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Introduction to shape sensitivity: three-dimensional and surface systems

by

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Abstract: In this paper we present some basic material for the shape optimization of structures. We emphasise the so called continuous approach with few results on numerical approximation with finite elements or boundary integrals.

1. Introduction

In this paper we present some basic material for the shape optimization of structures. We emphasise the so called continuous approach with few results on numerical approximation with finite elements or boundary integrals; this approach is traditional in mathematics and theoretical mechanics, whereas in mechanical engineering the tendency is to first approximate the behaviour of the structure with finite elements and afterwards to tackle optimization.

The choice of one of these approaches depends on the habits of thought; in many cases, discretisation in the first or second step yields the same results; this has been proved when one uses *conformal* finite elements (Moriano, 1988, Masmoudi, 1987). If one is interested in deriving necessary optimality conditions and finding explicit solutions, then the continuous approach is necessary; this is the route followed by Banichuk (1990), Prager (1972) and Rozvany (1996).

However, in connection with finite elements, the continuous approach is quite versatile: it enables the addition of design sensitivity to a commercial finite element code (Barros and Soares, 1987, Chenais and Knopf-Lenoir, 1988); but it also enables the inclusion of design sensitivity in an open finite element library such as Modulef (1985) and makes good use of existing software (Mehrez, Rousselet, Gauthier, Giuliano, 1991).

Moreover, formulae obtained with the continuous approach can be implemented with boundary elements (Masmoudi, 1987, Soares and Choi, 1984).

It should also be pointed out that these techniques may be used and are used in other fields of application; for example in acoustics (Masmoudi, 1987, Habbal, 1996) and in fluid mechanics (Pironneau, 1984).

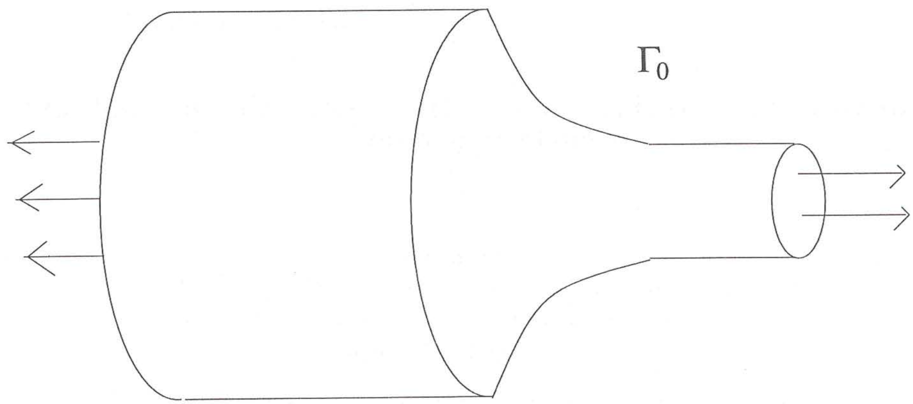

Figure 1.

What, however, is *shape optimization?* It is an optimal design problem where the design variable is the shape of the domain Ω occupied by the physical system; the best shape of a fillet in a tension bar will provide a classsical engineering example (Haug, Choi, Komkov, 1986): we want to find the best shape of Γ_0 to minimize volume with constraints on Von-Mises yield stress.

One of the first publications seems to be the one of Hadamard (1908) but the pioneers of research oriented toward the use of computers seem to be Céa, Gioan, Michel (1974). Since that date many papers have been devoted to this topic; for example Chenais (1977), Murat and Simon (1976), Rousselet (1976,1977,1982), Dems and Mróz (1984), Pironeau (1984). INRIA schools devoted to shape optimization have been organized by Pironneau (1982) and Céa and Rousselet (1983).

2. Optimization and continuum mechanics

As in conventional optimal design, the clue of the approach is to obtain first - order estimates of the variation of a functional of the state of the system; but for shape optimization one soon realizes that the set of possible domains has no standard vector space structure, so that it seems that classical differential calculus and calculus of variations cannot apply here.

Indeed, these techniques can be used if one realizes that for a given topology and regularity of the boundary, it is natural to look for domains as mappings of a given domain Ω; we shall denote

$$\omega_\Psi = (\Phi + \tilde{\Psi})(\Omega) = \{x \in E \ \ / \ \ x = \Phi(X) + \tilde{\Psi}(X) \ \ \forall \ X \in \Omega\}$$

where E is the usual Euclidean space (in one, two or three dimensions); Ψ is

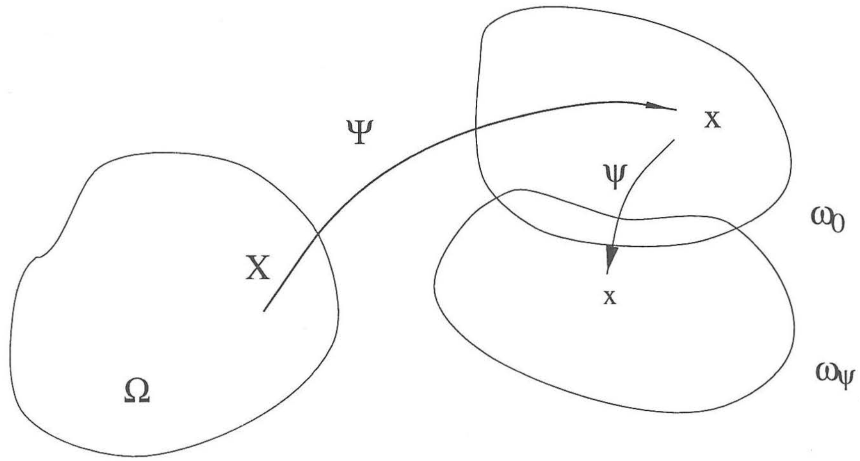

Figure 2.

an element of a vector space of functions; it will enable defition of variations of $\omega_0 = \Phi(\ \Omega)$; *in the sequel* ω *will be used instad of* ω_0.

Anyone familiar with the foundations of continuum mechanics should realise that this is what we are doing when we are using a Lagrangian representation of the movement of a continuous medium; this is the usual representation in solid mechanics. For the implementation of the analysis of large deformations of solids it is usual to use an updated Lagrangian formulation: this amounts to linearizing the behaviour of the solid around a configuration obtained with a fraction of the load.

Here we are going to linearize around the given domain ω, but we should keep in mind that in the overall process of optimization we shall update the domain ω around which we linearize the cost functional and the constraints.

Basic tools for this linearization are well-known in continuum mechanics, but were derived independently for shape optimization by several authors including Dervieux-Palmerio (1975), Murat-Simon (1976), Rousselet (1976). These tools are recalled in the next two sections.

3. Differential calculus and linearization around a given domain

To join domain sensitivity and surface sensitivity, we recall some basic notations of curvilinear coordinates; in fact the mapping

$$\begin{aligned}\Phi \ :\ & \Omega \longrightarrow \omega \\ & X \longmapsto x = \Phi(X)\end{aligned}$$

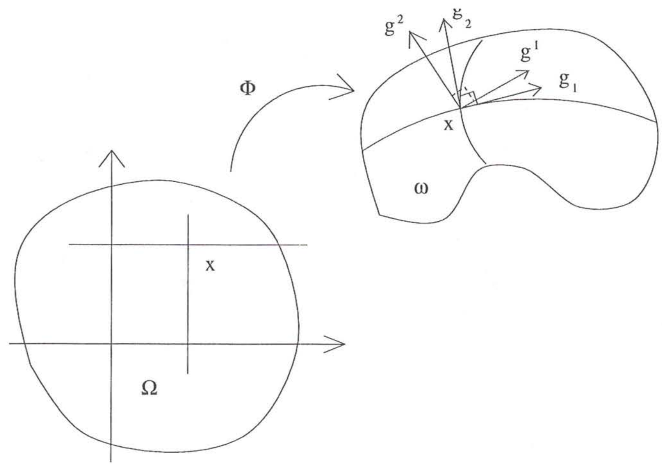

Figure 3.

defines *curvilinear coordinates* in ω.

We assume that all the domains Ω , ω are imbedded in a three-dimensional Euclidean space; entirely similar results hold in two dimensions.

We denote by $g_i(x) = \dfrac{\partial \Phi}{\partial X_i}$ the *local basis*; generally it is not orthonormal so that it is convenient to use the dual basis g^i defined by $g^i.g_j = \delta^i_j$; see drawing in two dimensions.

With these notations the matrix of $\dfrac{\partial \Phi}{\partial X}$ is

$$(g_1 \; g_2 \; g_3) \tag{1}$$

Note: *In the following repeated latin indices are summed from 1 to 3 and Greek indices from 1 to 2.*

Let $f \; : \omega \longrightarrow \mathbb{R}$ be a scalar funtion; if we set $f_{,i} = \dfrac{\partial f(\Phi(X))}{\partial X_i}$ the chain rule yields

$$\frac{\partial f}{\partial x} = f_{,i} g^i \tag{2}$$

it is usual to set

$$grad \; f = g^{ij} \; f_{,i} \; g_j \tag{3}$$

where

$$g^{ij} = g^i.g^j \tag{4}$$

For future reference we recall that

$$\int_{\omega} f(x)dx = \int_{\Omega} f(\Phi(X)) \mid D\Phi \mid dX \tag{5}$$

with

$$\mid D\Phi \mid = det(g_1\ g_2\ g_3) = \sqrt{g} \tag{6}$$

where $\qquad g = det(g_{ij}) \qquad$ with $\qquad g_{ij} = g_i.g_j$

For a vector field v defined in ω, the chain rule also yields :

$$\frac{\partial v}{\partial x} = v_{,i} g^i \tag{7}$$

where

$$v_{,i} = \frac{\partial v(\Phi(X))}{\partial X_i} \tag{8}$$

but if we express v in the local basis g_i and wish to express $\frac{\partial v}{\partial x}$ with these components it is classical to introduce Christoffel symbols:

$$\Gamma^i_{kj} = g^i.g_{k,j} \tag{9}$$

so that $\frac{\partial v}{\partial x} = v^i_{|j}\ g_i \otimes g^j$ where

$$v^i_{|j} = v^i{}_{,j} + \Gamma^i_{jk} v^k \tag{10}$$

and $g_i \otimes g^j$ is the linear mapping defined by

$$(g_i \otimes g^j)(h) = g_i h^j \tag{11}$$

The divergence operator is well-known in continuum mechanics; we recall here some formulae which have similar features when applied to surfaces. We first consider as a *definition* the following equality which should hold for any continuously differentiable function f with compact support in ω:

$$\int_{\omega} f\, div\, v\, dx = - \int_{\omega} \frac{\partial f}{\partial x} v\, dx \tag{12}$$

where component-wise:

$$\frac{\partial f}{\partial x} v = f_{,i}(g^i v) = f_{,i} v^i$$

to obtain an expression of $div\, v$ in local basis it is useful to state

LEMMA 3.1

(i) $$\frac{\partial g}{\partial g_{ij}} = g\, g^{ij}$$

(ii) $$\frac{\partial g}{\partial X_i} = 2g\Gamma^j_{ij} \qquad \text{or} \qquad \frac{\partial \sqrt{g}}{\partial X_i} = \sqrt{g}\,\Gamma^j_{ij}$$

Proof.
(i) Comes from $g_{ij}g^{jk} = \delta^k_i$
(ii) The proof uses (i) and some manipulations.

PROPOSITION 3.1 *Let* $v = v^i g_i$
(i) The following expressions hold

$$divv = \frac{1}{\sqrt{g}}(v^i\sqrt{g})_{,i} = v^i_{|i} = g^i.v_{,i}$$

(ii) The following identity holds

$$div(fv) = f div\, v + \frac{\partial f}{\partial x} v$$

Proof.
(i) The first identity comes from the definition (12) and (5), (6), (7).
(ii) Is straightforward in components.

The formula which provides *the first-order change of an integral over a domain* ω *with respect to changes of its shape* is well-known in continuum mechanics (see for example Germain, 1979) and is now widely used in shape optimal design (see e.g. Céa, 1975;1986, Masmoudi, 1987). Here we try to provide a presentation which is introductory to the more complex case of surface variation.
We recall from Section 2:

$$\omega_\Psi = (\Phi + \tilde{\Psi})(\Omega) = (Id + \Psi)(\omega)$$

with $\omega = \Phi(\Omega)$ and $\tilde{\Psi} = \Psi \circ \Phi$ and for any function $f:\ \tilde{f} = f \circ \Phi$

$$\tilde{f}(X) = f(\Phi(X)) \tag{13}$$

To make precise the first variation of a function f_Ψ defined on a variable domain ω_Ψ we set the

DEFINITION 3.1 *Let* f_Ψ *be a function defined on* ω_Ψ*; this function may depend explicitly on the vector field* Ψ *and implicitly through the position of the point* $x = x + \Psi(x)$ *where it is evaluated; we set*

$$\tilde{f}_\Psi(X) = f_\Psi(\Phi(X) + \Psi \circ \Phi(X))$$

and

$$\begin{aligned}\delta f_\Psi(x) &= \lim_{t\to 0}\frac{f_{t\Psi}(x+t\Psi(x))-f(x)}{t}\\ &= \frac{d}{dt}f_{t\Psi}\circ(\Phi+t\tilde{\Psi})\mid_{t=0}=\frac{\partial}{\partial t}\tilde{f}_{t\Psi}(X)\mid_{t=0}\\ &= \frac{\partial}{\partial t}f_{t\Psi}(\Phi(X))\mid_{t=0}+\frac{\partial}{\partial x}f_{t\Psi}\Psi(x)\mid_{t=0}\end{aligned}$$

Remark 1.

We note that δf is a function defined on ω; it is linear with respect to ψ ; if f does not depend explicitly on Ψ, the chain rule yields $\delta f = \frac{\partial f}{\partial x}\Psi(x)$. If f does not depend on x, δf is just the directional derivative with respect to Ψ. Moreover

$$\delta f_\Psi(x) = \frac{\partial f}{\partial \Psi} + \frac{\partial f}{\partial x}\Psi(x)$$

Remark 2.

The usual rules for computing derivatives of a sum or of a product of functions hold for the operator δ.

Remark 3.

In continuum mechanics, when a flow $t \longmapsto x(t)$ is defined on ω, the *material derivative* of $f(t,x(t))$ is

$$\lim_{\delta t\to 0}\frac{f(t,x(t+\delta t))-f(t,x(t))}{\delta t}$$

We note that δf is a particular case when $x(t) = X + t\Psi(X)$; this simple flow is what is needed to define the first order variation of ω. Here we call *material derivative* the δ operator.

To compute the variation of the integrals we need the following lemma.

LEMMA 3.2 *Let* $g = det(g_{ij})$ *then* $\delta\sqrt{g} = \sqrt{g}div\Psi$

Proof. We have

$$\delta g = \frac{\partial g}{\partial g_{ij}}\delta g_{ij}$$

as $g_{ij} = g_i.g_j$ we obtain

$$\delta g_{ij} = \tilde{\Psi}_i.g_j + g_i.\tilde{\Psi}_j$$

then using Lemma 3.1 we obtain

$$\delta g = 2gg^j.\tilde{\Psi}_j = 2g\ div\Psi$$

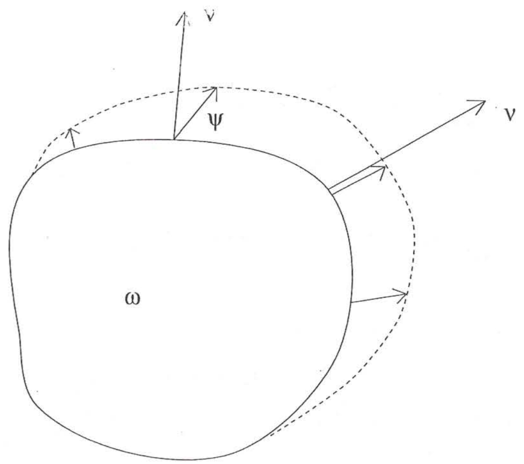

Figure 4.

PROPOSITION 3.2

$$\delta \int_\omega u \, d\omega = \int_\omega \delta u \, d\omega + \int_\omega u \, div\Psi \, d\omega$$

Proof. We obtain from (3.5), (3.6):

$$\int_\omega u \, d\omega = \int_\Omega \tilde{u}\sqrt{g} dX$$

The result then comes from the definition and Lemma 3.2.
Example.

$$vol(\omega) = \int_\omega d\omega \qquad \text{yields}$$

$$\delta vol(\omega) = \int_\omega div\Psi \, d\omega = \int_{\partial\omega} \Psi.\nu \, d\sigma$$

as could be expected; see the respective figure.

The last equality is obtained by using the Stoke's theorem.

We now state the *variation of a derivative.*

PROPOSITION 3.3 *Let u be a function defined in ω_Ψ; we have*

$$\delta \frac{\partial u}{\partial x} = \frac{\partial}{\partial x}\delta u - \frac{\partial u}{\partial x}\frac{\partial \Psi}{\partial x}$$

Proof. We note that

$$\frac{\partial u_{t\Psi}}{\partial x} = \frac{\partial \tilde{u}_{t\Psi}}{\partial X}\left(\frac{\partial(\Phi + t\tilde{\Psi})}{\partial X}\right)^{-1}$$

We use the definition of δ

$$\begin{aligned}
\delta\frac{\partial u_{t\Psi}}{\partial x} &= \frac{\partial}{\partial t}\left(\frac{\partial \tilde{u}_{t\Psi}}{\partial X}\right)_{|t=0}\left(\frac{\partial \Phi}{\partial X}\right)^{-1} + \frac{\partial \tilde{u}_{t\Psi}}{\partial X}_{|t=0}\frac{\partial}{\partial t}\left(\frac{\partial(\Phi + t\tilde{\Psi})}{\partial X}\right)^{-1}_{|t=0} \\
&= \frac{\partial}{\partial X}\left(\frac{\partial \tilde{u}_{t\Psi}}{\partial t}\right)_{|t=0}\left(\frac{\partial \Phi}{\partial X}\right)^{-1} - \frac{\partial \tilde{u}_0}{\partial X}\left(\frac{\partial \Phi}{\partial X}\right)^{-1}\frac{\partial \tilde{\Psi}}{\partial X}\left(\frac{\partial \Phi}{\partial X}\right)^{-1} \\
&= \frac{\partial}{\partial x}\delta u - \frac{\partial u}{\partial x}.\frac{\partial \Psi}{\partial x}
\end{aligned}$$

which proves the result.

4. Shape sensitivity for a model system

We apply the previous results to shape sensitivity of the simplest example: a membrane prestressed with an inplane tension T and submitted to a normal density of force f; the normal deflection is the solution of:

$$\left.\begin{array}{rl}
-T\Delta u = f & \text{in} \quad \omega \\
u = 0 & \text{on the part } \gamma_1 \text{ of the boundary} \\
 & \partial\omega \text{ where it is fixed.} \\
T\frac{\partial u}{\partial n} = 0 & \text{on } \gamma_2 \text{ where it is free}
\end{array}\right\} \tag{14}$$

We denote by V the space of kinematically admissible displacements; the principle of virtual work states that

$$\forall v \in V \;\; a(u,v) = l(v) \tag{15}$$

where

$$a(u,v) = \int_\omega T\frac{\partial u}{\partial x}\overline{\frac{\partial v}{\partial x}}\,dx \qquad \text{and} \qquad l(v) = \int_\omega fv\,dx \tag{16}$$

Note. *The overbar denotes the vector associated to a linear form and vice versa:*

$$\overline{\frac{\partial v}{\partial x}} \textit{ is the gradient of } v\ .$$

The variation of the solution is itself the solution of an equation as stated below.

PROPOSITION 4.1 *Let u be the solution of (15), then its first-order variation δu satisfies:*

$$\forall v \in V \qquad a(\delta u, v) = -(\delta a)(u, v) + (\delta l)(v) \tag{17}$$

where δa and δl are variations of a and l for fixed u and v :

$$\begin{aligned}(\delta a)(u,v) &= \int_\omega T\left(\frac{\partial u}{\partial x}.\frac{\partial \psi}{\partial x}.\frac{\overline{\partial v}}{\partial x}\,dx\right) + \frac{\partial v}{\partial x}.\frac{\partial \psi}{\partial x}.\frac{\overline{\partial u}}{\partial x}\,dx \\ &\quad + \int_\omega T\frac{\partial u}{\partial x}.\frac{\overline{\partial v}}{\partial x} div\psi\, dx \end{aligned} \tag{18}$$

$$(\delta l)(v) = \int_\Omega v\,\delta f\,dx + \int_\Omega f\,v\,div\Psi\,dx \tag{19}$$

The proof is a direct application of Propositions 3.2 and 3.3.

Shape sensitivity of a functional

We consider the simplest case

$$J = \int_\omega \alpha(u)dx \tag{20}$$

The proposition 3.2 yields

$$\delta J = \int_\omega \alpha'(u)\delta u\,dx + \int_\omega \alpha(u)div\Psi\,dx \tag{21}$$

As in conventional design sensitivity this expression is not explicit with respect to Ψ: δu is defined through equation (17); but this expression may be transformed.

PROPOSITION 4.2 *Let $L(u,v) = J(u) + a(u,v) - l(v)$ and set p the solution of*

$$\forall w \in V \qquad \frac{\partial L(u,p)}{\partial u}w = 0 \tag{22}$$

or $a(w,p) = -\dfrac{\partial J}{\partial u}w$ then

$$\delta J = (\delta L)(u,p)$$

where the variation of L is computed at u and p fixed; or more precisely:

$$\delta J = \int_\Omega \alpha(u)div\psi\,dx + (\delta a)(u,p) - (\delta l)(p) \tag{23}$$

with δa and δl given in the previous Proposition.

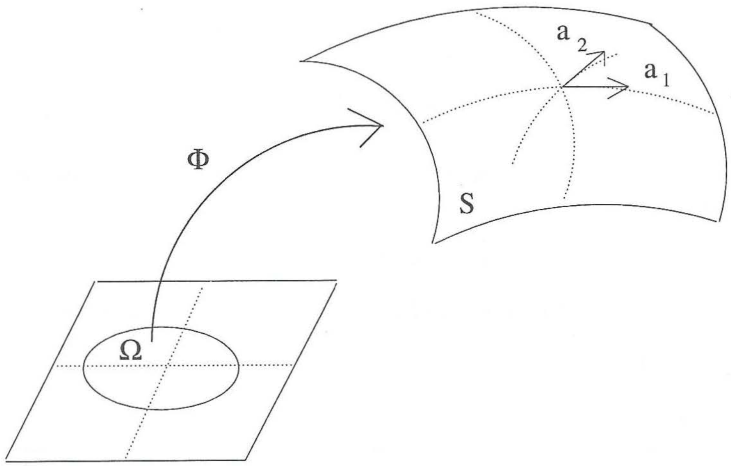

Figure 5.

5. Surface differential calculus

We consider now a surface S imbedded in a three dimensional space E^3, parametrized by a single-valued Φ from a reference open domain Ω of a two dimensional space E^2. The striking difference with Section 3 is that Φ is a mapping from a two dimensional space to a three dimensional space. With simplifications all the material presented would be adequate for plane curves, although the use of arc length would simplify some formulae.

To emphasize that Φ stems from a two - dimensional space, we denote by ξ the variable in Ω and Greek indices are implicitely running from 1 to 2; repeated indices mean summation, from 1 to 2.

The *local basis* is noted

$$a_\alpha = \frac{\partial \Phi}{\partial \xi^\alpha} \tag{24}$$

it is the basis of the tangent space to S at the point $m = \Phi(\xi)$.

The *dual basis is defined by*

$$a^\alpha . a_\beta = \delta^\alpha_\beta \tag{25}$$

where the dot means the usual scalar product of E^3. So $(a_1 a_2)$ is the matrix of

$$\frac{\partial \Phi}{\partial \xi} = a_\alpha \otimes e^\alpha \tag{26}$$

where $e^\alpha = e_\alpha$ is the standard basis of E^2 . We note that:

$$\begin{pmatrix} {}^t a^1 \\ {}^t a^2 \end{pmatrix} (a_1 \; a_2) = I_{\mathbb{R}^2} \tag{27}$$

or in tensor notations $(e_\alpha \otimes a^\alpha).(a_\alpha \otimes e^\alpha) = e_\alpha \otimes e^\alpha$, but

$$(a_1\, a_2)\begin{pmatrix} {}^t a^1 \\ {}^t a^2 \end{pmatrix} = a_1 \otimes a^1 + a_2 \otimes a^2 \tag{28}$$

is the matrix of Π , the orthogonal projection onto the tangent plane.
In the sequel we note

$$\tilde{f}(\xi) = f(\phi(\xi)) \ , \ x = \Phi(\xi) \ \text{ as in (13)}$$

Let now $f : S \longrightarrow \mathbb{R}$ be a real function defined on S. If we set

$$\frac{\partial f}{\partial m} = \frac{\partial \tilde{f}}{\partial \xi^\alpha} a^\alpha \tag{29}$$

it is easy to check that this linear mapping from the tangent plane to $\mathbb{R}$ is independent of the parametrization; we also have:

$$\frac{\partial f}{\partial m} a_\alpha = \frac{\partial \tilde{f}}{\partial \xi^\alpha}$$

or

$$\frac{\partial f}{\partial m}\frac{\partial \Phi}{\partial \xi} = \frac{\partial \tilde{f}}{\partial \xi} \ \text{ (the chain rule)}$$

In the following all the notions introduced are independent of the parametrization with the exception of the Christoffel symbols.

The integral over the surface may be written with a parametrization:

$$\int_S f(m)\, dS = \int_\Omega f(\Phi(\xi))\sqrt{a}\, d\xi \tag{30}$$

where

$$a = det(a_{\alpha\beta}) \tag{31}$$

with $a_{\alpha\beta} = a_\alpha . a_\beta$ or $\sqrt{a} = \| a_\alpha \times a_\beta \|$ (area element).

The differentiation of a vector field is here more intricate; this is intuitively obvious with a circle: let $T(\theta)$ be a unitary tangent vector field. It is clear that when $T(\theta)$ is near $T(\theta_0)$, the first-order change is not tangent but rather orthogonal to the circle; thus we need to introduce the orthogonal projection Π onto the tangent plane; recall that

$$\Pi = a_1 \otimes a^1 + a_2 \otimes a^2 \qquad \text{we set} \qquad a_{\alpha,\beta} = \frac{\partial a_\alpha}{\partial \xi^\beta}$$

then $\Pi a_{\alpha,\beta}$ is a tangent vector. Its decomposition in the local basis is classically expressed with Christoffel symbols (they *do* depend on the parametrization!):

$$\Pi a_{\alpha,\beta} = \Gamma^\lambda_{\alpha\beta} a_\lambda$$

with $\Gamma^{\lambda}_{\alpha\beta} = a^{\lambda}.a_{\alpha,\beta}$. Note that $\Gamma^{\lambda}_{\alpha\beta} = \Gamma^{\lambda}_{\beta\alpha}$ as $a_{\alpha,\beta} = a_{\beta,\alpha}$.

Similarly for a tangent vector field $v_t = v^{\alpha}a_{\alpha}$ as $\dfrac{\partial v_t}{\partial \xi^{\alpha}}$ is not tangent, we consider

$$\Pi\frac{\partial v_t}{\partial m} = v^{\alpha}_{|\beta}a_{\alpha} \otimes a^{\beta} \tag{32}$$

with

$$v^{\alpha}_{|\beta} = v^{\alpha}_{,\beta} + \Gamma^{\alpha}_{\lambda\beta}v^{\lambda} \tag{33}$$

$\Pi\frac{\partial v_t}{\partial m}$ is the so called covariant derivative of v; this definition is motivated by the following identity:

$$\Pi\frac{\partial v_t}{\partial m}a_{\mu} = \Pi\frac{\partial v}{\partial \xi^{\mu}}$$

and this formula comes from the chain rule; here are the details: by the definition,

$$\begin{aligned}
\Pi\frac{\partial v_t}{\partial m}a_{\mu} &= \left(v^{\alpha}_{|\beta}\, a_{\alpha} \otimes a^{\beta}\right) a_{\mu} = v^{\alpha}_{|\mu}a_{\alpha} \\
&= \left(v^{\alpha}_{,\mu} + \Gamma^{\alpha}_{\lambda\mu}v^{\lambda}\right) a_{\alpha} \\
&= v^{\alpha}_{,\mu}a_{\alpha} + \Gamma^{\alpha}_{\lambda\mu}a_{\alpha}v^{\lambda} \\
&= v^{\alpha}_{,\mu}a_{\alpha} + (\Pi a_{\alpha,\mu})\, v^{\lambda} \equiv v^{\alpha}_{,\mu}a_{\alpha} + v^{\alpha}\,(\Pi a_{\lambda,\mu}) \\
&= \Pi\left(v^{\alpha}a_{\alpha}\right)_{,\mu} \equiv \Pi\frac{\partial v}{\partial \xi^{\mu}}
\end{aligned}$$

We turn now to the *divergence of a tangent vector field* defined by an integration by parts.

For any continuously differentiable function f which is zero near the boundary of S:

$$\int_S f\ divv_t\ dS = -\int_S \frac{\partial f}{\partial m}v_t\ dS \tag{34}$$

To obtain an expression in the local basis it is convenient to note:

LEMMA 5.1 *(i)* $$\frac{\partial a}{\partial a_{\alpha\beta}} = aa^{\alpha\beta}$$

(ii) $$\frac{\partial a}{\partial \xi^{\alpha}} = 2a\Gamma^{\lambda}_{\alpha\lambda} \qquad or \qquad \frac{\partial \sqrt{a}}{\partial \xi^{\alpha}} = \sqrt{a}\Gamma^{\lambda}_{\alpha\lambda}$$

Proof: It is based on $(a^{\alpha\beta})(a_{\beta\gamma}) = \delta^{\alpha}_{\gamma}$ and

$$a_{\lambda\mu,\alpha} = \Gamma^{\gamma}_{\lambda\alpha}a_{\gamma\mu} + \Gamma^{\gamma}_{\mu\alpha}a_{\lambda\gamma}$$

which comes directly from the definition of Christoffel symbols.

PROPOSITION 5.1 *Let $v_t = v^\alpha a_\alpha$ be a tangent vector field, we then have the following expressions of the divergence*

$$div v_t = \frac{1}{\sqrt{a}}(\sqrt{a}v^\alpha)_{,\alpha} = v^\alpha_{|\alpha} = a^\alpha.\Pi\frac{\partial\tilde{v}_t}{\partial\xi^\alpha} = a^\alpha.\Pi\frac{\partial v_t}{\partial m}a_\alpha \tag{35}$$

Proof. The first equality comes from the definition and (30); then we obtain

$$div\, v_t = v^\alpha_{,\alpha} + v^\alpha\frac{(\sqrt{a})_{,\alpha}}{\sqrt{a}}$$

and with Lemma 5.1:

$$div\, v_t = v^\alpha_{,\alpha} + v^\alpha\Gamma^\lambda_{\alpha\lambda} = v^\alpha_{|\alpha}$$

(32) now gives

$$v^\alpha_{|\alpha} = a^\alpha.\Pi\frac{\partial v_t}{\partial m}a_\alpha = a^\alpha.\Pi\frac{\partial\tilde{v}_t}{\partial\xi^\alpha}$$

Because we are interested in variation of S , we shall have to consider vector fields Ψ which are transverse to S ; so now we recall how to compute derivatives of transverse vector fields.

It is usual to introduce a unitary normal vector

$$a_3 = \frac{a_1 \times a_2}{|| a_1 \times a_2 ||} \tag{36}$$

As $a^3.a^3 = 1$ we have $\frac{\partial a_3}{\partial m}.a_3 = 0$ so that $\dfrac{\partial a_3}{\partial m}$ may be considered as an operator of the tangent plane. Its expression in the local basis is usually written:

$$\frac{\partial a_3}{\partial m} = -b^\alpha_\beta a_\alpha \otimes a^\beta \tag{37}$$

so that $b^\alpha_\beta = -a^\alpha.\frac{\partial a_3}{\partial m}.a_\beta$ we also set $b_{\alpha\beta} = -a_\alpha.\frac{\partial a_3}{\partial m}.a_\beta = -a_\alpha.a_{3,\beta}$

Note that the lowering of indices is performed systematically with the metric tensor $a_{\alpha\beta}$:

$$b_{\alpha\beta} = a_{\alpha\lambda}b^\lambda_\beta$$

The derivative of a tangent vector a_α may be written:

$$a_{\alpha,\beta} = \Gamma^\lambda_{\alpha\beta}a_\lambda + b_{\alpha\beta}a_3 \tag{38}$$

Now let Ψ be a transversed vector field:

$$\psi = \psi_\lambda a^\lambda + \psi_3 a_3 = \psi^\lambda a_\lambda + \psi_3 a_3 \tag{39}$$

from the previous formula we can obtain:

$$\frac{\partial\tilde{\psi}}{\partial\xi^\beta} = \left(\psi_{\lambda|\beta} - b_{\lambda\beta}\psi_3\right)a^\lambda + \left(\psi_{3,\beta} + b^\lambda_\beta\psi_\lambda\right)a^3 \tag{40}$$

or

$$\frac{\partial \tilde{\psi}}{\partial \xi^{\beta}} = \left(\psi^{\lambda}_{|\beta} - b^{\lambda}_{\beta} \psi_3 \right) a_{\lambda} + \left(\psi_{3,\beta} + b_{\lambda\beta} \psi^{\lambda} \right) a_3 \tag{41}$$

from which we obtain

$$\frac{\partial \psi}{\partial m} = \psi^{\lambda}_{||\beta} a_{\lambda} \otimes a^{\beta} + \psi^{3}_{||\beta} a_3 \otimes a^{\beta} \tag{42}$$

with

$$\psi^{\lambda}_{||\beta} = \left(\psi^{\lambda}_{|\beta} - b^{\lambda}_{\beta} \psi_3 \right)$$

$$\psi^{3}_{||\beta} = \left(\psi_{3,\beta} + b_{\lambda\beta} \psi^{\lambda} \right)$$

An important operator for surface variation is the *tangential divergence of a vector field:*

$$div_S \psi = a^{\beta} . \frac{\partial \psi}{\partial m} a_{\beta} = \left(\psi^{\beta}_{|\beta} - b^{\beta}_{\beta} \psi^3 \right) = \psi^{\beta}_{||\beta} \tag{43}$$

We recognize that

$$\psi^{\beta}_{|\beta} = div \Pi \, \psi$$

and it is usual to set

$$H = -b^{\beta}_{\beta} \qquad \text{(mean curvature of } S\text{)},$$

so that we can also write:

$$div_S \psi = div \Pi \, \psi + H \psi^3 \tag{44}$$

We note that $div_S a^3 = H$.

6. Surface variations

Now we are to provide some basic formulas for *surface variation.*

The material derivative operator δ is defined in the same way as for domain variation

$$\delta f(m) = \frac{d}{dt} f_{t\psi} o (\Phi + t\tilde{\Psi})(\xi)_{|t=0} = \frac{\partial}{\partial t} \tilde{f}_{t\Psi}(\xi)_{|t=0} \tag{45}$$

We should emphasize some differences: S is a surface; Ψ is a transverse vector field to S;

$$S_{t\psi} = \{ m \mid \forall M \in S \qquad m = M + t\tilde{\psi}(M) \} \tag{46}$$

$f_{t\psi}$ is defined on $S_{t\psi}$.

First-order variation of integrals will be obtained with the following lemma.

LEMMA 6.1 *Let $a = det(a_{\alpha\beta})$ we have*

$$\delta\sqrt{a} = \sqrt{a}\, div_S \psi \tag{47}$$

The proof is left to the reader and its use to prove the following proposition.

PROPOSITION 6.1 *The first order variation of an integral is:*

$$\delta \int_S f_S \, dS = \int_S \delta f \, dS + \int_S f_S \, div_S \psi \, dS \tag{48}$$

Example.

$$\text{area}(S) = \int_S dS \qquad \text{implies}$$

$$\delta \ \text{area}(S) = \int_S div\Pi \, \psi \, dS + \int_s H\psi^3 \, dS$$

now a Green's formula yields

$$\int_S div\Pi \, \psi \, dS = \int_{\delta S} (\Pi\psi).n \, d\sigma$$

n being normal to S in the tangent plane, the interpretation is obvious for a circular arc.

The second term

$$\int_S H\psi^3 \, dS$$

means that for a given surface the first order variation is proportionnal to H; this is obvious for the one-dimensional example of the circle arc; with $\psi^3 = \delta R$;

$$\delta\text{length} = \int_S \frac{1}{R} \, \delta R \, dS = (\delta R)\alpha = (\delta R)\frac{\text{length}}{R}$$

if the arc of a circle converges to a segment of same length ($R \longrightarrow +\infty$) then δlength goes to zero

Now we study the *variation of a derivative. This is more difficult than in the volumic case.* We first state and "prove" a simple but *wrong* result.

$$\delta \frac{\partial u}{\partial m} = \frac{\partial \delta u}{\partial m} - \frac{\partial u}{\partial m} \Pi \frac{\partial \Psi}{\partial m} \tag{49}$$

The natural but *wrong* proof is as follows:

$$\frac{\partial u}{\partial m} = \frac{\partial \tilde{u}}{\partial \xi} \left(\frac{\partial \Phi}{\partial \xi} \right)^{-1} \qquad \text{now if} \qquad \Phi(\xi) = \Phi_0(\xi) + \tilde{\psi}(\xi)$$

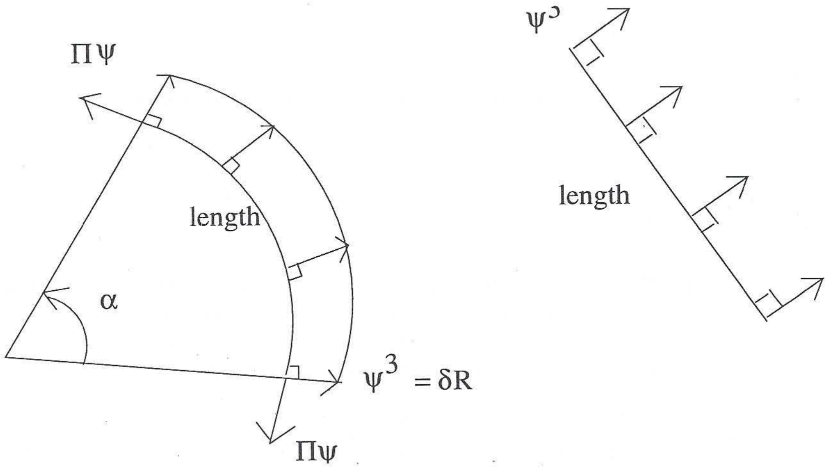

Figure 6.

$$\frac{\partial\Phi}{\partial\xi} = \frac{\partial\Phi_0}{\partial\xi} + \frac{\partial\tilde{\Psi}}{\partial\xi} = \frac{\partial\Phi_0}{\partial\xi}\left(I + \left(\frac{\partial\Phi_0}{\partial\xi}\right)^{-1}\frac{\partial\tilde{\Psi}}{\partial\xi}\right)$$

so that expanding up to first-order

$$\left(\frac{\partial\Phi}{\partial\xi}\right)^{-1} = \left(\frac{\partial\Phi_0}{\partial\xi}\right)^{-1} - \left(\frac{\partial\Phi_0}{\partial\xi}\right)^{-1}\frac{\partial\tilde{\Psi}}{\partial\xi}\left(\frac{\partial\Phi_0}{\partial\xi}\right)^{-1}$$

as in the volumic case; then expanding $u = u_0 + \delta u + \ldots$

$$\frac{\partial\tilde{u}}{\partial\xi}\left(\frac{\partial\Phi_0}{\partial\xi}\right)^{-1} = \frac{\partial u}{\partial m_0} = \frac{\partial u_0}{\partial m_0} + \frac{\partial\delta u}{\partial m_0} + \ldots \qquad \text{and}$$

$$\frac{\partial\tilde{u}}{\partial\xi}\left(\frac{\partial\Phi_0}{\partial\xi}\right)^{-1}\frac{\partial\tilde{\Psi}}{\partial\xi}\left(\frac{\partial\Phi_0}{\partial\xi}\right)^{-1} = \frac{\partial u}{\partial m_0}\Pi\frac{\partial\psi}{\partial m_0} \qquad \text{so that up to first-order}$$

$$\frac{\partial u}{\partial m_0} - \frac{\partial u_0}{\partial m_0} = \frac{\partial\delta u}{\partial m_0} + \ldots \frac{\partial u_0}{\partial m_0}\Pi\frac{\partial\psi}{\partial m_0} + \ldots \qquad \text{which is equivalent to (49)}$$

What is wrong? The crucial point is that

$$\frac{\partial\Phi_0}{\partial\xi}\left(\frac{\partial\Phi_0}{\partial\xi}\right)^{-1} \qquad \text{cannot be the identity!}$$

$\dfrac{\partial\Phi_0}{\partial\xi}$ is not on-to so it cannot have a right inverse (its image is a 2D tangent plane); it has a left inverse $B = e_\alpha \otimes a^\alpha$, the matrix of which is

$$\begin{pmatrix} {}^t a^1 \\ {}^t a^2 \end{pmatrix} \qquad \text{where } a^\alpha \text{ means the components of } a^\alpha \text{ in an orthonormal basis of } E^2.$$

Indeed, we have seen that

$$\frac{\partial \Phi_0}{\partial \xi} B \qquad \text{is the orthogonal projection onto the tangent plane;}$$

that means

$$I_{E^3} = \frac{\partial \Phi_0}{\partial \xi} B + a^3 \otimes a^3$$

Rather than modifying the previous proof, we are going to use more directly the basis vectors, but first of all the *right* proposition is as following.

PROPOSITION 6.2 *The first order variation of a derivative is:*

$$\delta \frac{\partial u}{\partial m} = \frac{\partial \delta u}{\partial m} - \frac{\partial u}{\partial m} \Pi \frac{\partial \Psi}{\partial m} + a^3 \left(a_3 . \frac{\partial \Psi}{\partial m} . \frac{\partial u}{\partial m} \right)$$

or component-wise

$$\delta \frac{\partial u}{\partial m} = (\delta \tilde{u})_{,\alpha} a^\alpha - \tilde{u}_{,\alpha} \left(a^\alpha . \tilde{\psi}_{,\mu} \right) a^\mu + \tilde{u}_{,\alpha} a^{\alpha\mu} \left(a^3 . \tilde{\psi}_{,\mu} \right) a^3$$

The proof rests on the following lemma.

LEMMA 6.2 *First order variation of basis vectors:*

$$(i) \qquad \delta a_\alpha = \frac{\partial \tilde{\psi}}{\partial \xi^\alpha} \qquad or \qquad \delta \frac{\partial \Phi}{\partial \xi} = \frac{\partial \tilde{\psi}}{\partial \xi}$$

$$(ii) \qquad \delta a^3 = -\left(a^3 . \frac{\partial \tilde{\psi}}{\partial \xi^\mu} \right) a^\mu = -a^3 . \frac{\partial \Psi}{\partial m} = -\psi^3_{||\beta} a^\beta$$

$$(iii) \qquad \delta a^\alpha = -\left(a^\alpha . \frac{\partial \tilde{\psi}}{\partial \xi^\mu} \right) a^\mu + a^3 a^{\alpha\mu} \left(a^3 . \frac{\partial \tilde{\psi}}{\partial \xi^\mu} \right)$$

$$or \qquad \delta B = -B \frac{\partial \Psi}{\partial m} \Pi + B \overline{\left(a^3 \frac{\partial \psi}{\partial m} \right)} a^3$$

(overbar means transposition; see Section 4)

Proof: We set $\Phi = \Phi_0 + \Psi$ and we have

$$a_\alpha = \frac{\partial \Phi}{\partial \xi^\alpha}$$

(i) so that

$$a_\alpha = a^0_\alpha + \frac{\partial \tilde{\psi}}{\partial \xi^\alpha} \qquad \text{which gives} \qquad \delta a_\alpha = \frac{\partial \tilde{\psi}}{\partial \xi^\alpha}$$

(ii) We use $a^3.a_\mu = 0$ so that $(\delta a^3).a_\mu = -a^3.\delta a_\mu$, moreover $a^3.a^3 = 1$ gives $(\delta a^3).a^3 = 0$; then as $\delta a^3 = \left(\delta a^3.a_\mu\right) a^\mu = -\left(a^3.\delta a_\mu\right) a^\mu$ we obtain

$$\delta a^3 = -\left(a^3.\frac{\partial \tilde{\psi}}{\partial \xi^\mu}\right) a^\mu$$

Then as

$$\frac{\partial \psi}{\partial m} = \frac{\partial \tilde{\psi}}{\partial \xi^\mu} a^\mu$$

we have obtained the second equality; the third one comes just from the notation (42).

$$\frac{\partial \psi}{\partial m} = \psi^\lambda_{||\beta}\, a_\lambda \otimes a^\beta + \psi^3_{||\beta}\, a_3 \otimes a^\beta$$

(iii) $a^\alpha.a^3 = 0$ implies $(\delta a^\alpha).a^3 = -(a^\alpha.\delta a^3)$ and $a^\alpha.a_\lambda = \delta^\alpha_\lambda$ gives $\delta a^\alpha.a_\lambda = a^\alpha.\delta a_\lambda$, so that

$$\begin{aligned}\delta a^\alpha &= -(a^\alpha.\delta a_\lambda)a^\lambda + (a^\alpha.\delta a^3)a^3 \\ &= -\left(a^\alpha.\frac{\partial \tilde{\psi}}{\partial \xi^\lambda}\right) a^\lambda + a^\alpha.a^\mu\left(a^3.\frac{\partial \tilde{\psi}}{\partial \xi^\mu}\right) a^3\end{aligned}$$

On the other hand $Bh = e_\alpha(a^\alpha.h)$, so that

$$\begin{aligned}\delta Bh &= e_\alpha(\delta a^\alpha.h) \\ &= -e_\alpha\left(a^\alpha.\frac{\partial \tilde{\psi}}{\partial \xi^\lambda}\right)(a^\lambda.h) + e_\alpha\left(a^\alpha.a^\mu\left(a^3.\frac{\partial \tilde{\psi}}{\partial \xi^\mu}\right)\right)(a^3.h)\end{aligned}$$

Proof of the Proposition 6.2.

$$\frac{\partial u}{\partial m} = \tilde{u}_{,\alpha}a^\alpha$$

so that

$$\delta\frac{\partial u}{\partial m} = (\delta\tilde{u})_{,\alpha}a^\alpha + \tilde{u}_{,\alpha}\delta a^\alpha$$

we note that $\tilde{u}$ is computed at a fixed point so that δ and $\dfrac{\partial}{\partial \xi^\alpha}$ commute; secondly we use (iii) of the previous Lemma:

$$\delta\frac{\partial u}{\partial m} = (\delta\tilde{u})_{,\alpha}a^\alpha + \tilde{u}_{,\alpha}\left(a^\alpha.\frac{\partial \tilde{\psi}}{\partial \xi^\lambda}\right) a^\lambda + \tilde{u}_{,\alpha}a^{\alpha\mu}\left(a^3.\frac{\partial \tilde{\psi}}{\partial \xi^\mu}\right) a^3$$

this is the component-wise formula of the proposition; the intrinsic formula stems from

$$\frac{\partial u}{\partial m} = \tilde{u}_{,\alpha}a^\alpha \qquad \text{and} \qquad \frac{\partial \psi}{\partial m} = \tilde{\psi}_{,\lambda}a^\lambda.$$

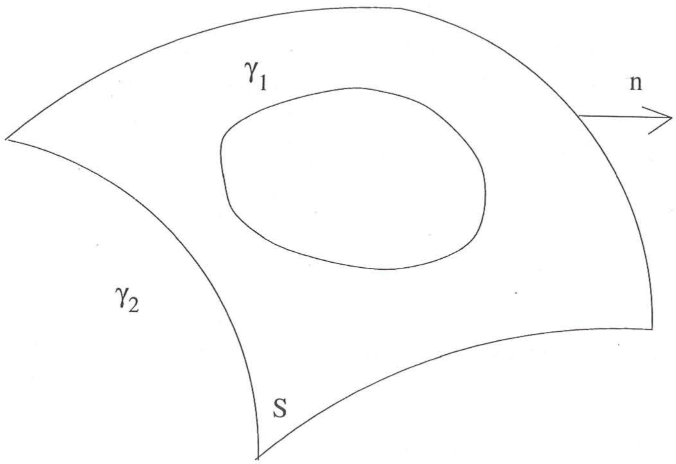

Figure 7.

7. Sensitivity analysis for a surface heat equation

We still consider a simple surface system; i.e. a stationary surface heat conduction equation; we set:

f surface density of heat source,
g line density of heat source,
q heat flux vector,
u deviation of temperature from the natural state.

We assume Fourier law for an isotropic homogeneous medium:

$$q = -c\frac{\tilde{\partial} u}{\partial m}$$

the conservation of heat gives: $div q = f$.
We assume prescribed zero deviation of the temperature on γ_1; $u = 0$; prescibed heat flux on γ_2; $q.n = -g$; note that the minus sign is a convention, q the pointing toward the cold subset, g is positive when heat is received and n is outward normal to the boundary and lies in the tangent plane to S.

Finally we have

$$\left\{\begin{array}{ll} div\, q = f & \text{in } S \\ u = 0 & \text{on } \gamma_1 \\ q.n = \overline{-g} & \text{on } \gamma_2 \\ q = -c\dfrac{\partial u}{\partial m} & \end{array}\right. \tag{50}$$

$$\text{or componentwise} \qquad \left\{ \begin{array}{ll} q^{\alpha}_{|\alpha} = f & \text{in } S \\ u^{\alpha} = 0 & \text{on } \gamma_1 \\ q^{\alpha}.n_{\alpha} = -g & \\ q^{\alpha} = -c\, a^{\alpha\beta} u_{,\beta} & \end{array} \right. \tag{51}$$

In a standard way we consider the variational formulation:

$$\forall v \in V \qquad a(u,v) = l(v) \tag{52}$$

where

$$V = \left\{ v \in H^1(S) \;\mid\; v_{|\gamma_1} = 0 \right\} \tag{53}$$

$$a(u,v) = \int_S c \frac{\partial u}{\partial m} . \overline{\frac{\partial v}{\partial m}}\, dS \tag{54}$$

$$l(v) = \int_S f v \, dS + + \int_{\gamma_2} g v \, d\sigma \tag{55}$$

As in the volumic case δu is the solution of an equation with the same bilinear form a.

PROPOSITION 7.1 *Let u be the solution of (50) or (52), then its variation δu satisfies*

$$\forall v \in V \qquad a(du, v) = -(\delta a)(u,v) + (\delta l)(v)$$

where δa and δl are the variations of a and l for fixed u and v :

$$\begin{aligned} (\delta a)(u,v) \;\; &= \;\; -\int_S c \left(\frac{\partial u}{\partial m} \Pi \frac{\partial \psi}{\partial m} . \overline{\frac{\partial v}{\partial m}} + \frac{\partial v}{\partial m} \Pi \frac{\partial \psi}{\partial m} . \overline{\frac{\partial u}{\partial m}} \right) dS \\ &\quad + \int_S c \frac{\partial u}{\partial m} . \overline{\frac{\partial v}{\partial m}} div_S \psi \, dS \\ (\delta l)(v) \;\; &= \;\; \int_S v\, \delta f \, dS + \int_S f\, v\, div_S \psi \, dS + \int_{\gamma_2} v\, \delta g \, d\sigma \\ &\quad + \int_{\gamma_2} v\, g\, div_{\gamma_2} \psi \, d\sigma \end{aligned}$$

As in the volumic case, the *proof* is simple if one uses the previous results: Propositions 6.1 and 6.2 . As a touch of "humour" we note that the "wrong" Proposition 6.2 would give here the same Proposition 7.1 . This is because the term

$$\left(a_3 . \frac{\partial \Psi}{\partial m} . \frac{\partial u}{\partial m} \right) a_3$$

has a zero scalar product with $\dfrac{\partial v}{\partial m}$ which is a tangential vector.

Surface sensitivity of a functional

The simplest case is

$$J(u) = \int_S \alpha(u)\, dS$$

With proposition 6.1 we obtain

$$\delta J = \int_S \alpha'(u)\, \delta u\, dS + \int_S \alpha(u)\, div_S \psi\, dS$$

To make this expression explicit with respect to Ψ we use the same Proposition 6.1 to obtain $\delta J = (\delta L)(u,p)$ where $L = J + a(u,p) - l(p)$ and δL is computed at fixed u and p:

$$\delta J = \int_S \alpha(u)\, div_S \psi\, dS + \delta a(u,p) \; - \; \delta l(p)$$

where δa and δl are given in Proposition 7.1 and p is solution of an adjoint state.

8. Boundary expression of shape sensitivity

We turn here to the volumic case of section 4. It is possible to obtain a different expression of the shape sensitivity of a functional: formula (23) may be transformed to a formula which involves boundary integrals. We need some auxiliary lemmas.

LEMMA 8.1 *The solution u of (14) satisfies*

$$\forall w \in \omega \qquad a(u,w) = l(w) + l_{\gamma_1}(w) \tag{56}$$

where W is the space of virtual displacements which do not necessarily satisfy $w = 0$ on γ_1 and

$$l_{\gamma_1}(w) = \int_{\gamma_1} T w \frac{\partial u}{\partial n}\, d\sigma \tag{57}$$

The proof just uses the Stockes formula:

$$\int_\omega -T\, \Delta u\, w\, dx = \int_\omega T \frac{\partial u}{\partial x}\frac{\partial \overline{w}}{\partial x} dx \; - \; \int_{\partial\omega} T w \frac{\partial u}{\partial n}\, d\sigma$$

which gives Lemma 8.1 as $T\dfrac{\partial u}{\partial n} = 0$ on γ_2

LEMMA 8.2 *The following identities hold*

$$(i) \qquad \frac{\partial u}{\partial x}\frac{\partial \psi}{\partial x}\frac{\partial \overline{p}}{\partial x} = \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\psi\right)\frac{\partial \overline{p}}{\partial x} \; - \; \overline{\psi}\frac{\partial^2 u}{\partial x^2}\frac{\partial \overline{p}}{\partial x}$$

$$(ii) \qquad \frac{\partial p}{\partial x}\frac{\partial \psi}{\partial x}\frac{\partial \overline{u}}{\partial x} = \frac{\partial}{\partial x}\left(\frac{\partial p}{\partial x}\psi\right)\frac{\partial \overline{u}}{\partial x} - \overline{\psi}\frac{\partial^2 p}{\partial x^2}\frac{\partial \overline{u}}{\partial x}$$

$$(iii) \qquad \frac{\partial u}{\partial x}\frac{\partial \psi}{\partial x}\frac{\partial \overline{p}}{\partial x} + \frac{\partial p}{\partial x}\frac{\partial \psi}{\partial x}\frac{\partial \overline{u}}{\partial x} =$$

$$\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\psi\right)\frac{\partial \overline{p}}{\partial x} + \frac{\partial}{\partial x}\left(\frac{\partial p}{\partial x}\psi\right)\frac{\partial \overline{u}}{\partial x} - \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\frac{\partial \overline{p}}{\partial x}\right)\psi$$

$$(iv) \qquad \frac{\partial u}{\partial x}\frac{\partial \overline{p}}{\partial x} div\psi = div\left(\left(\frac{\partial u}{\partial x}\frac{\partial \overline{p}}{\partial x}\right)\psi\right) - \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\frac{\partial \overline{p}}{\partial x}\right)\psi$$

$$(v) \qquad -\frac{\partial u}{\partial x}\frac{\partial \psi}{\partial x}\frac{\partial \overline{p}}{\partial x} - \frac{\partial p}{\partial x}\frac{\partial \psi}{\partial x}\frac{\partial \overline{u}}{\partial x} + \frac{\partial u}{\partial x}\frac{\partial \overline{p}}{\partial x} div\psi =$$

$$-\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\psi\right)\frac{\partial \overline{p}}{\partial x} - \frac{\partial}{\partial x}\left(\frac{\partial p}{\partial x}\psi\right)\frac{\partial \overline{u}}{\partial x} + div\left(\left(\frac{\partial u}{\partial x}\frac{\partial \overline{p}}{\partial x}\right)\psi\right)$$

$$(vi) \qquad p\,\delta f + pf\, div\Psi = div(pf\psi) - f\frac{\partial p}{\partial x}\psi + p\left(\delta f - \frac{\partial f}{\partial x}\psi\right)$$

and if f does not depend explicitly on ω:

$$p\,\delta f + pf\, div\Psi = div(pf\psi) - f\frac{\partial p}{\partial x}\psi$$

The *proof* uses the definitions and is left to the reader.

PROPOSITION 8.1 *Let u be the solution of the model system (14) and $J_\omega(u)$ be the functional (20), then its variation given by (23) may be also expressed as*

$$\begin{aligned}\delta J &= -T\int_{\gamma_1}\frac{\partial u}{\partial n}\frac{\partial p}{\partial n}(\psi.n)\,d\sigma \\ &\quad + \int_{\gamma_2}\alpha(u)(\psi.n)\,d\sigma + \int_{\gamma_2}\left(T\frac{\partial u}{\partial\sigma}\frac{\partial \overline{p}}{\partial\sigma} - pf\right)(\psi.n)\,d\sigma\end{aligned} \qquad (58)$$

Proof. Lemma 8.2 (v) enables us to derive from (18):

$$\begin{aligned}(\delta a)(u,p) &= -T\int_\omega\left(\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\psi\right)\frac{\partial \overline{p}}{\partial x} + \frac{\partial}{\partial x}\left(\frac{\partial p}{\partial x}\psi\right)\frac{\partial \overline{u}}{\partial x}\right)dx \\ &\quad + T\int_\omega div\left(\left(\frac{\partial u}{\partial x}\frac{\partial \overline{p}}{\partial x}\right)\psi\right)dx\end{aligned} \qquad (59)$$

Next we use Lemma 8.2 (vi) with (19) and assume for simplicity that f does not depend explicitly on ω:

$$\delta f = \frac{\partial f}{\partial x}.\psi$$

$$(\delta l)(f) = \int_\omega div(pf\psi)\, dx \; - \; \int_\omega f\frac{\partial p}{\partial x}\psi\, dx \tag{60}$$

Then we note that Lemma 8.1 for the adjoint state (22) gives

$$\forall w \in W \qquad a(p,w) = - < \frac{\partial J}{\partial w}, w > + \int_{\gamma_1} Tw\frac{\partial p}{\partial n}\, d\sigma$$

so that:

$$\begin{aligned} -T\int_\omega \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\psi\right)\frac{\partial \overline{p}}{\partial x} = \\ < \frac{\partial J}{\partial u}, \frac{\partial u}{\partial x}w > \; - \; \int_{\gamma_1} T\left(\frac{\partial u}{\partial x}\psi\right)\frac{\partial p}{\partial n}\, d\sigma \end{aligned} \tag{61}$$

Similarly as the state u of the system satisfies:

$$\forall w \in W \qquad a(u,w) = \int_\omega fw\, dx + \int_{\gamma_1} Tw\frac{\partial u}{\partial n}\, d\sigma$$

we have

$$\begin{aligned} -\,T\int_\omega \frac{\partial}{\partial x}\left(\frac{\partial p}{\partial x}\psi\right)\frac{\partial \overline{u}}{\partial x} = \\ -\int_\omega f\frac{\partial p}{\partial x}\psi\, dx \; - \; \int_{\gamma_1} T\left(\frac{\partial p}{\partial x}\psi\right)\frac{\partial u}{\partial n}\, d\sigma \end{aligned} \tag{62}$$

Finally we recall from Proposition 4.3 that if

$$J_\omega(u) = \int_\omega \alpha(u)\, dx \tag{63}$$

$$\delta J = \int_\omega \alpha(u)\, div(\psi)\, dx + \delta a(u,p) \; - \; \delta l(p)$$

so that (59), (60), (61), (62) provide

$$\begin{aligned} \delta J \;\; = \;\; & \int_\omega \alpha(u)\, div(\psi)\, dx + < \frac{\partial J}{\partial u}, \frac{\partial u}{\partial x}w > \\ & - \int_{\gamma_1} T\left(\frac{\partial u}{\partial x}\psi\right)\frac{\partial p}{\partial n}\, d\sigma \; - \; \int_{\gamma_1} T\left(\frac{\partial p}{\partial x}\psi\right)\frac{\partial u}{\partial n}\, d\sigma \\ & + T\int_\omega div\left(\left(\frac{\partial u}{\partial x}\frac{\partial \overline{p}}{\partial x}\right)\psi\right)\, dx \; - \; \int_\omega div(pf\psi)\, dx \end{aligned} \tag{64}$$

Then we note that for our functional (63)

$$< \frac{\partial J}{\partial u}, \frac{\partial u}{\partial x}\psi > = \int_\omega \alpha'(u)\frac{\partial u}{\partial x}.\psi\, dx$$

so that the first two terms of (64) provide:

$$\int_\omega \alpha(u)\, div(\psi)\, dx + \int_\omega \alpha'(u)\frac{\partial u}{\partial x}.\psi\, dx =$$

$$\int_\omega div(\alpha(u)\psi)\, dx = \int_{\gamma_2} \alpha(u)\psi.n\, d\sigma \tag{65}$$

Using Green's formula in (64) we obtain:

$$\begin{aligned}\delta J &= \int_{\gamma_2} \alpha(u)\psi.n\, d\sigma - \int_{\gamma_1} T\left(\frac{\partial u}{\partial x}\psi\right)\frac{\partial p}{\partial n}\, d\sigma \\ &\quad - \int_{\gamma_1} T\left(\frac{\partial p}{\partial x}\psi\right)\frac{\partial u}{\partial n}\, d\sigma + \int_{\partial\omega} T\left(\frac{\partial u}{\partial x}\frac{\partial \overline{p}}{\partial x}\right)(\psi.n)\, d\sigma \\ &\quad - \int_{\partial\omega} (pf\psi.n)\, d\sigma \end{aligned}\tag{66}$$

Then we note that on γ_1 $u = 0$ and $p = 0$ so that $\frac{\partial u}{\partial x} = \frac{\partial u}{\partial n}n$ and $\frac{\partial p}{\partial x} = \frac{\partial p}{\partial n}n$ and on γ_2 where $\frac{\partial u}{\partial n} = 0$ we have $\frac{\partial u}{\partial x} = \frac{\partial u}{\partial \sigma^\alpha}a^\alpha$ so that

$$\begin{aligned}\delta J &= -\int_{\gamma_1} T\left(\frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\right)(\psi.n)\, d\sigma + \int_{\gamma_2} \alpha(u)\psi.n\, d\sigma \\ &\quad + \int_{ga_2}\left(T\frac{\partial u}{\partial \sigma}\frac{\partial p}{\partial \sigma} - pf\right)(\psi.n)\, d\sigma\end{aligned}$$

Remark. When one uses finite elements to solve (14), it has been observed that the boundary expression (58) is not very accurate; theoretical support of this fact will be given in Section 9.

9. Use of finite elements and boundary integrals

We consider the model system of section 4 and to make things simpler we assume $u = 0$ is the *only boundary condition.* We shall give error estimates of δJ when we replace u and p by finite elements approximations; many results of this type may be found in Masmoudi (1987).

First we consider the boundary expression (58) which in the case of $u = 0$ on $\partial\omega$ is

$$\delta J^B = -T\int_{\partial\omega} \frac{\partial u}{\partial n}\frac{\partial p}{\partial n}(\psi.n)\, d\sigma \tag{67}$$

We denote u_h and p_h finite elements approximations of u and p; h denotes the mesh size. We set

$$\delta J_h^B = -T\int_{\partial\omega} \frac{\partial u_h}{\partial n}\frac{\partial p_h}{\partial n}(\psi.n)\, d\sigma \tag{68}$$

For simplification we assume that there is no error in the approximation of the geometry; we need an error estimate of the normal derivative of u and p on $\partial\omega$; an accurate estimation may be based on Rannacher and Scott (1982):

$$\| u - u_h \|_{1,\infty;\Omega} \leq c h^k \| u \|_{k+1,\infty;\Omega} \tag{69}$$

where

$$\| u \|_{k,\infty;\Omega} = \| u \|_{L^\infty(\Omega)} + \sum_{l=0}^{l=k} \left\| \frac{\partial^l u}{\partial x^l} \right\|_{L^\infty(\Omega)}$$

and k is the degree of polynomials used in the finite element approximation. We note that for $k = 1$, the second derivatives of the solution u should be essentially bounded

$$\left(\frac{\partial^2 u}{\partial x^2} \in L^\infty(\Omega) \right) ;$$

this is an assumption which, for example, excludes reintrant corners in $\partial\Omega$ (Grisvard, 1985).

PROPOSITION 9.1 *If data are smooth enough such that (69) holds then*

$$| \delta J^B - \delta J_h^B | \leq c h^k \| u \|_{k+1,\infty;\Omega} \| p \|_{k+1,\infty;\Omega} \| \psi.n \|_{0,\infty;\Gamma}$$

Proof.

$$\begin{aligned} | \delta J^B - \delta J_h^B | \leq\ & T \int_{\partial\omega} \left| \frac{\partial u}{\partial n} - \frac{\partial u_h}{\partial n} \right| \left| \frac{\partial p}{\partial n} \right| | \psi.n | \, d\sigma \\ & + T \int_{\partial\omega} \left| \frac{\partial u}{\partial n} - \frac{\partial u_h}{\partial n} \right| \left| \frac{\partial p}{\partial n} - \frac{\partial p_h}{\partial n} \right| | \psi.n | \, d\sigma \\ & + T \int_{\partial\omega} \left| \frac{\partial u}{\partial n} \right| \left| \frac{\partial p}{\partial n} - \frac{\partial p_h}{\partial n} \right| | \psi.n | \, d\sigma \end{aligned}$$

from which we obtain:

$$\begin{aligned} | \delta J^B - \delta J_h^B | \leq\ & T \left(\left\| \frac{\partial u}{\partial n} - \frac{\partial u_h}{\partial n} \right\|_{0,\infty;\gamma} \left\| \frac{\partial p}{\partial n} \right\|_{0,\infty;\gamma} \right. \\ & + \left\| \frac{\partial u}{\partial n} - \frac{\partial u_h}{\partial n} \right\|_{0,\infty;\gamma} \left\| \frac{\partial p}{\partial n} - \frac{\partial p_h}{\partial n} \right\|_{0,\infty;\gamma} \\ & \left. + \left\| \frac{\partial u}{\partial n} \right\|_{0,\infty;\gamma} \left\| \frac{\partial p}{\partial n} - \frac{\partial p_h}{\partial n} \right\|_{0,\infty;\gamma} \right) \| \psi.n \|_{0,\infty;\gamma} \end{aligned}$$

We note that (69) implies:

$$\left\| \frac{\partial u}{\partial n} - \frac{\partial u_h}{\partial n} \right\|_{0,\infty;\gamma} \leq c h^k \| u \|_{k+1,\infty;\omega}$$

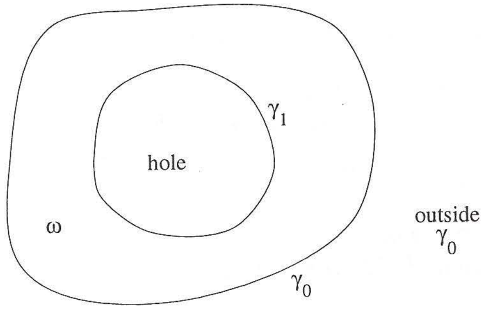

Figure 8.

and equivalently for p from which we obtain the proposition.

Second we consider the domain expression. We only state the result; we set δJ^D the expression given by (23); δJ_h^D means that u and p are replaced by a finite element approximation u_h and p_h; k stands for the degree of polynomial approximation and k' the order of derivatives of ψ which are essentially bounded.

PROPOSITION 9.2 *If the data are smooth enough then*

$$| \, \delta J^D - \delta J_h^D \, | \leq c(u) \, h^{k+k'} \, (||p||_{k+1;\Omega} + 1) \, ||\psi||_{k'+1,\infty;\Omega}$$

The *proof* is technical but the result may be understood directly. It means that if the vector field ψ has essentially bounded second derivatives, the error estimate is in h^{k+1} and, moreover, if the second derivatives are small, it will be multiplied by a small constant; this error estimate is to be compared with h^k of Proposition 9.1 ; numerical evidence of this result may be found in Rochette (1990).

Third, we consider the use of boundary integrals to solve the state equation. For simplicity, we consider a membrane with no density of force and prescribed *constant displacement* on two pieces of the boundary.

$$\left.\begin{array}{rl} -T\,\Delta u = 0 & \text{in } \omega \\ u = b & \text{on } \gamma_1 \\ u = 0 & \text{on } \gamma_0 \end{array}\right\} \qquad (70)$$

The *transformation* of this boundary value problem into a boundary integral equation is performed by introducing the classical *elementary solution* of the Laplacian Δ:

$$E(x,z) = -\frac{1}{2\pi} \log |x - z| \qquad \text{(in two dimensions);} \qquad (71)$$

classically $\Delta_z E(x,y) = \delta(x-z)$ holds; and if we consider

$$v(x) = \int_\gamma E(x,y) q(y) \, d\sigma_y \qquad (72)$$

where γ is the boundary of Ω, this function satisfies

$$\left.\begin{array}{ll} \Delta v = 0 & \text{outside } \gamma \\ v & \text{is continuous in } \mathbb{R}^2 \\ \dfrac{\partial v^i}{\partial n} - \dfrac{\partial v^e}{\partial n} = q & \text{on } \gamma \end{array}\right\} \tag{73}$$

where $v^i = v_{|\omega}$ $v^e = v_{R^2-\omega}$

So, the solution of (70) is given by

$$\forall x \in \omega \qquad u(x) = T \int_\gamma E(x,y)q(y)\, d\sigma_y \tag{74}$$

where q is solution of

$$\left.\begin{array}{ll} T \displaystyle\int_\gamma E(x,y)q(y)\, d\sigma_y = b(x) & \forall x \in \gamma_1 \\ T \displaystyle\int_\gamma E(x,y)q(y)\, d\sigma_y = 0 & \forall x \in \gamma_0 \end{array}\right\} \tag{75}$$

Now, we note $u = 0$ outside of γ_0 and $u = b$ in the hole surrounded by γ_1 are the solution of (70) with the right boundary conditions, so that using (73) we obtain

$$\frac{\partial u}{\partial n} = q \qquad \text{on } \gamma \tag{76}$$

If we consider now the simple functional

$$J_\omega = \int_\omega \left|\frac{\partial u}{\partial x}\right|^2 dx$$

we note that

$$\frac{\partial J}{\partial u}.w = \int_\omega \frac{\partial u}{\partial x}\frac{\partial w}{\partial x}\, dx$$

so that the adjoint state is $p = -u$ and

$$\delta J^B = T \int_\gamma \left|\frac{\partial u}{\partial n}\right|^2 (\psi.n)\, d\sigma = T \int_\omega q^2(\psi.n)\, d\sigma.$$

Moreover, it is easy to obtain with Green's formula the following expression of J_ω: we note that the expressions of J_ω and δJ^B may be easily computed with the solution of (75). Remark that in this case we do not need to use (74).

$$J_\omega = \int_{\gamma_1} T\, b\, q\, d\sigma$$

The case of an equation with a non zero right-hand side may also be computed with integral equations but we need to use the second Green's formula;

we skip the details and refer to Masmoudi (1987). *Before stating the error estimate of δJ,* we should recall that many error estimates for the solution of boundary integral equations have been obtained by Nedelec (1976,1977); of the next proposition the *proof* is still in Masmoudi (1987).

PROPOSITION 9.3 *For smooth enough data*

$$| \, \delta J^I \; - \; \delta J_h^I \, | \leq \; c(u) \; h^{min(2k+1,l+1)} \; ||q||_{k+1;\gamma} \; ||\Pi||_{k+1,\gamma} \; ||\Psi.n||$$

where:

- *l means the degree of polynomials used to approximate the boundary;*
- *k the degree of finite elements approximation;*
- *q is the solution of an equation of the type of (75) set on γ;*
- *Π is the solution of a similar equation for the adjoint state.*

Remark. We note that for $k = 2$ we should use $l = 4$ so that the error estimate is in h^5; finally we should note that with a smooth approximation of the boundary the error estimate of δJ is quite good; this is in contrast with what we obtained with finite elements.

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