are the fixed values of y at the ends, A and B, of the curve L_t, and

(2.41)
$$s = \left(\frac{\partial \tilde{x}_i}{\partial y}\frac{\partial \tilde{x}_i}{\partial y}\right)^{\frac{1}{2}} \neq 0, \quad dl = s\,dy.$$

Denote by $\boldsymbol{\lambda}$ the unit vector tangent to the curve L_t, of the components

(2.42)
$$\lambda_i = \frac{1}{s}\frac{\partial \tilde{x}_i}{\partial y}.$$

It can easily be shown that

(2.43)
$$\frac{Ds}{Dt} \equiv \frac{\partial s}{\partial t}\bigg|_{y=\text{const}} = sv_{i,j}\lambda_i\lambda_j.$$

By differentiating the right hand side of Eq. (2.40) with respect to t, using Eq. (2.43) and returning to the arc length variable, we obtain

(2.44)
$$\frac{d}{dt}I_L = \int_{L_t}\left(\frac{Df}{Dt} + fv_{i,j}\lambda_i\lambda_j\right)dl.$$

According to the notation (2.3), $(\cdot)_{,\lambda}$ coincides with the derivative $\partial/\partial l$ with respect to the arc length along the curve L. We have

(2.45)
$$\frac{\partial \boldsymbol{\lambda}}{\partial l} = k\boldsymbol{\varkappa},$$

where k is the curvature of L_t and $\boldsymbol{\varkappa}$ is the unit principal normal to L_t. The expression (2.44) can be rearranged as follows:

(2.46)
$$\frac{d}{dt}I_L = \int_{L_t}\left\{\frac{Df}{Dt} - f_{,\lambda}v_\lambda - fkv_\varkappa + \frac{\partial}{\partial l}(fv_\lambda)\right\}dl.$$

The last term of the integrand in Eq. (2.46) can be integrated and we finally obtain

$$(2.47) \qquad \frac{d}{dt} I_L = \int\limits_{L_t} \frac{\delta_L f}{\delta t}\, dl - \int\limits_{L_t} fk v_{\varkappa}\, dl + (f v_{\lambda})\Big|_A^B .$$

In the above expression we have introduced the following time derivative of a function $f(x_i, t)$ relative to a moving curve

$$(2.48) \qquad \frac{\delta_L f}{\delta t} \equiv \frac{\partial f}{\partial t} + f_{,i} v_i^{\perp} = \frac{Df}{Dt} - f_{,\lambda} v_{\lambda},$$

where

$$(2.49) \qquad \mathbf{v}^{\perp} = \mathbf{v} - v_{\lambda}\boldsymbol{\lambda}$$

is the vector component of $\mathbf{v}$ orthogonal to the curve. The derivative $\delta_L/\delta t$ plays here an analogical role as the derivative $\delta/\delta t$ in the analysis of moving surfaces. It can easily be checked that $\delta_L/\delta t$ represents the time derivative following the normal trajectory of the moving curve. Therefore, this derivative can be more generally defined, in analogy to (2.23), as the partial derivative with respect to time while the appropriately chosen "convected coordinate" of a line point is held fixed.

If the moving curve constitutes (a part of) the boundary of a moving regular surface, then the derivative (2.48) can be expressed equivalently as

$$(2.50) \qquad \frac{\delta_L f}{\delta t} = \frac{\delta f}{\delta t} + f_{,\mu} v_{\mu},$$

where the unit vector $\boldsymbol{\mu}$ is orthogonal to $\boldsymbol{\lambda}$ and to the surface normal $\mathbf{n}$. This follows from the decomposition

$$(2.51) \qquad \mathbf{v} = v_n \mathbf{n} + v_{\mu}\boldsymbol{\mu} + v_{\lambda}\boldsymbol{\lambda} .$$

The expression (2.47) will be needed to determine the second time derivative of a surface integral.

2.4. Second derivative of volume integral

Similarily as the first derivative of I_V, the second time derivative of volume integral can also be expressed in several alternative forms. Starting from the first expression in Eq. (2.29) and applying the differentiation once more, we obtain

$$(2.52) \qquad \frac{d^2}{dt^2} I_V = \frac{d}{dt} \int\limits_{V_t} \left(\frac{Df}{Dt} + f v_{i,i} \right) d\mathcal{V}$$

$$= \int\limits_{V_t} \left\{ \frac{D^2 f}{Dt^2} + 2\frac{Df}{Dt} v_{i,i} + f\left((v_{i,i})^2 + \frac{D}{Dt}(v_{i,i}) \right) \right\} d\mathcal{V} .$$

However, since

$$(2.53) \qquad \frac{D}{Dt}(v_{i,i}) = \left(\frac{\partial v_i}{\partial t} \right)_{,i} + v_{i,ij} v_j = \left(\frac{Dv_i}{Dt} \right)_{,i} - v_{i,j} v_{j,i},$$

the expression (2.52) takes the form

$$
(2.54) \qquad \frac{d^2}{dt^2} I_V = \int\limits_{V_t} \left\{ \frac{D^2 f}{Dt^2} + 2 \frac{Df}{Dt} v_{i,i} + f\left((v_{i,i})^2 + \left(\frac{Dv_i}{Dt}\right)_{,i} - v_{i,j} v_{j,i} \right) \right\} d\mathcal{V}.
$$

Starting from the second form of Eq. (2.29), we obtain

$$
(2.55) \qquad \frac{d^2}{dt^2} I_V = \frac{d}{dt} \int\limits_{V_t} \left\{ \frac{\partial f}{\partial t} + (fv_i)_{,i} \right\} d\mathcal{V} = \int\limits_{V_t} \left\{ \frac{\partial^2 f}{\partial t^2} + 2\left(\frac{\partial f}{\partial t} v_i\right)_{,i} + \left(f \frac{\partial v_i}{\partial t}\right)_{,i} + \right.
$$

$$
\left. + ((fv_i)_{,i} v_j)_{,j} \right\} d\mathcal{V} = \int\limits_{V_t} \frac{\partial^2 f}{\partial t^2} d\mathcal{V} + \int\limits_{\hat{S}_t} \left\{ 2\frac{\partial f}{\partial t} v_n + f \frac{\partial v_i}{\partial t} n_i + (fv_i)_{,i} v_n \right\} da.
$$

The surface integral in Eq. (2.55) involves all components of the transformation velocity vector on S_t. To express the second time derivative of I_V in terms of the normal velocity v_n only, let us start from the third form of Eq. (2.29) and apply the formula (2.37). The result is

$$
(2.56) \qquad \frac{d^2}{dt^2} I_V = \frac{d}{dt} \left(\int\limits_{V_t} \frac{\partial f}{\partial t} d\mathcal{V} + \int\limits_{\hat{S}_t} f v_n da \right) = \int\limits_{V_t} \frac{\partial^2 f}{\partial t^2} d\mathcal{V} + \int\limits_{\hat{S}_t} \left\{ \frac{\partial f}{\partial t} v_n \right.
$$

$$
\left. + \frac{\delta}{\delta t} (fv_n) - 2fv_n^2 K_m \right\} da + \sum \int\limits_{L_t} f(v_n^+ v_\mu^+ + v_n^- v_\mu^-) dl = \int\limits_{V_t} \frac{\partial^2 f}{\partial t^2} d\mathcal{V}
$$

$$
+ \int\limits_{\hat{S}_t} \left\{ 2\frac{\partial f}{\partial t} v_n + f_{,n} v_n^2 + f\left(\frac{\delta v_n}{\delta t} - 2v_n^2 K_m \right) \right\} da + \sum \int\limits_{L_t} f(v_n^+ v_\mu^+ + v_n^- v_\mu^-) dl,
$$

where the sum of the line integrals is taken over all edges of the surface $\hat{S}_t$, and the $(+)$ and $(-)$ signs refer to the quantities evaluated on the two regular surface sections intersecting along an edge L_t (cf. the comment following the formula (2.37)).

In view of Eqs. (2.24), (2.26) and (2.11), the transformation derivative $\delta v_n / \delta t$ is expressed as follows:

$$
(2.57) \qquad \frac{\delta v_n}{\delta t} = \frac{\delta v_i}{\delta t} n_i + v_i \frac{\delta n_i}{\delta t} = \left(\frac{\partial v_i}{\partial t} + v_{i,j} n_j v_n \right) n_i - v_i g^{\alpha\beta} v_{n,\alpha} \tilde{x}_{i,\beta}
$$

$$
= \frac{Dv_i}{Dt} n_i - 2v_{n,\alpha} v^\alpha - b_{\alpha\beta} v^\alpha v^\beta.
$$

From the definitions of v_n and the transformation derivative, it follows that $\delta v_n / \delta t$ coincides with the second time derivative of length of the corresponding normal trajectory of the moving surface. The value of the expression (2.57) is thus invariant with respect to the choice of the analytic description (e.g. of the surface parametrization or transformation field **w**) of a geometrically given shape transformation process.

On substituting $f = \text{const} = 1$ in the expression (2.56), we obtain as a corollary the following formula for the second time derivative of volume of the domain V_t:

$$
(2.58) \qquad \frac{d^2}{dt^2} \int\limits_{V_t} d\mathcal{V} = \int\limits_{\hat{S}_t} \left(\frac{\delta v_n}{\delta t} - 2v_n^2 K_m \right) da + \sum \int\limits_{L_t} (v_n^+ v_\mu^+ + v_n^- v_\mu^-) dl.
$$

2.5. Second derivative of surface integral

Consider again the integral (2.30) over the moving regular surface S_t, and denote by C a typical corner point on the piecewise smooth boundary line $\hat{L}_t$ of S_t. As in the case of the volume integral, we can obtain several alternative forms for the second time derivative of the surface integral by the repeated use of one of the expressions for its first derivative. We explore here one possibility only, namely, by differentiating Eq. (2.36) and substituting Eq. (2.47). This yields

$$(2.59) \quad \frac{d^2}{dt^2} I_S = \int_{S_t} \left\{ \frac{\delta}{\delta t} \left(\frac{\delta f}{\delta t} - 2fv_n K_m \right) - 2\left(\frac{\delta f}{\delta t} - 2fv_n K_m \right) v_n K_m \right\} da$$

$$+ \oint_{\hat{L}_t} \left\{ \left(\frac{\delta f}{\delta t} - 2fv_n K_m \right) v_\mu + \frac{\delta_L}{\delta t} (fv_\mu) - fkv_\mu v_\varkappa \right\} dl + \Sigma \{ (v_\mu^+ v_\lambda^+ + v_\mu^- v_\lambda^-) f \}|_C .$$

At a point C, the symbols $(+)$ and $(-)$ refer to the quantities evaluated on the two smooth segments of the curve L_t which intersect at C. The unit vectors $\boldsymbol{\lambda}^+$ and $\boldsymbol{\lambda}^-$ tangent to the segments at C are chosen to point towards the outside of the corresponding segments (Fig. 3). Note that the pair $(v_\lambda^+, v_\lambda^-)$ is uniquely defined by the pair (v_μ^+, v_μ^-), irrespective
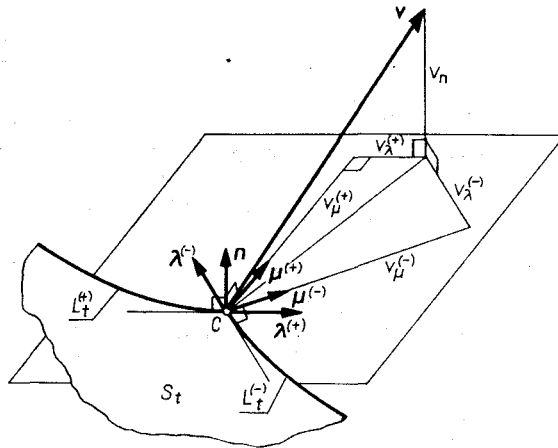

Fig. 3. Decomposition of transformation velocity vector at a corner point.

of the value of v_n, provided the angle of intersection of the segments is not equal to 0 nor to π. By substituting Eqs. (2.27) and (2.50) in Eq. (2.59), we obtain

$$(2.60) \quad \frac{d^2}{dt^2} I_S = \int_{S_t} \left\{ \frac{\delta^2 f}{\delta t^2} - 4 \frac{\delta f}{\delta t} v_n K_m + f \left(2K_g v_n^2 - g^{\alpha\beta} v_{n;\alpha\beta} v_n - 2K_m \frac{\delta v_n}{\delta t} \right) \right\} da$$

$$+ \oint_{\hat{L}_t} \left\{ 2 \frac{\delta f}{\delta t} v_\mu + f_{,\mu} v_\mu^2 + f \left(\frac{\delta_L v_\mu}{\delta t} - 2K_m v_n v_\mu - kv_\mu v_\varkappa \right) \right\} dl + \Sigma \{ (v_\mu^+ v_\lambda^+ + v_\mu^- v_\lambda^-) f \}|_C .$$

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By using Eqs. (2.24) and (2.26), the second transformation derivative of a spatial field $f(x_i, t)$ can be expressed explicitly as follows:

$$(2.61) \quad \frac{\delta^2 f}{\delta t^2} \equiv \frac{\delta}{\delta t}\left(\frac{\delta f}{\delta t}\right) = \frac{\partial^2 f}{\partial t^2} + 2\frac{\partial^2 f}{\partial t \partial x_i} n_i v_n + \frac{\partial^2 f}{\partial x_i \partial x_j} n_i n_j v_n^2$$

$$+ \frac{\partial f}{\partial x_i} n_i \frac{\delta v_n}{\delta t} - \frac{\partial f}{\partial x_i} \tilde{x}_{i,\beta} g^{\alpha\beta} v_{n,\alpha} v_n.$$

We can rearrange the expression (2.60) to eliminate the derivatives of f in the directions tangent to S_t, appearing in the surface integral on account of the last term in Eq. (2.61). From Eqs. (2.19) and (2.8) we have

$$(2.62) \quad \int_{S_t} \{f v_n v_{n;\alpha\beta} g^{\alpha\beta} + f_{,i} \tilde{x}_{i,\beta} g^{\alpha\beta} v_{n,\alpha} v_n\} da = \oint_{\hat{L}_t} f v_n v_{n,\mu} dl - \!\int\!\!\!\int_{S_t} v_{n,\alpha} v_{n,\beta} g^{\alpha\beta} da.$$

By substituting Eqs. (2.61) and (2.62) in Eq. (2.60), we obtain

$$(2.63) \quad \frac{d^2}{dt^2} I_S = \int_{S_t} \left| \frac{\partial^2 f}{\partial t^2} + 2\left(\left(\frac{\partial f}{\partial t}\right)_{,n} - 2\frac{\partial f}{\partial t} K_m\right) v_n + (f_{,ij} n_i n_j - 4f_{,n} K_m) \right.$$

$$+ 2fK_g) v_n^2 + (f_{,n} - 2fK_m)\frac{\delta v_n}{\delta t} + fg^{\alpha\beta} v_{n,\alpha} v_{n,\beta} \right] da + \oint_{L_t} \left\{\left(2\frac{\partial f}{\partial t} + 2f_{,n} v_n\right.\right.$$

$$\left. - 2fK_m v_n - fkv_x\right) v_\mu + f_{,\mu} v_\mu^2 + f\left(\frac{\delta_L v_\mu}{\delta t} - v_n v_{n,\mu}\right) \right\} dl + \Sigma\{(v_\mu^+ v_\lambda^+ + v_\mu^- v_\lambda^-)f\}|_c.$$

If we substitute $f = \text{const} = 1$ in Eq. (2.60), then we arrive at the following formula for the second time derivative of area of the moving regular surface:

$$(2.64) \quad \frac{d^2}{dt^2} \int_{S_t} da = \int_{S_t} \left(2K_g v_n^2 - g^{\alpha\beta} v_{n;\alpha\beta} v_n - 2K_m \frac{\delta v_n}{\delta t}\right) da$$

$$+ \oint_{\hat{L}_t} \left(\frac{\delta_L v_\mu}{\delta t} - 2K_m v_n v_\mu - kv_\mu v_x\right) dl + \Sigma(v_r^+ v_\lambda^+ + v_\mu^- v_\lambda^-)|_c.$$

3. Time derivatives of volume and surface functionals

3.1. Derivatives of volume functional

Consider the functional of a field $\mathbf{u}$ and of a domain V_t,

$$(3.1) \qquad\qquad J_V(\mathbf{u}) = \int_{V_t} h(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}) d\mathcal{V},$$

where V_t is the variable domain considered above, $\mathbf{u} = (u_1, \ldots, u_N) = \mathbf{u}(\mathbf{x}, t)$ is a vector function of class C^3 on the four-dimensional region Ω_t containing $\overline{V}_t$, $\nabla\mathbf{u}$ is the space gradient of $\mathbf{u}$ in the components $(\nabla\mathbf{u})_{Ij} = \partial u_I/\partial x_j = u_{I,j}$, $I = 1, \ldots, N$, and h is a real-valued function of class C^3, specified for $\mathbf{x}$ from an open region in E_3 containing $\overline{V}_t$.

By using the last expression in Eq. (2.29) for the derivative of volume integral and identifying f with h, so that

$$f(\mathbf{x}, t) = h\big(\mathbf{x}, \mathbf{u}(\mathbf{x}, t), \nabla \mathbf{u}(\mathbf{x}, t)\big),$$

(3.2)
$$\frac{\partial f}{\partial t} = \frac{\partial h}{\partial u_I}\, \dot{u}_I + \frac{\partial h}{\partial(u_{I,j})}\, \dot{u}_{I,j}, \qquad (\dot{\;}) \equiv \frac{\partial(\,\cdot\,)}{\partial t}\bigg|_{\mathbf{x} = \mathrm{const}},$$

we obtain

(3.3)
$$\frac{d}{dt}\, J_V(\mathbf{u}) = \int_{V_t} \left(\frac{\partial h}{\partial u_I}\, \dot{u}_I + \frac{\partial h}{\partial(u_{I,j})}\, \dot{u}_{I,j} \right) d\mathcal{V} + \int_{\hat{S}_t} h v_n\, da$$

$$= \int_{V_t} \left\{ \frac{\partial h}{\partial u_I} - \left(\frac{\partial h}{\partial(u_{I,j})} \right)_{,j} \right\} \dot{u}_I\, d\mathcal{V} + \int_{\hat{S}_t} \left\{ h v_n + \frac{\partial h}{\partial(u_{I,j})}\, n_j \dot{u}_I \right\} da$$

$$= \int_{V_t} A_I \dot{u}_I\, d\mathcal{V} + \int_{\hat{S}_t} B v_n\, da + \int_{\hat{S}_t} C_I\, \frac{\delta u_I}{\delta t}\, da,$$

where

(3.4)
$$A_I = \frac{\partial h}{\partial u_I} - \frac{\partial}{\partial x_j} \left(\frac{\partial h}{\partial(u_{I,j})} \right),$$

$$B = h - C_I u_{I,n},$$

$$C_I = \frac{\partial h}{\partial(u_{I,j})}\, n_j = \frac{\partial h}{\partial(u_{I,n})}^{(2)}.$$

The expression (3.3) is equivalent to that derived e.g. by GELFAND and FOMIN [19] for the first (weak) variation of the functional (3.1).

When the field $\mathbf{u}$ corresponds to the extremum of the functional (3.1) for the *fixed* domain V_t (within the class of smooth fields $\mathbf{u}$ unconstrained on the boundary $\hat{S}_t$ of V_t), then from Eq. (3.3) it follows that

(3.5)
$$A_I = 0 \quad \text{in} \quad V_t, \qquad C_I = 0 \quad \text{on} \quad \hat{S}_t,$$

and the derivative is simply expressed by

(3.6)
$$\frac{d}{dt}\, J_V(\mathbf{u}) = \int_{\hat{S}_t} h v_n\, da,$$

that is, in terms of the boundary flux of h through the normal component of the transformation velocity vector.

The second time derivative of the functional (3.1) can be calculated by using any of the expressions (2.54), (2.55), (2.56) and identifying f with h as in the expressions (3.2). An alternative way is to differentiate the last expression in Eq. (3.3) with the help of Eqs. (2.29) and (2.37), which yields

---

(^{2}) When writing the derivative $\partial h/\partial(u_{I,n})$ at a surface point, h is regarded as a function of the variables $(\mathbf{x}, \mathbf{u}, u_{,n}, \tilde{\mathbf{u}}_{,\alpha})$, and the last equality in Eq. (3.4) results then from the chain rule of differentiation.

(3.7) $\dfrac{d^2}{dt^2} J_V(\mathbf{u}) = \displaystyle\int_{V_t} (A_I \ddot{u}_I + \dot{A}_I \dot{u}_I)\,dv + \int_{\hat{S}_t} \left\{ A_I \dot{u}_I v_n + B\left(\dfrac{\delta v_n}{\delta t} - 2v_n^2 K_m \right) \right.$

$$+ C_I \left(\dfrac{\delta^2 u_I}{\delta t^2} - 2\dfrac{\delta u_I}{\delta t} v_n K_m \right) + \dfrac{\delta B}{\delta t} v_n + \dfrac{\delta C_I}{\delta t}\dfrac{\delta u_I}{\delta t} \bigg\}\, da$$

$$+ \sum \int_{L_t} \left\{ \left(B v_n + C_I \dfrac{\delta u_I}{\delta t} \right)^{+} v_\mu^{+} + \left(B v_n + C_I \dfrac{\delta u_I}{\delta t} \right)^{-} v_\mu^{-} \right\}\, dl.$$

3.2. Derivatives of the volume functional with discontinuity surface

Consider now a fixed domain $V_t = V_0$ in E_3 composed of two variable subdomains $V_t^{(1)}$ and $V_t^{(2)}$ separated by a regular moving interface S_t^D (Fig. 4). The shape transformation of the subdomains is due to the motion of the surface S_t^D alone. All the assumptions con-
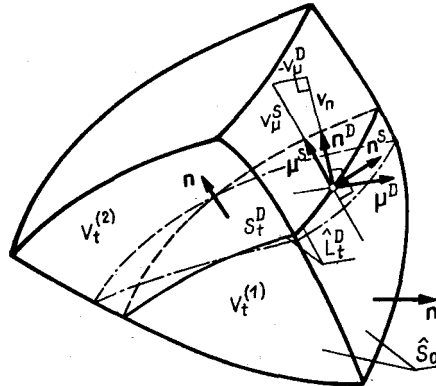

FIG. 4. Moving discontinuity surface S_t^D within a volume domain bounded by piecewise regular surface

cerning the domain V_t are now supposed to hold for each of the subdomains $V_t^{(1)}$ and $V_t^{(2)}$ considered separately. Denote by $\mathbf{n}$ the unit outward normal to the exterior surface S_0, while on the surface S_t^D we introduce the notation

(3.8) $\mathbf{n} = \mathbf{n}^{(1)} = -\mathbf{n}^{(2)}, \quad v_n = v_n^{(1)} = -v_n^{(2)},$

where the superscripts (1) and (2) refer to the quantities defined on S_t^D (directly or in the limit sense) regarded as a boundary of $V_n^{(1)}$ and $V_n^{(2)}$, respectively. A jump across S_t^D is denoted by $[\![\cdot]\!]$, viz.

(3.9) $[\![f]\!] = f^{(2)} - f^{(1)}.$

We introduce the restriction that the field $\mathbf{u}$ is continuous across S_t^D at each t, i.e. $[\![\mathbf{u}]\!] = 0$, $[\![\delta \mathbf{u}/\delta t]\!] = 0$, etc. According to the assumption introduced above, the field $\mathbf{u}(\mathbf{x}, t)$ is of class C^3 except on S_t^D. The well known compatibility conditions require that the jump across S_t^D of the gradient and of the time derivative of $\mathbf{u}$ are necessarily of the form

(3.10) $[\![u_{I,j}]\!] = [\![u_{I,n}]\!] n_j, \quad [\![\dot{u}_I]\!] = -[\![u_{I,n}]\!] v_n.$

Our aim is to derive expressions for the first and second time derivatives of the functional

$$(3.11) \qquad J_D(\mathbf{u}) = \int_{V_t^{(1)}} h^{(1)}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u})\, d\mathscr{V} + \int_{V_t^{(2)}} h^{(2)}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u})\, d\mathscr{V},$$

where $h^{(1)}$ and $h^{(2)}$ are real-valued functions of class C^3, specified for $\mathbf{x}$ from open domains containing $\overline{V_t^{(1)}}$ and $\overline{V_t^{(2)}}$, respectively. The functions $h^{(1)}$ and $h^{(2)}$ need not be related to each other.

By applying the last expression in Eq. (3.3) separately to each of the subdomains $V_t^{(1)}$ and $V_t^{(2)}$ and combining the results, we obtain

$$(3.12) \qquad \frac{d}{dt} J_D(\mathbf{u}) = \int_{V_t^{(1)}} A_I^{(1)} \dot{u}_I d\mathscr{V} + \int_{V_t^{(2)}} A_I^{(2)} \dot{u}_I d\mathscr{V} + \int_{\hat{S}_0} C_I \dot{u}_I da$$

$$- \int_{S_t^p} [\![C_I]\!] \frac{\delta u_I}{\delta t} da - \int_{S_t^p} [\![B]\!] v_n da,$$

where $A_I^{(r)}$ in $V_t^{(r)}$, $r = 1, 2,$ and C_I on $\hat{S}_0$ as well as $B^{(r)}$ and $C_I^{(r)}$ on both sides of S_t^p are defined by Eqs. (3.4) with h replaced by the respective $h^{(r)}$, with the assumed convention (3.8) for $\mathbf{n}$ on S_t^p.

If the field $\mathbf{u}$ corresponds to the stationary value of the functional (3.11) with respect to arbitrary (weak) variations within the considered class of fields $\mathbf{u}$ for the *fixed* position of S_t^p, then the derivative (3.12) must vanish identically provided $v_n = 0$ over S_t^p. It follows that in that case we have

$$(3.13) \qquad A_I^{(1)} = 0 \quad \text{in } V_{t}^{(1)}, \quad A_I^{(2)} = 0 \quad \text{in } V_{ij}^{(2)}, \quad C_I = 0 \quad \text{on } \hat{S}_0,$$

$$(3.14) \qquad [\![C_I]\!] = \left[\!\left[\frac{\partial h}{\partial(u_{I,j})} \right]\!\right] n_j = \left[\!\left[\frac{\partial h}{\partial(u_{I,n})} \right]\!\right] = 0 \quad \text{on } S_t^p,$$

and the expression (3.12) reduces to

$$(3.15) \qquad \frac{d}{dt} J_D(\mathbf{u}) = - \int_{S_t^p} [\![B]\!] v_n da.$$

If, moreover, the field $\mathbf{u}$ renders the functional $J_D(\mathbf{u})$ a weak relative extremum [3] value within the considered class of $\mathbf{u}$ for the *variable* position of S_t^p as well, then the integral in Eq. (3.15) must vanish for all v_n, so that

$$(3.16) \qquad [\![B]\!] = [\![h]\!] - \frac{\partial h}{\partial(u_{I,n})} [\![u_{I,n}]\!] = 0 \quad \text{on } S_t^p.$$

The derivative $\partial h / \partial(u_{I,n})$ can be regarded here as the limit value from either side of S_t^p on account of Eq. (3.14).

The conditions (3.14) and (3.16) are the multidimensional analogs of the classical Weierstrass–Erdmann corner conditions for piecewise-smooth one-dimensional extremals (cf. e.g. GELFAND and FOMIN [19]).

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[3] That is, the relative (local) minimum or maximum with respect to the norm $\sup_{\xi}(|\mathbf{u}| + |\nabla\mathbf{u}|)$.

On account of continuity of **u**, the jump across S_t^D of the second partial derivatives of $\mathbf{u}(\mathbf{x}, t)$ must satisfy the following compatibility conditions (cf. Thomas [15, 16]).

$$[\![u_{I,jk}]\!] = [\![u_{I,nn}]\!]n_j n_k + g^{\alpha\beta}[\![u_{I,n}]\!]_{,\alpha}(n_j \tilde{x}_{k,\beta} + n_k \tilde{x}_{j,\beta}) - [\![u_{I,n}]\!]b^{\alpha\beta}\tilde{x}_{j,\alpha}\tilde{x}_{k,\beta},$$

(3.17)
$$[\![\dot{u}_{I,j}]\!] = \left(-[\![u_{I,nn}]\!]v_n + \frac{\delta}{\delta t}[\![u_{I,n}]\!]\right)n_j - g_{\mathbf{1}}^{\alpha\beta}([\![u_{I,n}]\!]v_n)_{,\alpha}\tilde{x}_{J,\beta},$$

$$[\![\ddot{u}_I]\!] = [\![u_{I,nn}]\!]v_n^2 - 2v_n \frac{\delta}{\delta t}[\![u_{I,n}]\!] - [\![u_{I,n}]\!]\frac{\delta v_n}{\delta t},$$

$$u_{I,nn} \equiv u_{I,jk}n_j n_k, \qquad \ddot{u}_I \equiv \partial^2 u_I/\partial t^2.$$

The expression for the second time derivative of the functional (3.11) is obtained by applying the formula (3.7) separately to the regions $V_t^{(1)}$ and $V_t^{(2)}$ and combining the results. In view of the assumptions made, we arrive at

(3.18)
$$\frac{d^2}{dt^2}J_D(\mathbf{u}) = \int_{V_t^{(1)}}(A_I^{(1)}\ddot{u}_I + \dot{A}_I^{(1)}\dot{u}_I)d\mathcal{V} + \int_{V_t^{(2)}}(A_I^{(2)}\ddot{u}_I + \dot{A}_I^{(2)}\dot{u}_I)d\mathcal{V}$$

$$+ \int_{\hat{S}_0}(C_I\ddot{u}_I + \dot{C}_I\dot{u}_I)da - \int_{S_t^D}\left\{[\![A_I\dot{u}_I]\!]v_n + [\![B]\!]\left(\frac{\delta v_n}{\delta t} - 2v_n^2 K_m\right)\right.$$

$$+ [\![C_I]\!]\left(\frac{\delta^2 u_I}{\delta t^2} - 2\frac{\delta u_I}{\delta t}v_n K_m\right) + v_n\frac{\delta}{\delta t}[\![B]\!] + \frac{\delta}{\delta t}[\![C_I]\!]\frac{\delta u_I}{\delta t}\right\}da$$

$$- \oint_{\hat{L}_t^D}\left\{\left([\![B]\!]v_n + [\![C_I]\!]\frac{\delta u_I}{\delta t}\right)^D v_\mu^D + [\![C_I^S\dot{u}_I]\!]v_\mu^S\right\}dl.$$

In the above expression, $\hat{L}_t^D$ denotes the boundary of S_t^D obtained as the intersection curve of the surfaces S_t^D and $\hat{S}_0$. The quantities appearing in the line integral along $\hat{L}_t^D$ and distinguished by the superscript D or S denote the limit values evaluated on the surface S_t^D or $\hat{S}_0$, respectively, with the notation $v_\mu^D = v_\mu^{D(1)} = v_\mu^{D(2)}$ and $v_\mu^S = v_\mu^{S(1)} = -v_\mu^{S(2)}$. Note that the tangential surface velocities v_μ^D and v_μ^S at a point on a smooth segment L_t^D of $\hat{L}_t^D$ result uniquely, by simple geometry, from the value $v_n = v_{\mu,n}^D$ at that point (Fig. 4).

If the conditions (3.13) and (3.14) are satisfied, then the expression (3.18) reduces to

(3.19)
$$\frac{d^2}{dt^2}J_D(\mathbf{u}) = \int_{V_t^{(1)}}\dot{A}_I^{(1)}\dot{u}_I d\mathcal{V} + \int_{V_t^{(2)}}\dot{A}_I^{(2)}\dot{u}_I d\mathcal{V} + \int_{\hat{S}_0}\dot{C}_I\dot{u}_I da$$

$$- \int_{S_t^D}\left\{[\![B]\!]\left(\frac{\delta v_n}{\delta t} - 2v_n^2 K_m\right) + v_n\frac{\delta}{\delta t}[\![B]\!] + \frac{\delta}{\delta t}[\![C_I]\!]\frac{\delta u_I}{\delta t}\right\}da - \oint_{\hat{L}_t^D}[\![B^D]\!]v_n v_\mu^D dl.$$

3.3. First derivative of the sum of volume and surface functionals

Consider a functional of the field **u** in the form of the sum of the volume and surface functionals

(3.20)
$$J(\mathbf{u}) = J_V(\mathbf{u}) + J_S(\mathbf{u}) = \int_{V_t}h(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u})d\mathcal{V} + \int_{\hat{S}_t}g(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u})da,$$

with the assumptions concerning V_t, **u** and h as in the point 3.1 above. The function g may be prescribed over regular sections S_t of the surface $\hat{S}_t$ independently of each other. For each regular section S_t, g is assumed to be of class C^2 specified for **x** from a neighbourhood of S_t. From the relation (2.24) and the chain rule, we have

$$(3.21) \qquad \frac{\delta g}{\delta t} = \frac{\partial g}{\partial u_I} \dot{u}_I + \frac{\partial g}{\partial(u_{I,j})} \dot{u}_{I,j} + g_{,n} v_n,$$

where

$$(3.22) \qquad g_{,n} = \frac{\partial g}{\partial x_j} n_j + \frac{\partial g}{\partial u_I} u_{I,n} + \frac{\partial g}{\partial(u_{I,j})} u_{I,jk} n_k.$$

By using the second form of Eq. (3.3) and the formula (2.37) and substituting Eq. (3.21), we obtain

$$(3.23) \qquad \frac{d}{dt} J(\mathbf{u}) = \int_{S_t} A_I \dot{u}_I \, d\mathscr{V} + \int_{\hat{S}_t} \left\{ C_I \dot{u}_I + \frac{\partial g}{\partial u_I} \dot{u}_I + \frac{\partial g}{\partial(u_{I,j})} \dot{u}_{I,j} + (h + g_{,n} \right.$$
$$\left. - 2gK_m) v_n \right\} da + \sum \int_{L_t}' (g^+ v_\mu^+ + g^- v_\mu^-) \, dl.$$

Over a regular surface section, we may regard g also as a function of the independent variables $(\mathbf{x}, \mathbf{u}, \mathbf{u}_{,n}, \tilde{\mathbf{u}}_{,\alpha})$ with the relationships

$$(3.24) \qquad \begin{aligned} \frac{\partial g}{\partial(u_{I,j})} \dot{u}_{I,j} &= \frac{\partial g}{\partial(u_{I,n})} \dot{u}_{I,n} + \frac{\partial g}{\partial(\tilde{u}_{I,\alpha})} \dot{\tilde{u}}_{I,\alpha}, \\ \frac{\partial g}{\partial(u_{I,n})} &= \frac{\partial g}{\partial(u_{I,j})} n_j, \qquad \frac{\partial g}{\partial(\tilde{u}_{I,\alpha})} = \frac{\partial g}{\partial(u_{I,j})} \tilde{x}_{j,\beta} g^{\alpha\beta}. \end{aligned}$$

With the help of the Green theorem (2.19), the expression (3.23) can thus be rearranged as follows:

$$(3.25) \qquad \frac{d}{dt} J(\mathbf{u}) = \int_{V_t} A_I \dot{u}_I \, d\mathscr{V} + \int_{\hat{S}_t} \left\{ C_I + \frac{\partial g}{\partial u_I} - \left(\frac{\partial g}{\partial(\tilde{u}_{I,\alpha})} \right)_{;\alpha} \right\} \dot{u}_I \, da$$
$$+ \int_{\hat{S}_t} \frac{\partial g}{\partial(u_{I,n})} \dot{u}_{I,n} \, da + \int_{\hat{S}_t} (h + g_{,n} - 2gK_m) v_n \, da$$
$$+ \sum \int_{L_t}' \left\{ (g^+ v_\mu^+ + g^- v_\mu^-) + \left(\left(\frac{\partial g}{\partial(u_{I,\mu})} \right)^+ + \left(\frac{\partial g}{\partial(u_{I,\mu})} \right)^- \right) \dot{u}_I \right\} dl,$$

where

$$(3.26) \qquad \frac{\partial g}{\partial(u_{I,\mu})} = \frac{\partial g}{\partial(u_{I,j})} \mu_j.$$

Suppose now that the field **u** corresponds to the stationary value of $J(\mathbf{u})$ with respect to arbitrary (weak) variations of **u** (unconstrained over the boundary) for the fixed boundary of V_t. By standard argument of the calculus of variations, from Eq. (3.25) it follows that in that case we must have

$$A = 0 \quad \text{in } V_t,$$

(3.27)
$$C_I = -\frac{\partial g}{\partial u_I} + \left(\frac{\partial g}{\partial(\tilde{u}_{I,\alpha})}\right)_{;\alpha} \quad \text{and} \quad \frac{\partial g}{\partial(u_{I,n})} = 0 \quad \text{on } \hat{S}_t,$$

$$\left(\frac{\partial g}{\partial(u_{I,\mu})}\right)^+ = -\left(\frac{\partial g}{\partial(u_{I,\mu})}\right)^- \quad \text{on every } L_t,$$

and Eq. (3.25) reduces then to

(3.28)
$$\frac{d}{dt} J(\mathbf{u}) \doteq \int_{\hat{S}_t} (h + g_{,n} - 2gK_m)v_n\,da + \int_{\hat{L}_t} (g^+ v_\mu^+ + g^- v_\mu^-)\,dl.$$

4. Example: time derivatives of the potential energy in nonlinear elasticity

The general results of the preceding sections can now be applied to various particular problems of mechanics. To illustrate this application, consider a nonlinear elastic body occupying a region V_t in its undeformed state and assume this region to undergo a shape transformation process with varying t. This transformation process may correspond, for instance, to body growth, phase transformation, or to conceptual redesign procedure where some material domains are added to or removed from the body. The deformation process described by a displacement field $u_i(\mathbf{x}, t)$ corresponds also to a change of body configuration but transformation and deformation fields are regarded as separate fields, coupled through governing equations for the body.

The Cartesian coordinates x_i are interpreted as the material coordinates, and the displacement field $\mathbf{u}(\mathbf{x}, t)$ is assumed to be of class C^2 in the four-dimensional domain Ω_t containing $\overline{V}_t$.[4] The deformation gradient $\mathbf{F}$ is defined by $\mathbf{F} = \mathbf{I} + \nabla\mathbf{u}$, that is $F_{ij} = \delta_{ij} + u_{i,j}$. The material is assumed to be hyperelastic, obeying the constitutive relations of the form

(4.1)
$$\sigma_{ij} = \frac{\partial W}{\partial F_{ij}},$$

where σ is the first (nonsymmetric) Piola–Kirchhoff stress tensor (related to the symmetric Cauchy stress σ^c by the formula $\sigma_{ij}F_{kj} = \det(\mathbf{F})\,\sigma_{ik}^c$), and W is the specific strain energy (per unit volume in the undeformed state), assumed to be a given function of $(\mathbf{x}, \mathbf{F})$ of class C^2 specified for $\mathbf{x}$ from an open domain containing $\overline{V}_t$. The nominal body forces b_i (per unit undeformed volume) are assumed to be continuously differentiable functions of $\mathbf{x}$. The body surface is composed of two piecewise regular parts $\hat{S}_t^u$ and $\hat{S}_t^T$. Over $\hat{S}_t^u$ the displacements $\mathbf{u} = \overline{\mathbf{u}}$ are specified as the restriction to $\hat{S}_t^u$ of a given spatial vector field $\overline{\mathbf{u}}(\mathbf{x})$ of class C^2 defined in a neighbourhood of $\hat{S}_t^u$. Over each regular section S_t^T of $\hat{S}_t^T$ (possibly, independently of each other) the nominal tractions $\mathbf{T} = \overline{\mathbf{T}}$ (per unit undeformed area) are prescribed as the restriction to S_t^T of a given spatial vector field $\overline{\mathbf{T}}(x)$ of class C^1 defined in a neighbourhood of S_t^T.

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[4] Physically, $\mathbf{u}$ may be defined only over the body domain V_t, but the smooth extension of $\mathbf{u}$ on the domain Ω_t is assumed to exist.

Consider the potential energy functional

(4.2)
$$\pi(u) = \int_{V_t} \{W(\mathbf{x}, \nabla u + \mathbf{I}) - b_i u_i\} d\mathcal{V} - \int_{\hat{S}_t^T} \overline{T}_i u_i \, da,$$

which is assumed to vanish in the undeformed state ($u_i \equiv 0$) for any shape of V_t. Now, we can identify (for $N = 3$) the function $W - b_i u_i$ with h and the function equal to $-\overline{T}_i u_i$ on $\hat{S}_t^T$ and zero on $\hat{S}_t^u$ with g in Eq. (3.20). From Eqs. (3.23), (3.22), (3.4) and (4.1), the following expression for the time derivative of $\pi(\mathbf{u})$ is obtained:

(4.3)
$$\frac{d}{dt} \pi(u) = - \int_{V_t} (\sigma_{ij,j} + b_i) \dot{u}_i \, d\mathcal{V} + \int_{\hat{S}_t^T} (\sigma_{ij} n_j - \overline{T}_i) \dot{u}_i \, da + \int_{\hat{S}_t^T} \{W - b_i u_i - (\overline{T}_i u_i)_{,n}\}$$

$$+ 2\overline{T}_i u_i K_m \} v_n \, da + \int_{\hat{S}_t^u} \{(W - b_i u_i) v_n + \sigma_{ij} n_j \dot{u}_i\} da$$

$$- \int_{\hat{L}_t^T} (\overline{T}_i^+ v_\mu^+ + \overline{T}_i^- v_\mu^-) u_i \, dl - \int_{\hat{L}_t^{Tu}} \overline{T}_i u_i v_\mu^T \, dl.$$

In the above expression, $\hat{L}_t^T$ and $\hat{L}_t^{Tu}$ denote the set of the edges of intersection of the regular surface sections S_t^{T+} with S_t^{T-} and S_t^T with S_t^u, respectively, with the corresponding meaning of the symbols $(+)$, $(-)$ and (T) in the integral expressions. The condition $\mathbf{u} = \overline{\mathbf{u}}$ on S_t^u yields

(4.4)
$$\frac{\delta u_i}{\delta t} = \frac{\delta \overline{u}_i}{\delta t} = \overline{u}_{i,n} v_n, \qquad \dot{u}_i = \frac{\delta u_i}{\delta t} - u_{i,n} v_n = (\overline{u}_{i,n} - u_{i,n}) v_n.$$

The last expression can be substituted in Eq. (4.3) to eliminate $\dot{u}_i$ from the integral over $\hat{S}_t^u$.

Suppose that the derivative (4.3) is calculated when the body is in equilibrium, that is when

(4.5)
$$\sigma_{ij,j} + b_i = 0 \quad \text{in} \quad V_t,$$
$$\sigma_{ij} n_j = \overline{T}_i \quad \text{on} \quad \hat{S}_t^T.$$

The conditions (4.5) are equivalent to vanishing of the derivative (4.3) with respect to kinematically admissible fields $\dot{\mathbf{u}}$ with $\hat{S}_t$ held fixed, that is

(4.6)
$$\left(\frac{d}{dt}\right)_s \pi(u) = - \int_{V_t} (\sigma_{ij,j} + b_i) \dot{u}_i \, dv + \int_{\hat{S}_t^T} (\sigma_{ij} n_j - \overline{T}_i) \dot{u}_i \, da = 0.$$

In view of Eq. (4.6), the expression (4.3) takes the form

(4.7)
$$\frac{d}{dt} \pi(u) = \left(\frac{d}{dt}\right)_d \pi(u) = \int_{\hat{S}_t^T} \{W - (b_i + \overline{T}_{i,n}) u_i - (u_{i,n} - 2u_i K_m) \overline{T}_i\} v_n \, da$$

$$+ \int_{\hat{S}_t^u} \{W - b_i \overline{u}_i - (u_{i,n} - \overline{u}_{i,n}) \sigma_{ij} n_j\} v_n \, da - \int_{\hat{L}_t^T} (\overline{T}_i^+ v_\mu^+ + \overline{T}_i^- v_\mu^-) u_i \, dl - \int_{\hat{L}_t^{Tu}} \overline{T}_i \overline{u}_i v_\mu^T \, dl.$$

This expression provides a generalization of the result of DEMS and MRÓZ [2]. Let us note that the total derivative (4.3) can be presented as a sum of the state and domain derivatives, (4.6) and (4.7). In view of stationarity of the potential energy with respect

to the state field **u**, the state derivative (4.6) vanishes and the total time derivative equals the domain derivative expressed by the surface and line integrals explicitly in terms of the state field **u** and normal transformation velocity v_n (since $v_\mu^\pm$ on the edges are definite functions of $v_n^\pm$).

Consider now the case when the external body surface S_t is fixed[5] but the elastic body is composed of two variable subdomains $V_t^{(1)}$ $V_t^{(2)}$ separated by the moving regular interface S_t^D. The displacement field $\mathbf{u}(\mathbf{x}, t)$ is assumed to be continuous on S_t^D and twice continuously differentiable elsewhere but its derivatives may be discontinuous across S_t^D, satisfying Eqs. (3.10) and (3.17). The process of shape transformation with moving interface S_t^D can be regarded, for instance, as a phase transformation process, damage progression, or redesign of an elastic composite structure with different material properties within $V_t^{(1)}$ and $V_t^{(2)}$. The strain energy functions $W^{(1)}$ and $W^{(2)}$ on both sides of S_t^D are of class C^2 and are in, general, independently specified for **x** from open domains containing $\overline{V_t^{(1)}}$ and $\overline{V_t^{(2)}}$, respectively. Similarly, we regard the body forces in $V_t^{(1)}$ and $V_t^{(2)}$ as two independently specified spatial fields $\mathbf{b}^{(1)}(\mathbf{x})$ and $\mathbf{b}^{(2)}(\mathbf{x})$ of class C^1. The boundary conditions on the fixed body surface $\hat{S}_t \equiv \hat{S}_0$ are identical as in the previous case. The potential energy functional is taken in the form

$$(4.8) \quad \pi^D(u) = \int_{V_t^{(1)}} \{W^{(1)}(\mathbf{x}, \nabla \mathbf{u}+\mathbf{I}) - b_i^{(1)} u_i\} d\mathscr{V} + \int_{V_t^{(2)}} \{W^{(2)}(\mathbf{x}, \nabla \mathbf{u}+\mathbf{I})$$

$$- b_i^{(2)} u_i\} d\mathscr{V} - \int_{\hat{S}_0^T} \overline{T}_i u_i \, da.$$

The term $\overline{T}_i u_i$ on S_0^T is assumed, for simplicity, to be continuous across a moving edge L_t^D of intersection of S_t^D with S_0^T so that no line integral appears in the expression for the first time derivative of the surface integral in Eq. (4.8). From the condition $\mathbf{u} = \bar{\mathbf{u}}$ on $\hat{S}_0^u$ it follows that $\dot{\mathbf{u}} = 0$ on $\hat{S}_0^u$. Identifying the function $W^{(r)} - b_i^{(r)} u_i$ with $h^{(r)}$ in Eq. (3.11) ($r = 1, 2$) and using Eqs. (3.12), (3.4), and (4.1) with $W^{(r)}$ and $\boldsymbol{\sigma}^{(r)}$ in place of W and $\boldsymbol{\sigma}$, we arrive at the following expression for the time derivative of the potential energy:

$$(4.9) \quad \frac{d}{dt} \pi^D(u) = -\int_{V_t^{(1)}} (\sigma_{ij,j}^{(1)} + b_i^{(1)}) \dot{u}_i \, d\mathscr{V} - \int_{V_t^{(2)}} (\sigma_{ij,j}^{(2)} + b_i^{(2)}) \dot{u}_i \, d\mathscr{V}$$

$$+ \int_{\hat{S}_0^T} (\sigma_{ij} n_j - \overline{T}_i) \dot{u}_i \, da - \int_{S_t^D} [\![\sigma_{ij}]\!] n_j \frac{\delta u_i}{\delta t} \, da - \int_{S_t^D} \{[\![W]\!] - n_j [\![\sigma_{ij} u_{i,n}]\!] - [\![b_i]\!] u_i\} v_n \, da.$$

Suppose that the derivative (4.9) is calculated at the equilibrium state of the body, that is when the conditions (4.5) (with $\boldsymbol{\sigma}$ replaced by the respective $\boldsymbol{\sigma}^{(r)}$) are satisfied except on S_t^D and there is

$$(4.10) \qquad\qquad\qquad\qquad [\![\sigma_{ij}]\!] n_j = 0 \quad \text{on } S_t^D.$$

The conditions (4.5) and (4.10) are equivalent to vanishing of the state derivative of $\pi^D(\mathbf{u})$ with respect to kinematically admissible fields $\dot{\mathbf{u}}$ and with fixed S_t^D. The expression (4.9) becomes now the domain derivative in the form

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[5] In the sense that there is no shape transformation of $\hat{S}_t$, that is, $v_n = 0$ on $\hat{S}_t$, but the displacements need not vanish on $\hat{S}_t$.

(4.11) $\qquad \dfrac{d}{dt}\,\pi^D(\mathbf{u}) = \left(\dfrac{d}{dt}\right)_d \pi^D(u) = -\int\limits_{S_t^D} \{[\![W]\!] - \sigma_{ij} n_j [\![u_{i,n}]\!] - [\![b_i]\!] u_i\}\, v_n\, da.$

If the potential energy functional (4.8) is required to attain a stationary value (or a weak relative minimum) for varying S_t^D as well, then from Eq. (4.11) (or from Eq. (3.16)) it follows that

(4.12) $\qquad\qquad\qquad [\![W]\!] - \sigma_{ij} n_j [\![u_{i,n}]\!] - [\![b_i]\!] u_i = 0 \qquad$ on S_t^D.

This relation can be written down in two other equivalent forms, on account of Eq. (3.10). The relationships (4.11) and (4.12) reduce to those derived and discussed by ESHELBY [8], KNOWLES [20], JAMES [13], ABEYRATNE [9], GURTIN [14] and DEMS and MRÓZ [2, 3].

Let us now discuss the second time derivative of the potential energy (4.8) at the equilibrium state. The assumed order of differentiability in $V_t^{(1)}$ and $V_t^{(2)}$ of all functions involved is now increased by one with respect to that assumed previously. It is possible to apply the general expression (3.18) with appropriate identification of the integrand functions. An alternative way is to differentiate the expression (4.9) with the help of Eq. (3.23) and substitute the equilibrium conditions. The result is

(4.13) $\qquad \dfrac{d^2}{dt^2}\,\pi^D(\mathbf{u}) = -\int\limits_{V_t^{(1)}} \dot{\sigma}_{ij,j}^{(1)} \dot{u}_i\, d\mathscr{V} - \int\limits_{V_t^{(2)}} \dot{\sigma}_{ij,j}^{(2)} \dot{u}_i\, d\mathscr{V} + \int\limits_{\hat{S}_0^T} \dot{\sigma}_{ij} n_j \dot{u}_i\, da$

$\qquad\qquad\qquad - \int\limits_{S_t^D} \left\{ D\left(\dfrac{\delta v_n}{\delta t} - 2v_n^2 K_m\right) + v_n\,\dfrac{\delta D}{\delta t} + \dfrac{\delta}{\delta t}([\![\sigma_{ij}]\!]n_j)\,\dfrac{\delta u_i}{\delta t} \right\} da - \int\limits_{\hat{L}_t^D} D v_n v_\mu^D\, dl,$

where

$\qquad\qquad\qquad\qquad D = [\![W]\!] - [\![\sigma_{ij} u_{i,n}]\!] n_j - [\![b_i]\!] u_i.$

This form is convenient in applications when $\dot{\mathbf{u}}$ satisfies the incremental conditions of equilibrium since it contains explicitly the terms appearing in these conditions. An alternative expression (not given here) can be obtained from Eq. (4.13) by using the divergence theorem and rearranging with help of the differentiation rule (2.24).

5. Derivative of a volume functional with constraints imposed on the state field

The general results presented in Sect. 3 shall now be applied in the case when the time derivative of a functional of a state field $\mathbf{u}$ defined over a variable domain V_t,

(5.1) $\qquad\qquad\qquad J(\mathbf{u}) = \int\limits_{V_t} g(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u})\, d\mathscr{V},$

is to be determined in the presence of certain constraints imposed upon the field $\mathbf{u}$. For simplicity, the boundary S_t of V_t is assumed to be regular and the vector $\mathbf{u}$ is taken to be three-dimensional, of the components u_i (though an extension to N-dimensional $\mathbf{u}$ is immediate). The function g is of class C^2 and is specified for $\mathbf{x}$ from some neighbourhood of $\bar{V}_t$.

We begin with general considerations, not pretending to be completely rigorous in a mathematical sense. Suppose that the field $\mathbf{u}$ is constrained by an operator equation within the domain V_t,

(5.2) $\qquad\qquad A(\mathbf{u}) = 0 \quad$ in $V_t \quad$ (or $A_i(\mathbf{u})(\mathbf{x}) = 0 \quad$ for $\mathbf{x} \in V_t$)

and by the so-called essential boundary conditions

(5.3) $\tilde{\mathbf{G}}(\mathbf{u}) = \mathbf{0}$ on S_t (or $\tilde{G}_i(\mathbf{u})(\mathbf{x}) = 0$ for $\mathbf{x} \in S_t$),

where $\mathbf{A}$ and $\tilde{\mathbf{G}}$ are nonlinear operators (with *functions* as their arguments and values), assumed to be (Gateaux) differentiable. We shall proceed in a formal way, leaving the corresponding function spaces unspecified. In general, the surface operator $\tilde{\mathbf{G}}$ defined on the varying boundary surface can be regarded either as specified by or as specifying the operator $\mathbf{G}$ defined in a neighbourhood of the surface S_t, such that $\tilde{\mathbf{G}}(\mathbf{u})(\mathbf{x}) = \mathbf{G}(\mathbf{u})(\mathbf{x})$ for $\mathbf{x} \in S_t$. A form of the operator $\mathbf{G}$ depends on the shape transformation process; however, in the course of differentiation we may regard this process and this operator as specified. The derivatives $\partial(\mathbf{G}(\mathbf{u}))/\partial t$ and $(\mathbf{G}(\mathbf{u}))_{,n}$ refer to the time-dependent *spatial* field obtained as the value of the operator $\mathbf{G}$ acting on the field $\mathbf{u}$ which varies in time. The distinction between $\mathbf{G}$ and $\tilde{\mathbf{G}}$ will be illustrated in the subsequent discussion of the particular case.

Following the usual technique, consider an augmented functional

(5.4) $J^a(\mathbf{u}) = \int\limits_{V_t} g(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}) \, d\mathscr{V} - \int\limits_{V_t} \lambda_i A_i(\mathbf{u}) \, d\mathscr{V} - \int\limits_{S_t} \lambda_i \tilde{G}_i(\mathbf{u}) \, da,$

where $\boldsymbol{\lambda}$ is the Lagrange multiplier field, assumed continuous and continuously differentiable. In Eq. (5.4), the field $\mathbf{u}$ is regarded as nonconstrained, however, the derivative of $J^a(\mathbf{u})$ shall be evaluated at the (known) state $\mathbf{u}$ which satisfies the conditions (5.2) and (5.3). The total time derivative of $J^a(\mathbf{u})$ corresponds to variation of $\mathbf{u}$, λ and of the domain V_t, so that, in analogy to Eq. (3.23) and on substituting the conditions (5.2) and (5.3),

(5.5) $\dfrac{d}{dt} J^a(\mathbf{u}) = \left(\dfrac{d}{dt}\right)_s J^a(\mathbf{u}) + \left(\dfrac{d}{dt}\right)_d J^a(\mathbf{u}),$

where the state derivative equals

(5.6) $\left(\dfrac{d}{dt}\right)_s J^a(\mathbf{u}) = \int\limits_{V_t} \left\{ \dfrac{\partial g}{\partial u_i} - \left(\dfrac{\partial g}{\partial(u_{i,j})}\right)_{,j} \right\} \dot{u}_i \, d\mathscr{V} - \int\limits_{V_t} \lambda_i \dfrac{\partial}{\partial t}(A_i(\mathbf{u})) \, d\mathscr{V}$

$$+ \int\limits_{S_t} \left\{ \dfrac{\partial g}{\partial(u_{i,j})} n_j \dot{u}_i - \lambda_i \dfrac{\partial}{\partial t}(G_i(\mathbf{u})) \right\} da$$

and the domain derivative is expressed by

(5.7) $\left(\dfrac{d}{dt}\right)_d J^a(\mathbf{u}) = \int\limits_{S_t} \{g - \lambda_i (G_i(\mathbf{u}))_{,n} v_n\} \, da.$

Denoting the (Gateaux) derivatives of the operators $\mathbf{A}$ and $\tilde{\mathbf{G}}$ by $\mathbf{A}'$ and $\tilde{\mathbf{G}}'$, respectively, we can write

(5.8) $\dfrac{\partial}{\partial t}(A_i(\mathbf{u})) = A_i'(\mathbf{u})(\dot{\mathbf{u}}), \quad \dfrac{\partial}{\partial t}(G_i(\mathbf{u}))|_{S_t} = \tilde{G}_i'(\mathbf{u})(\dot{\mathbf{u}}).$

The operators $\mathbf{A}'$ and $\tilde{\mathbf{G}}'$ are, by definition, linear with respect to the second argument. Suppose that we are able to determine the adjoint operators $(\mathbf{A}')^*$ and $(\tilde{\mathbf{G}}')^*$ such that for all fields $\dot{\mathbf{u}}$, $\boldsymbol{\lambda}$

(5.9) $\int\limits_{V_t} \lambda_i A_i'(\mathbf{u})(\dot{\mathbf{u}}) \, dv + \int\limits_{S_t} \lambda_i \tilde{G}_i'(\mathbf{u})(\dot{\mathbf{u}}) \, da = \int\limits_{V_t} \dot{u}_i (\mathbf{A}')_i^*(\mathbf{u})(\boldsymbol{\lambda}) \, d\mathscr{V} + \int\limits_{S_t} \dot{u}_i (\tilde{\mathbf{G}}')_i^*(\mathbf{u})(\boldsymbol{\lambda}) \, da.$

On substituting Eqs. (5.8) and (5.9), the expression (5.6) takes the form

$$(5.10) \quad \left(\frac{d}{dt}\right)_s J^a(\mathbf{u}) = \int_{V_t} \left\{ \left| \frac{\partial g}{\partial u_i} - \left(\frac{\partial g}{\partial (u_{i,j})} \right)_{,j} - (A')_i^*(\mathbf{u})(\lambda) \right\} \dot{u}_i \, d\mathscr{V}$$

$$+ \int_{S_t} \left\{ \frac{\partial g}{\partial (u_{i,j})} n_j - (\tilde{G}')_i^*(\mathbf{u})(\lambda) \right\} \dot{u}_i \, da.$$

Now we require the state derivative (5.10) to vanish identically for all fields $\dot{\mathbf{u}}$, and obtain in that way the following linear equations for the field λ:

$$(5.11) \qquad (A')_i^*(\mathbf{u})(\lambda) = \frac{\partial g}{\partial u_i} - \left(\frac{\partial g}{\partial (u_{i,j})} \right)_{,j} \quad \text{in } V_t,$$

$$(5.12) \qquad (G')_i^*(\mathbf{u})(\lambda) = \frac{\partial g}{\partial (u_{i,j})} n_j \quad \text{on } S_t.$$

Suppose that the system of equations (5.11) with the boundary conditions (5.12) has a solution λ. For that field λ the total time derivative of $J^a(\mathbf{u})$, at $\mathbf{u}$ satisfying the constraints (5.2) and (5.3), reduces to the domain derivative (5.7). In turn, the functional $J^a(\mathbf{u})$ has been so constructed that for any field $\dot{\mathbf{u}}$ compatible with the constraints, that is, for $\dot{\mathbf{u}}$ satisfying

$$(5.13) \qquad \frac{\partial}{\partial t}(A(\mathbf{u})) = A'(\mathbf{u})(\dot{\mathbf{u}}) = 0 \quad \text{in } V_t,$$

$$(5.14) \qquad \frac{\delta}{\delta t}(\tilde{G}(\mathbf{u})) = \tilde{G}'(\mathbf{u})(\dot{\mathbf{u}}) + (G(\mathbf{u}))_{,n} v_n = 0 \quad \text{on } S_t,$$

the derivative (5.5) of $J^a(\mathbf{u})$ coincides with the time derivative of the original functional (5.1). This can be verified by substituting Eqs. (5.11), (5.12) and (5.9) in the expression of type (3.3) for the derivative of the relation (5.1) which leads to the right hand side expression in Eq. (5.7), on account of the relations (5.13) and (5.14). Hence the time derivative of the functional (5.1) in the presence of the constraints (5.2) and (5.3) is expressed by

$$(5.15) \qquad \left(\frac{d}{dt}\right)_c J(\mathbf{u}) = \int_{S_t} \left\{ g - \lambda_i (G_i(\mathbf{u}))_{,n} \right\} v_n \, da$$

provided that the field λ satisfies Eqs. (5.11) and (5.12). Note that in this formula the field $\dot{\mathbf{u}}$ has been eliminated, and that the normal derivative $(G(\mathbf{u}))_{,n}$ depends in general on the shape transformation process as does the operator G itself.

The equations (5.11) and (5.12) can be regarded as definition of the adjoint field $\mathbf{u}^a(\mathbf{x}) = \lambda(\mathbf{x})$ within the same domain V_t, but satisfying different field equations and boundary conditions. It is seen that in order to determine the time derivative (5.15), we need a solution of the primary problem defined by Eqs. (5.2) and (5.3) and of an adjoint problem defined by Eqs. (5.11) and (5.12).

Consider now a particular case when the functional (5.1) is considered with the constraining conditions of the form

$$A_i(\mathbf{u}) \equiv \frac{\partial h}{\partial u_i} - \left(\frac{\partial h}{\partial(u_{i,j})}\right)_{,j} = 0 \quad \text{in } V_t,$$

(5.16)
$$\tilde{G}_i(\mathbf{u}) = \frac{\partial h}{\partial(u_{i,j})}\,\tilde{n}_j - \bar{T}_i = 0 \quad \text{on } S_t,$$

where $h = h(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}) = \bar{h}(\mathbf{x}, \mathbf{u}) + \bar{\bar{h}}(\mathbf{x}, \nabla\mathbf{u})$ with the functions $\bar{h}$ and $\bar{\bar{h}}$ of class C^2 and C^3, respectively, specified for $\mathbf{x}$ from some neighbourhood of V_t. $\bar{T} = \bar{T}(\mathbf{x})$ is the continuously differentiable spatial vector field prescribed in a neighbourhood of S_t, and $\tilde{n}$ is a *surface* field of the unitnormal vector.

To identify the operator $\mathbf{G}$ discussed previously, let S_t be a surface configuration in a shape transformation process with nonvanishing normal transformation velocity v_n. Each point $\mathbf{x}$ from a neighbourhood of S_t lies at some instant $t = \tau$ on the moving surface S_τ, therefore, we can construct the *spatial* field $\mathbf{n} = \mathbf{n}(\mathbf{x})$ by assigning to $\mathbf{x}$ the unit vector normal to that S_τ^j at $\mathbf{x}$. The operator $\mathbf{G}$ is defined by the second formula in Eq. (5.16) in which the surface field $\tilde{n}$ is replaced by the spatial field $\mathbf{n}$. Evidently, the field $\mathbf{n}$ and thus also the operator $\mathbf{G}$ are dependent on the shape transformation process. However, in any specified process with non-vanishing v_n, the derivatives

(5.17)
$$\frac{\partial n_i}{\partial t}\bigg|_{\mathbf{x}=\text{const}} = 0 \quad \text{and} \quad n_{i,n} = \frac{\partial n_i}{\partial x_j}\,n_j = \frac{1}{v_n}\frac{\delta n_i}{\delta t} = \frac{1}{v_n}\frac{\delta\tilde{n}_i}{\delta t}$$

are well defined and therefore the derivatives $\partial(\mathbf{G}(\mathbf{u}))/\partial t$ and $(\mathbf{G}(\mathbf{u}))_{,n}$ have a clear sense. Of course, on S_t we have $\tilde{n} = \mathbf{n}$ and in the following the tilda will be in many cases omitted.

From Eq. (5.15) we immediately obtain the following expression for the time derivative of the relation (5.1) in the presence of the constraints (5.16)

(5.18)
$$\left(\frac{d}{dt}\right)_c |\!(\mathcal{J}(\mathbf{u})| = \int_{S_t}\left\{g - \lambda_i\left(\frac{\partial h}{\partial(u_{i,j})}\,n_j\right)_{,n} + \lambda_i\bar{T}_{i,n}\right\}v_n\,da,$$

and there remains to determine the adjoint operators $(\mathbf{A}')^*$ and $(\tilde{\mathbf{G}}')^*$ which occur in Eqs. (5.11) and (5.12) for the adjoint field λ. However, it is preferable (and instructive) to repeat the whole derivation procedure outlined previously with a slight modification which allows to avoid construction of the operator $\mathbf{G}$ and to remove the restriction $v_n \neq 0$.

The argmented functional has now the form

(5.19)
$$J^a(\mathbf{u}) = \int_{V_t} g(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u})\,d\mathcal{V} - \int_{V_t}\lambda_i\left\{\frac{\partial h}{\partial u_i} - \left(\frac{\partial h}{\partial(u_{i,j})}\right)_{,j}\right\}d\mathcal{V}$$

$$-\int_{S_t}\lambda_i\left\{\frac{\partial h}{\partial(u_{i,j})}\,\tilde{n}_j - \bar{T}_i\right\}da,$$

where the field λ is assumed to be of class C^2. The time derivative of Eq. (5.19) is calculated with help of Eqs. (3.3), (2.37) and (2.2) but the decomposition (2.24) is not applied to the vector $\tilde{n}$. At a state $\mathbf{u}$ satisfying the constraint conditions (5.16), the time derivative of Eq. (5.19) takes the form (5.5) with

$$(5.20) \quad \left(\frac{d}{dt}\right)_s J^a(\mathbf{u}) = \int_{V_t} \left\{ \frac{\partial g}{\partial u_i} \dot{u}_i - \left(\frac{\partial g}{\partial(u_{i,j})}\right)_{,j} \dot{u}_i - \lambda_i \frac{\partial^2 h}{\partial u_j \partial u_i} \dot{u}_j \right.$$

$$\left. + \lambda_i \left(\frac{\partial^2 h}{\partial(u_{k,m})\partial(u_{i,j})} \dot{u}_{k,m}\right)_{,j} \right\} d\mathscr{V} + \int_{S_t} \left\{ \frac{\partial g}{\partial(u_{i,j})} n_j \dot{u}_i - \lambda_i \frac{\partial^2 h}{\partial(u_{k,m})\partial(u_{i,j})} \dot{u}_{k,m} n_j \right\} da$$

and

$$(5.21) \quad \left(\frac{d}{dt}\right)_d J^a(\mathbf{u}) = \int_{S_t} \left\{ \left(g - \lambda_i \left(\left(\frac{\partial h}{\partial(u_{i,j})}\right)_{,n} n_j - \bar{T}_{i,n}\right)\right) v_n - \lambda_i \frac{\partial h}{\partial(u_{i,j})} \frac{\delta \tilde{n}_j}{\delta t} \right\} da.$$

By applying twice the divergence theorem to the last term in the volume integral in Eq. (5.20), we can rearrange this expression as follows:

$$(5.22) \quad \left(\frac{d}{dt}\right)_s J^a(\mathbf{u}) = \int_{V_t} \left\{ \frac{\partial g}{\partial u_i} - \left(\frac{\partial g}{\partial(u_{i,j})}\right)_{,j} - \frac{\partial^2 h}{\partial u_i \partial u_j} \lambda_j + \left(\frac{\partial^2 h}{\partial(u_{i,j})\partial(u_{k,m})} \lambda_{k,m}\right)_{,j} \right\} \dot{u}_i d\mathscr{V}$$

$$+ \int_{S_t} \left\{ \frac{\partial g}{\partial(u_{i,j})} - \frac{\partial^2 h}{\partial(u_{i,j})\partial(u_{k,m})} \lambda_{k,m} \right\} n_j \dot{u}_i da.$$

Requiring this expression to vanish identically for all $\mathbf{u}$, we obtain the equations for the adjoint problem

$$(5.23) \quad (A')_i^*(\mathbf{u})(\lambda) \equiv \frac{\partial^2 h}{\partial u_i \partial u_j} \lambda_j - \left(\frac{\partial^2 h}{\partial(u_{i,j})\partial(u_{k,m})} \lambda_{k,m}\right)_{,j} = \frac{\partial g}{\partial u_i} - \left(\frac{\partial g}{\partial(u_{i,j})}\right)_{,j} \quad \text{in } V_t,$$

$$(\tilde{G}')_i^*(\mathbf{u})(\lambda) \equiv \frac{\partial^2 h}{\partial(u_{i,j})\partial(u_{k,m})} \lambda_{k,m} \tilde{n}_j = \frac{\partial g}{\partial(u_{i,j})} \tilde{n}_j \quad \text{on } S_t.$$

By the same argument as is the general case, the time derivative of the functional (5.1) in the presence of the constraints (5.16) is equal to the domain derivative (5.21) of the argumented functional, and is thus, on account of Eq. (2.26), expressed by

$$(5.24) \quad \left(\frac{d}{dt}\right)_c J(\mathbf{u}) = \int_{S_t} \left\{ \left(g - \lambda_i \left(\left(\frac{\partial h}{\partial(u_{i,j})}\right)_{,n} n_j - \bar{T}_{i,n}\right)\right) v_n + \lambda_i \frac{\partial h}{\partial(u_{i,j})} \tilde{x}_{j,\beta} g^{\alpha\beta} v_{n,\alpha} \right\} da,$$

provided that the field λ satisfies Eq. (5.23). For $v_n \neq 0$, the equivalence of Eqs. (5.24) and (5.18) follows from the formulae (5.17) and (2.26).

The case considered above can easily be interpreted in the context of the nonlinear theory of elasticity. Identifying $\mathbf{u}$ with a displacement field and assuming that the first Piola-Kirchhoff stress tensor σ and the body force vector $\mathbf{b}$ are generated by the potential h, that is

$$(5.25) \quad \sigma_{ij} = \frac{\partial h}{\partial(u_{i,j})}, \quad b_i = -\frac{\partial h}{\partial u_i},$$

Eqs. (5.16) can be regarded as equilibrium equations and traction boundary conditions. In turn, the adjoint field λ may be identified with a field $\mathbf{u}^a$ of displacements of the adjoint body. The adjoint body problem is similar to that occurring when small displacements $\mathbf{u}^a$

are superposed on the initial field **u**. The corresponding stress $\boldsymbol{\sigma}^a$ is *linearly* related to the gradient of $\mathbf{u}^a$ by

(5.26)
$$\sigma_{ij}^a = \frac{\partial^2 h}{\partial(u_{i,j})\,\partial(u_{k,m})}\,\lambda_{k,m} \equiv C_{ijkm}^a(\nabla\mathbf{u})u_{k,m}^a,$$

where $C_{ijkm}^a = C_{kmij}^a$ are the tangential stiffness moduli at the state **u**. The term

(5.27)
$$-\frac{\partial^2 h}{\partial u_i\,\partial u_j}\,\lambda_j \equiv \frac{\partial b_j}{\partial u_i}\,u_j^a = \frac{\partial b_i}{\partial u_j}\,u_j^a$$

represents the linearized increment of the displacement-sensitive body forces **b**. Denote by $\mathbf{b}^a$ and $\boldsymbol{\sigma}^{(i)}$ the (artificially superposed at the state **u**) fields of additional body forces and initial stresses (induced, e.g. by an initial distortion field), defined by

(5.28)
$$\sigma_{ij}^{(i)} = -\frac{\partial g}{\partial(u_{i,j})}, \qquad b_i^a = \frac{\partial g}{\partial u_i}.$$

Eqs. (5.23) for the adjoint problem can be rewritten in the form of equilibrium conditions:

(5.29)
$$(\sigma_{ij}^a + \sigma_{ij}^{(i)})_{,j} + \frac{\partial b_i}{\partial u_j}u_j^a + b_i^a = 0 \quad \text{in } V_t,$$

$$(\sigma_{ij}^a + \sigma_{ij}^{(i)})n_j = 0 \quad \text{on } S_t.$$

The interpretation of the adjoint system is similar to that discussed by Dems and Mróz [2] who started from the virtual work principle deriving the variation of an arbitrary functional associated with the boundary transformation. To show that their result (93) is in agreement with the present formula (5.24), we use the identity

(5.30)
$$\int\limits_{S_t} \{\lambda_i\sigma_{ij}\tilde{x}_{j,\beta}g^{\alpha\beta}v_{n,\alpha} + (\lambda_{i,\alpha}\sigma_{ij}\tilde{x}_{j,\beta}g^{\alpha\beta} + \lambda_i\sigma_{ij,\alpha}\tilde{x}_{j,\beta}g^{\alpha\beta}$$

$$+ \lambda_i\sigma_{ij}n_j b_{\alpha\beta}g^{\alpha\beta})v_n\}\,da = \int\limits_{S_t} (v_n\lambda_i\sigma_{ij}\tilde{x}_{j,\beta}g^{\alpha\beta})_{;\alpha}\,da = 0$$

which results from the relations (2.8) and (2.10) and from the Green theorem (2.19) applied to a regular closed surface S_t. By substituting Eqs. (5.25), (5.30), (2.12) and $\lambda \equiv u^a$, the expression (5.24) can be rearranged as follows:

(5.31)
$$\left(\frac{d}{dt}\right)_c J(\mathbf{u}) = \int\limits_{S_t} \{g + u_i^a\bar{T}_{i,n} - u_{i,\alpha}^a\sigma_{ij}\tilde{x}_{j,\beta}g^{\alpha\beta} - 2u_i^a\sigma_{ij}n_j K_m - u_i^a(\sigma_{ij,}n_j$$

$$+ \sigma_{ij,\alpha}\tilde{x}_{j,\beta}g^{\alpha\beta})\}v_n\,da = \int\limits_{S_t} \{g + u_i^a\bar{T}_{i,n} - u_{i,j}^a\sigma_{ij} + u_{i,n}^a\sigma_{ij}n_j - 2u_i^a\sigma_{ij}n_j K_m$$

$$- u_i^a\sigma_{ij,j}\}v_n\,da.$$

Substitution of the equilibrium conditions (5.16) yields

(5.32)
$$\left(\frac{d}{dt}\right)_c J(\mathbf{u}) = \int\limits_{S_t} \{g + (u_i^a\bar{T}_i)_{,n} - u_{i,j}^a\sigma_{ij} - 2u_i^a\bar{T}_i K_m + u_i^a b_i\}v_n\,da.$$

The final formula is in agreement with the result derived by Dems and Mróz [2].

6. Concluding remarks

The present paper provides a systematic derivation of expressions for time derivatives of surface and volume integrals and functionals defined over varying domains. There are numerous physical applications of such derivatives and here we have presented some examples in the context of the nonlinear theory of elasticity. The previous results are extended by considering piecewise regular boundary surfaces with edges and corners of intersection. The extended application in sensitivity analysis and optimal shape design has been discussed recently in the literature [1–7]. The application of such derivatives in phase transformation problems was discussed in [8, 9, 13, 14]. We hope that the present paper can provide the foundation for systematic treatment of a variety of problems where the deformation process is accompanied by a shape transformation process.

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