Second order derivatives, Newton method,application to shape optimization

Arian Novruzi, Jean R. Roche

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Second order derivatives, Newton method, application to shape optimization.

Arian Novruzi and Jean R. Roche

N° 2555

Mai 1995

PROGRAMME 6

Rapport de recherche

ISSN 0249-6399

Second order derivatives, Newton method, application to shape optimization.

Arian Novruzi and Jean R. Roche*

Programme 6 — Calcul scientifique, modélisation et logiciel numérique
Projet NUMATH

Rapport de recherche n2555 — Mai 1995 — 25 pages

Abstract: We describe a Newton method applied to the evaluation of a critical point of a total energy associated to a shape optimization problem. The key point of this methods is the Hessian of the shape functional. We give an expression of the Hessian as well as the relation with the second-order Eulerian semi-derivative. An application to the electromagnetic shaping of liquid metals process is studied. The unknown surface i represented by piecewise linear closed Jordan curves. Each step of the algorithm requires solving two exterior elliptic boundary values problems. This is done by using an integral repreentation of solutions on this surfaces. A comparison with a Quasi-Newton algorithm is worked out.

Key-words: free boundary, electromagnetic shaping, optimization, Newton, computational methods.

(Résumé : tsvp)

*roche@iecn.u-nancy.fr

Dérivée de second ordre, méthode de Newton, application à l'optimisation de formes.

Résumé : On décrit une méthode de Newton appliquée à l'évaluation d'un point critique d'une énergie associée à un problème d'optimisation des formes. On donne une expression de l'Hessien ainsi qu'une relation avec les semi-dérivées euleriene de deuxième ordre. On développe une application au formage électromagnétique des métaux liquides. La surface inconnue est représentée par une courbe linéaire par morceaux. A chaque itération on résoud deux problèmes extérieurs de type elliptique. Ceci est fait en utilisant une représentation intégrale de la solution sur la frontière. Des résultats des calculs et de la comparaison avec une méthode de Quasi-Newton est présentée.

Mots-clé : frontière libre, formage électromagnétique, optimisation des formes, Newton

Unité de recherche INRIA Lorraine, Technopôle de Nancy-Brabois, Campus scientifique,
615 rue du Jardin Botanique, BP 101, 54600 VILLERS LÈS NANCY
Unité de recherche INRIA Rennes, Irisa, Campus universitaire de Beaulieu, 35042 RENNES Cedex
Unité de recherche INRIA Rhône-Alpes, 46 avenue Félix Viallet, 38031 GRENOBLE Cedex 1
Unité de recherche INRIA Rocquencourt, Domaine de Voluceau, Rocquencourt, BP 105, 78153 LE CHESNAY Cedex
Unité de recherche INRIA Sophia-Antipolis, 2004 route des Lucioles, BP 93, 06902 SOPHIA-ANTIPOLIS Cedex

Éditeur
INRIA, Domaine de Voluceau, Rocquencourt, BP 105, 78153 LE CHESNAY Cedex (France)
ISSN 0249-6399

0. Introduction.

Our purpose is to analyze in detail the realisation of a Newton method in shape optimization problems and to apply it to a particular problem. We compare cost and efficiency of Newton methods with Quasi-Newton methods applied to the same problem. This problem concerns electromagnetic shaping and levitation of molten metals.

A lot of litterature about models of this phenomenon appeared in the last years; we refer for example, to [Shercliff 1981], [Mestel 1982], [Brancher & Sero Guillaume, 1983], [Besson, Bourgeois, Chevallier, Rappaz & Touzani, 1991], [Henrot & Pierre, 1989].

Under suitable assumptions, the equilibrium liquid metal configurations are described by a set of equations containing an equilibrium relation at the boundary between electromagnetic and superficial tension forces (and gravity in three dimensional models). It involves the curvature of the boundary and an elliptic exterior boundary value problem. This equilibrium shape is shown to be the stationary state of the total energy under the constraint that the surface (the volume in 3-d) is prescribed.

Optimization techniques to compute a critical point of the energy need evaluation of the first shape derivative, in the case of the Quasi-Newton method, and of the second order shape derivative in the Newton method case. Section 1 is devoted to the study of different approaches of shape derivatives, see [Murat&Simon,1976], [Murat,1988], [Zolesio,1986], [Zolesio & Delfour,1991], [Sokolowski & Zolesio,1992] and [Goto & Fujii, 1990]. We give a precise description of the second shape derivative used in our Newton method, in particular we relate them to the second order Eulerian shape semi-derivatives as described in [Zolesio & Delfour,1991].

Using our approach we compute the first and second order derivatives of the total energy of the electromagnetic shaping problem mentioned above (we remark that the second order derivative is a bilinear and symmetric integral operator on the boundary of the domain).

To carry out Newton and Quasi-Newton methods we consider domains ω with a piecewise boundary $\partial\omega$ as in [Pierre & Roche,91,93]. As a consequence we compute at each iteration a discrete approximation of the continuous derivative. Therefore, we do not have a genuine Newton or Quasi-Newton method and we lose in particular the quadratic rate of convergence of the continuos algorithm. However we obtain a superlinear rate of convergence without too much increasing the cost of each iteration. Indeed, in the Newton method case we have to solve n extra exterior elliptic problems to compute the Hessian. But since these problems have the same matrix of discretization as the initial state problem we need only one LDL^t decomposition at each iteration. Then each iteration of the Newton method has a computational cost between 1.2 and 3 times more expensive than a Quasi-Newton method.

1- Shape derivatives.

1.1- Shape derivatives of a cost function.

Here we want to make precise the notion of second derivative with respect to shape, having in mind to apply it to a Newton algorithm. For this we compare below two classical points of vue.

Assume E is a real valued function defined on the set:

$$\mathcal{O} = \{\omega \subset \mathbb{R}^N; \omega \text{ a bounded and open subset of class } \mathcal{C}^2\} \tag{1.1}$$

and let Ω denote the exterior of ω. Following [Delfour & Zolesio, 1991], let $V : [0,\tau] \times \mathbb{R}^N \to \mathbb{R}^N$ be a given velocity field for some fixed $\tau > 0$.

Assume that:

$$(1.2)\qquad \begin{cases} \forall x \in \mathbb{R}^N; V(\cdot,x) \in C^0\big([0,\tau];\mathbb{R}^N\big), \\ \exists c > 0, \forall x,y \in \mathbb{R}^N; ||V(\cdot,y) - V(\cdot,x)||_{C^0([0,\tau];\mathbb{R}^N)} \leq c|y-x| \end{cases}$$

where $V(\cdot,x)$ denotes the function $t \to V(t,x)$. Associate to (1.2) the solution $x(t;X)$ of the ordinary differential equation

$$(1.3)\qquad \frac{dx}{dt}(t) = V(t,x(t))\,;\ t \in [0,\tau]\,;\ x(0) = X \in \mathbb{R}^N$$

and introduce the family of homeomorphisms

$$(1.4)\qquad X \to T_t^V(X) := x(t,X) : \mathbb{R}^N \to \mathbb{R}^N.$$

Definition 1.1. [Delfour & Zolesio, 1991] *Let V satisfying the property (1.2). If the following limit exists :*

$$(1.5)\qquad \lim_{t \searrow 0} \frac{E(T_t^V(\omega)) - E(\omega)}{t}$$

we say that E has an Eulerian semiderivative and we denote it by $\mathrm{d}E(\omega;V)$.

The shape functional E is said to be shape differentiable at ω if the Eulerian semiderivative exists for all V and the map: $V \to \mathrm{d}E(\omega;V)$ is linear and continuous in $\overline{\mathcal{V}}^{m,k}$, see [Delfour & Zolesio, 1991].

Definition 1.2. [Delfour & Zolesio, 1991] *Let V,W satisfy the property (1.2). Assume that for all $t \in [0,\tau]$, $dE(T_t^W(\omega),V(t))$ exists. The functional E is said to have a second-order Eulerian semiderivative at ω in the directions (V,W) if the following limit exists :*

$$(1.6)\qquad \lim_{t \searrow 0} \frac{dE(T_t^W(\omega),V(t)) - dE(\omega,V(0))}{t}$$

Whenever it exists, it is denoted by $d^2E(\omega;V,W)$.

Now we present another point of view; let $\overline{C}^2 = \{\theta : \mathbb{R}^N \to \mathbb{R}^N\ ;\ \theta$ is a diffeomorphism of class $C^2\}$. Then we can define:

$$(1.7)\qquad \begin{cases} \omega : \overline{C}^2 \to \mathcal{P}(\mathbb{R}^N) \\ \omega : \theta \to \omega(\theta) = \{\theta(x) : x \in \omega_0\} \in \mathcal{O} \end{cases}$$

where $\mathcal{P}(\mathbb{R}^N)$ is the set of all subsets of $\mathbb{R}^N$ and $\omega_0 \in \mathcal{O}$ is fixed. Now instead of the functional E we consider the cost function G defined in the following way :

$$(1.8)\qquad \begin{cases} G : \overline{C}^2 \to \mathbb{R} \\ G(\theta) = E\big(\omega(\theta)\big) \end{cases}$$

We remark that finding the critical points of E is essentially equivalent to finding the critical points of G.

Now we are going to consider the Frechet derivatives G' and G'' and relate them to the classical shape derivatives, (see [Murat & Simon,1976], [Simon,1988]).

If for all ξ in $\overline{C}^2$ the following limit exists:

$$\lim_{t \searrow 0} \frac{G(\theta + t\xi) - G(\theta)}{t} \tag{1.9}$$

we denote it by $G'(\theta)(\xi)$. We assume that it defines an operator $G' : \overline{C}^2 \to \mathcal{L}(\overline{C}^2, \mathbb{R})$ linear and continuous.

In the same way we define G'' the Frechet derivative of G' and then the value of $G''(\theta)$ in (ξ, η) is given by:

$$G''(\theta)(\xi, \eta) = \lim_{t \searrow 0} \frac{G'(\theta + t\,\eta)(\xi) - G'(\theta)(\xi)}{t}. \tag{1.10}$$

First we are going to give an expression of $G'(\theta)(\xi)$ and $G''(\theta)(\xi, \eta)$ in terms of $\mathrm{d}E(\omega(\theta), V)$ and $\mathrm{d}^2 E(\omega(\theta); V, W)$ where V and W are velocities corresponding to some perturbations of the identity, given by :

$$V(t, x) = \xi \circ \theta^{-1}\big((T_t^V)^{-1}(x)\big) \text{ where } T_t^V(x) = (I + t\,\xi \circ \theta^{-1})(x) \tag{1.11}$$

and

$$W(t, x) = \eta \circ \theta^{-1}\big((T_t^W)^{-1}(x)\big) \text{ where } T_t^W(x) = (I + t\,\eta \circ \theta^{-1})(x) \tag{1.12}$$

where I denotes the identity transformation and $\circ$ the composition operation.

We remark that:

$$\frac{dT_t^V(x)}{dt}(t) = V(t, T_t^V(x)). \tag{1.13}$$

Clearly, the velocity W satisfies a similar equation.

Lemma 1.1. *If $G'(\theta)(\xi)$ exists and V is given by (1.11) then*

$$G'(\theta)(\xi) = \mathrm{d}E\big(\omega(\theta); V\big). \tag{1.14}$$

Proof.

$$\begin{aligned} G'(\theta)(\xi) &= \lim_{t \searrow 0} \frac{1}{t}\big(G(\theta + t\,\xi) - G(\theta)\big) \\ &= \lim_{t \searrow 0} \frac{1}{t}\big(E(\omega(\theta + t\,\xi)) - E(\omega(\theta))\big) \\ &= \lim_{t \searrow 0} \frac{1}{t}\Big(E(T_t^V(\omega(\theta))) - E\big(\omega(\theta)\big)\Big) \\ &= \mathrm{d}E\big(\omega(\theta); V\big). \end{aligned}$$

Remark 1. By the Theorem 2.3 from [Delfour & Zolesio, 1991] under the assumption that $\mathrm{d}E\big(\omega(\theta); V\big)$ exists and is continuous in V for all $V \in \overline{\mathcal{V}}^{m,k}$ we have

$$G'(\theta)(\xi) = \mathrm{d}E\big(\omega(\theta); V\big) = \mathrm{d}E\big(\omega(\theta); V(0)\big). \tag{1.15}$$

Lemma 1.2. *Let $\theta, \xi, \eta \in \overline{C}^2$ and V, W defined by (1.11) and (1.12) . Assume the application $V \to \mathrm{d}E(\omega(\theta), V)$ is continuous in a neighborhood of V with respect to the topology on $\overline{\mathcal{V}}^{m,k}$. Then if $G''(\theta)(\xi,\eta)$ exists, we have;*

(1.16)
$$G''(\theta)(\xi,\eta) = \mathrm{d}^2 E\big(\omega(\theta); V, W\big) - \mathrm{d}E\big(\omega(\theta), \dot{V}(0)\big) - \mathrm{d}E\big(\omega(\theta), [DV(0)]W(0)\big),$$

where
$$\dot{V}(0)(x) = \lim_{t \searrow 0} \big[V(t,x) - V(0,x)\big]/t,$$

and $[DV(0)]$ is the Jacobian matrix of $V(0)$.

Proof.

$$G''(\theta)(\xi,\eta) = \lim_{t \searrow 0} \frac{1}{t}\big(G'(\theta + t\,\eta)(\xi) - G'(\theta)(\xi)\big) \tag{1.17}$$

From the lemma 1.1 and the previous remark 1 we have:

$$G'(\theta + t\,\eta)(\xi) = \mathrm{d}E\big(T_t^W(\omega(\theta)), U(0)\big) \tag{1.18}$$

where

$$T_{t'}^U(x) = \big(I + t'\,\xi \circ (\theta + t\,\eta)^{-1}\big)(x)$$
$$U(t', x) = \xi \circ (\theta + t\,\eta)^{-1}\big((T_{t'}^{U^{-1}}(x)\big),\ U(0,x) = \xi \circ (\theta + t\,\eta)^{-1}(x).$$

and $G'(\theta)(\xi) = \mathrm{d}E(\omega(\theta), V(0))$. Clearly, $U(0,x)$ is a function of t. Let Z be the velocity field:

$$Z(t) = U(0) \ \ (= \xi \circ (\theta + t\,\eta)^{-1}) \tag{1.19}$$

We have :

$$Z(0) = \xi \circ \theta^{-1} = V(0). \tag{1.20}$$

and

$$\dot{Z}(0) = -[D(\xi \circ \theta^{-1})] \circ \eta \circ \theta^{-1} = -[DV(0)]W(0) \tag{1.21}$$

where $[D(\xi \circ \theta^{-1})]$ is the Jacobian matrix of $\xi \circ \theta^{-1}$.
Then by theorem 2.5 in [Delfour & Zolesio, 1991] we obtain :

$$\begin{aligned} G''(\theta)(\xi,\eta) &= \lim_{t \searrow 0} \frac{1}{t}\big(\,\mathrm{d}E(T_t^W(\omega(\theta); U(0)) - \mathrm{d}E(\omega(\theta), V(0))\big) \\ &= \lim_{t \searrow 0} \frac{1}{t}\big((\,\mathrm{d}E(T_t^W(\omega(\theta); Z(t)) - \mathrm{d}E(\omega(\theta), Z(0))\big) \\ &= \frac{d}{dt}\Big|_{t=0}\big(\,\mathrm{d}E(T_t^W(\omega(\theta); Z(t)) \\ &= \mathrm{d}^2 E(\omega(\theta); Z, W) \\ &= \mathrm{d}^2 E(\omega(\theta); Z(0), W(0)) + \mathrm{d}E(\omega(\theta); \dot{Z}(0)) \\ &= \mathrm{d}^2 E(\omega(\theta); V(0), W(0)) + \mathrm{d}E(\omega(\theta); \dot{Z}(0)). \end{aligned} \tag{1.22}$$

Also by the theorem 2.5 in [Delfour & Zolesio, 1991]:

$$\mathrm{d}^2 E(\omega(\theta); V, W) = \mathrm{d}^2 E(\omega(\theta); V(0), W(0)) + \mathrm{d}E(\omega(\theta); \dot{V}(0)) \cdot \tag{1.23}$$

By (1.21) we have:

$$\mathrm{d}E(\omega(\theta); \dot{Z}(0)) = -\,\mathrm{d}E(\omega(\theta); [DV(0)]W(0)) \tag{1.24}$$

Then by (1.22), (1.23), (1.24) we obtain:

(1.25)

$$G''(\theta)(\xi, \eta) = \mathrm{d}^2 E\big(\omega(\theta); V, W\big) - \mathrm{d}E\big(\omega(\theta), \dot{V}(0)\big) - \mathrm{d}E\big(\omega(\theta), [DV(0)]W(0)\big).$$

The following theorem gives a relation between the first and second-order eulerian semi-derivatives E (method of velocity) and the Frechet derivatives of G for arbitrary velocities.

Theorem 1.3. *Let $\mathbb{V}$ and $\mathbb{W}$ be two vector fields regular enough. Let $\theta \in \overline{C}^2$ and*

$$\begin{aligned} \xi &= \mathbb{V}(0) \circ \theta \\ \eta &= \mathbb{W}(0) \circ \theta \end{aligned} \tag{1.26}$$

Then

$$G''(\theta)(\xi, \eta) = \mathrm{d}^2 E\big(\omega(\theta); \mathbb{V}, \mathbb{W}\big) - \mathrm{d}E\big(\omega(\theta); \dot{\mathbb{V}}(0)\big) - dE\big(\omega(\theta), [D\mathbb{V}(0)]\mathbb{W}(0)\big). \tag{1.27}$$

Proof. By [Delfour & Zolesio, 1991] remark 2.4:

$$\mathrm{d}^2 E\big(\omega(\theta), \mathbb{V}, \mathbb{W}\big) = \mathrm{d}^2 E\big(\omega(\theta), \mathbb{V}(0), \mathbb{W}(0)\big) + \mathrm{d}E\big(\omega(\theta), \dot{\mathbb{V}}(0)\big) \tag{1.28}$$

where

$$\dot{\mathbb{V}}(0) = \lim_{t \to 0} \frac{\mathbb{V}(\cdot, t) - \mathbb{V}(\cdot, 0)}{t}.$$

Let us introduce:

$$V(x, t) = \mathbb{V}(0)(I + t\ \mathbb{V}(0))^{-1}(x) \tag{1.29}$$

$$W(x, t) = \mathbb{W}(0)(I + t\ \mathbb{W}(0))^{-1}(x) \tag{1.30}$$

Then :

$$T_t^V(x) = \big(I + t\ \mathbb{V}(0)\big)(x) \text{ and } T_t^W(x) = \big(I + t\ \mathbb{W}(0)\big)(x). \tag{1.31}$$

By [Delfour & Zolesio, 1991] remark 2.4;

$$\mathrm{d}^2 E(\omega(\theta); V, W) = \mathrm{d}^2 E\big(\omega(\theta); V(0), W(0)\big) + \mathrm{d}E\big(\omega(\theta); \dot{V}(0)\big). \tag{1.32}$$

But

$$\begin{aligned} V(0) &= \mathbb{V}(0) \text{ and } W(0) = \mathbb{W}(0) \\ \dot{V}(0) &= -[DV(0)]V(0) \quad \text{by [Delfour \& Zolesio, 1991] remark 2.2} \\ &= -[D\mathbb{V}(0)]\mathbb{V}(0) \end{aligned} \tag{1.33}$$

Then

$$d^2E(\omega(\theta); V, W) = d^2E(\omega(\theta); \mathbb{V}(0), \mathbb{W}(0)) - dE(\omega(\theta); [D\mathbb{V}(0)]\mathbb{V}(0)) \tag{1.34}$$

By substitution in (1.28):

$$d^2E(\omega(\theta), \mathbb{V}, \mathbb{W}) = d^2E(\omega(\theta), V, W) + dE(\omega(\theta), \dot{\mathbb{V}}(0) + [D\mathbb{V}(0)]\mathbb{V}(0)). \tag{1.35}$$

Let $\widetilde{V}$ and $\widetilde{W}$ be given by (1.11) and (1.12).
Then by Lemma 1.2:
(1.36)

$$G''(\theta)(\xi, \eta) = d^2E(\omega(\theta), \widetilde{V}, \widetilde{W}) - dE(\omega(\theta), \dot{\widetilde{V}}(0)) - dE(\omega(\theta), [D\widetilde{V}(0)]\widetilde{W}(0))$$

But

$$\widetilde{V}(x,t) = \xi \circ \theta^{-1}((I + t\ \xi \circ \theta^{-1})^{-1}(x)) = \mathbb{V}(0)((I + t\ \mathbb{V}(0))^{-1}(x)) = V(x,t) \tag{1.37}$$

and in the same way:

$$\widetilde{W}(x,t) = W(x,t) \tag{1.38}$$

then

$$\dot{\widetilde{V}}(0) = \dot{V}(0) = -[D\mathbb{V}(0)]\mathbb{V}(0) \tag{1.39}$$

by [Delfour & Zolesio, 1991] remark 9 and the definition of V.
Thus:

$$G''(\theta)(\xi, \eta) = d^2E(\omega(\theta), \mathbb{V}, \mathbb{W}) - dE(\omega(\theta), \dot{\mathbb{V}}(0)) - dE(\omega(\theta), [D\mathbb{V}(0)]\mathbb{W}(0)). \tag{1.40}$$

1.2-Shape derivatives of the solution to a Dirichlet problem.

Now we are going to introduce the derivatives with respect to the shape of the solution φ of the exterior Dirichlet problem :

$$-\Delta\varphi = \mu_0 j_0 \quad \text{in } \Omega \tag{1.41}$$

$$\varphi = 0 \quad \text{on } \partial\Omega \tag{1.42}$$

$$\varphi(x) = O(1) \text{ as } |x| \to \infty. \tag{1.43}$$

when j_0 has compact support and is regular enough.

Let $\theta, \xi \in \overline{C}^2$; we denote by $\varphi(\theta + t\ \xi)$ a solution of the exterior Dirichlet problem:

$$\begin{cases} -\Delta\varphi(\theta + t\ \xi) = \mu_0 j_0 \text{ on } \Omega(\theta + t\ \xi) \\ \varphi(\theta + t\ \xi) = 0 \text{ in } \partial\Omega(\theta + t\ \xi) \\ \varphi(\theta + t\ \xi) = O(1) \text{ on } |x| \to \infty. \end{cases} \tag{1.44}$$

If j_0 is a square integrable function with compact support in the interior of $\Omega(\theta + t\xi)$ for all $|t| < \varepsilon$ then there exists $\varphi(\theta + t\xi)$ solution of the exterior Dirichlet problem (1.44) for all $|t| < \varepsilon$, see [Kress, 1989].

Following [Murat & Simon, 1975], [Goto & Fujii, 1990], [Simon, 1988], [Sokolowski & Zolesio, 1992] we consider the first derivative of φ at θ from $\overline{C}^2$ to $L^\infty(\mathbb{R}^2)$. If it exists we have:

$$\varphi'(\theta)(\xi) = \lim_{t \searrow 0} \frac{\varphi(\theta + t\,\xi) - \varphi(\theta)}{t}. \tag{1.45}$$

If the application $\varphi' : \overline{C}^2 \to \mathcal{L}(\overline{C}^2, L^\infty(\mathbb{R}^2))$ has a derivative at θ then we denote it by $\varphi''(\theta)$ and $\varphi''(\theta) \in \mathcal{L}_2(\overline{C}_2, L^\infty(\mathbb{R}^2))$. If $\varphi''(\theta)$ exists then it is given by :

$$\varphi''(\theta)(\xi,\eta) = \lim_{t \searrow 0} \frac{\varphi'(\theta + t\,\eta)(\xi) - \varphi'(\theta)(\xi)}{t}. \tag{1.46}$$

The authors mentioned before characterized the first and the second derivatives of the solution φ.

Lemma 1.4. *Let be $\theta, \xi, \eta \in \overline{C}^2$. Assume that $\varphi'(\theta)$ and $\varphi''(\theta)$ exist. Then :*

$$\begin{cases} -\Delta\varphi'(\theta)(\xi) = 0 \text{ on } \Omega(\theta) \\ \quad \varphi'(\theta)(\xi) = -V(0)\nabla\varphi \text{ in } \partial\Omega(\theta) \\ \quad \varphi'(\theta)(\xi) = O(1) \text{ if } |x| \to \infty \end{cases} \tag{1.47}$$

and

$$\begin{cases} -\Delta\varphi''(\theta)(\xi,\eta) = 0 \text{ in } \Omega(\theta) \\ \quad \varphi''(\theta)(\xi,\eta) = -\big(V(0)\nabla^2\varphi W(0) + V(0)\nabla\varphi'(\theta)(\eta) + W(0)\nabla\varphi'(0)(\xi)\big) \\ \qquad\qquad \text{on } \partial\Omega(\theta) \\ \quad \varphi''(\theta)(\xi,\eta) = O(1) \text{ if } |x| \to \infty \end{cases} \tag{1.48}$$

where V, W are given by (1.11) and (1.12), that is $V(0) = \xi \circ \theta^{-1}$ and $W(0) = \eta \circ \theta^{-1}$.

In the next sections we are going to compute the Hessian of a cost function with respect to shapes, and we will see the way to implement a Newton method applied to the Kuhn and Tucker first-order necessary conditions.

2.-Variational Formulation.

The simplified model of the electromagnetic shaping problem studied here concerns the case of a vertical column of liquid metal falling down into an electromagnetic field induced by vertical conductors. We assume the frequency of the imposed current is very high so that the magnetic field does not penetrate into the metal. In other words we neglect the skin effect. The electromagnetic forces are reduced to the magnetic pressure acting on the interface.

Under suitable assumptions, [Henrot&Pierre,89], [Pierre&Roche,91,93], the equilibrium configurations are given by a local critical point of the following total energy:

$$E(\omega(\theta)) = -\frac{1}{2\mu_0} \int_{\Omega(\theta)} |\nabla\varphi|^2 + \sigma P(\omega(\theta)) \tag{2.1}$$

where $P(\omega(\theta))$ is the perimeter of $\omega(\theta)$, i.e. the length of $\partial\omega(\theta)$ when $\partial\omega(\theta)$ is regular enough (for instance of class C^1)

$$P(\omega(\theta)) = \int_{\partial\omega(\theta)} d\gamma, \qquad d\gamma = \text{ length measure on } \partial\omega(\theta). \tag{2.2}$$

In (2.1), σ is the surface tension of the liquid and φ is solution of:

$$-\Delta\varphi = \mu_0 j_0 \quad \text{in } \Omega(\theta) \tag{2.3}$$

$$\varphi = 0 \quad \text{on } \partial\Omega(\theta) \tag{2.4}$$

$$\varphi(x) = O(1) \text{ as } |x| \to \infty \tag{2.5}$$

where $\vec{j_0} = (0, 0, j_0)$ denotes the density current vector and μ_0 is the vacuum permeability.

The variational formulation of (2.1)-(2.5) consists in considering the equilibrium domain $\omega(\theta)$ as a stationary point for the total energy (2.1), under the constraint that measure of $\omega(\theta)$ is given by S_0.

We will show that the equilibrium relation is given on the boundary of $\partial\omega(\theta)$ by:

$$\frac{1}{2\mu_0}|\nabla\varphi|^2 + \sigma\mathcal{C} = \Lambda \qquad \text{on } \partial\omega(\theta) \tag{2.6}$$

where $\mathcal{C}$ the curvature of $\partial\omega(\theta)$ (seen from the metal), σ the surface tension of the liquid and $|.|$ denotes the euclidean norm. The constant Λ is an unknown of the problem as well as the boundary $\partial\omega(\theta)$.

This problem or very similar ones have been considered by several authors. We refer the reader to the following papers and to references in them for the physical analysis of the simplifying assumptions that the above model requires: see [Shercliff, 1981], [Sero-Guillaume, 1983], [Brancher & Sero-Guillaume, 1983], [Sneyd & Moffatt, 1982] , [Brancher & al. , 1983], [Gagnoud & al. , 1986], [Mestel, 1982], [Etay & al., 1988], [Coulaud&Henrot,94].

To establish the equilibrium relation (2.6) and to compute the second derivatives we introduce the Lagrangian:

$$\begin{cases} L : \mathcal{O} \times \mathbb{R} \to \mathbb{R} \\ \quad (\omega, \Lambda) \to L(\omega, \Lambda) = E(\omega) + \Lambda(m(\omega) - S_0) \end{cases} \tag{2.7}$$

We will consider the functional :

$$\begin{cases} L : \overline{C}^2 \times \mathbb{R} \to \mathbb{R} \\ \quad (\theta, \Lambda) \to L(\theta, \Lambda) = E(\omega(\theta)) + \Lambda(m(\omega(\theta)) - S_0) \end{cases} \tag{2.8}$$

where in order to simplify the notations, we have used letter L as in (2.7), but it will be clear from the context whether L is a function of (ω, Λ) or (θ, Λ).

Using the formal framework introduced in section 1 we are going to compute the first and second derivatives of L.

Lemma 2.1. *If $\theta, \xi \in \overline{C}_2$ and L is defined by (2.8) then*

$$L'(\theta, \Lambda)(\xi) = \mathrm{d}L\big((\omega(\theta), \Lambda); V\big) = \frac{1}{2\mu_0}\int_{\partial\omega(\theta)} \big(|\nabla\varphi|^2 + \sigma\mathcal{C} + \Lambda\big)(V \cdot \overline{n})\, \mathrm{d}\gamma \tag{2.9}$$

where V is given by (1.11).

Moreover, traces of φ and $\nabla\varphi$ on $\partial\omega(\theta)$ exist and are (at least) square integrable on $\partial\omega(\theta)$.

Very similar results can be found for instance in [Zolesio, 1984], [Sero Guillaume, 1989], [Descloux, 1990].

A complete proof under precise regularity assumptions is given in [Pierre & Roche, 1990].

According to (2.9) the variational formulation for the continuous problem (2.1)-(2.5) consists in finding (θ, Λ) such that

$$L'(\theta,\Lambda)(\xi) = 0 \tag{2.10}$$

for every $\xi \in \overline{C}^2$.

The fact that $L'(\theta, \Lambda)$ is an integral equation over $\partial\omega(\theta)$ makes the numerical approach possible. To implement Newton method we are going to compute the second derivative $L''(\theta)(\xi,\eta)$. First let us state two technical lemmas.

Lemma 2.2. *Let ω be a compact subset of $\mathbb{R}^2$ without empty interior and of class $\mathcal{C}^2$. Let be $V \in \mathcal{C}^2(\mathbb{R}^2,\mathbb{R}^2)$ with compact support. If s and s_t denote a parametrization by arc length of the boundary of ω and $\omega_t = (I+tV)(\omega)$, then if $x_t = (I+tV)(x)$:*

$$\frac{\mathrm{d}s_t}{\mathrm{d}s}(x_t) = \big(1 + t\ (\overline{s}\cdot\frac{\partial V}{\partial s}) + o(t)\big)(x) \tag{2.11}$$

where $\overline{s}$ is the tangent to $\partial\omega$.

Proof.

Let δs be the distance between two points on $\partial\omega$ then

$$(\delta s)^2 = \big(x + \varepsilon\overline{s} + o(\varepsilon) - x\big)^2 = \big(\varepsilon\overline{s} + o(\varepsilon)\big)^2 + \varepsilon^2\overline{s}.\overline{s} + o(\varepsilon^2) = \varepsilon^2 + o(\varepsilon^2) \tag{2.12}$$

Let δs_t be the distance between two points on $\partial\omega_t$ then

$$\begin{aligned}(\delta s_t)^2 &= \big[x + \varepsilon\overline{s} + o(\varepsilon) + t\ V(x+\varepsilon\overline{s}+o(\varepsilon)) - x - t\ V(x)\big]^2\\ &= \left[\varepsilon\overline{s} + t\ \varepsilon(\overline{s}\cdot[DV(x)]) + o(\varepsilon)\right]^2\\ &= \varepsilon^2 + 2\,t\ \varepsilon^2(\overline{s}\cdot[DV(x)])\cdot\overline{s} + t^2\varepsilon^2(\overline{s}\cdot[DV(x)]) + o(\varepsilon^2)\\ &= \varepsilon^2 + 2\ t\varepsilon^2(\overline{s}\cdot\frac{\partial V}{\partial s}) + t^2\varepsilon^2(\frac{\partial V}{\partial s})^2 + o(\varepsilon^2)\end{aligned} \tag{2.13}$$

Then :

$$\begin{aligned}\frac{\mathrm{d}s_t}{\mathrm{d}s} &= \lim_{\varepsilon\to 0}\frac{\delta s_t}{\delta s} = \big[1 + 2t(\overline{s}\cdot\frac{\partial V}{\partial s}) + t^2(\frac{\partial V}{\partial s})^2\big]^{1/2}\\ &= 1 + t\ (\overline{s}\cdot\frac{\partial V}{\partial s}) + o(t).\end{aligned} \tag{2.14}$$

Lemma 2.3. *With the same hypotheses as in Lemma 2.2, if we denote by $\overline{n},\overline{s},\overline{n}_t$ and $\overline{s}_t$ the normal and tangential unitary vectors to the boundary of ω and ω_t, $x_t = (I+tV)(x)$ then we have:*

$$\overline{s}_t(x_t) = \overline{s} + t\ (\overline{n}\cdot\frac{\partial V}{\partial s})\overline{n} + o(t) \tag{2.15}$$

$$\overline{n}_t(x_t) = \overline{n} - t\ (\overline{n}\cdot\frac{\partial V}{\partial s})\overline{s} + o(t) \tag{2.16}$$

Moreover if $\mathcal{C}$ and $\mathcal{C}_t$ are the curvature of ω and ω_t respectively then :

$$\mathcal{C}_t(x_t) = \mathcal{C} - t\big[\mathcal{C}(\overline{s}\cdot\frac{\partial V}{\partial s}) + \frac{\partial}{\partial s}(\overline{n}\cdot\frac{\partial V}{\partial s})\big] + o(t). \tag{2.17}$$

Proof.

It is easy to verify that :

$$\overline{s}_t = \frac{\partial x_t}{\partial s_t} = \frac{\partial(x+tV(x))}{\partial s_t} = (\overline{s} + t\frac{\partial V}{\partial s})\frac{\mathrm{d}s}{\mathrm{d}s_t} \tag{2.18}$$

then as

$$\begin{aligned}\frac{\mathrm{d}s}{\mathrm{d}s_t} &= 1 - t\ (\overline{s}\cdot\frac{\partial V}{\partial s}) + o(t)\\ \overline{s}_t &= \overline{s} + t\ \frac{\partial V}{\partial s} - t\ \overline{s}\cdot(\overline{s}\cdot\frac{\partial V}{\partial s}) + o(t)\\ &= \overline{s} + t\ \big((\overline{n}\cdot\frac{\partial V}{\partial s})\cdot\overline{n} + (\overline{s}\cdot\frac{\partial V}{\partial s})\cdot\overline{s} - (\overline{s}\cdot\frac{\partial V}{\partial s})\cdot\overline{s}\big) + o(t)\\ &= \overline{s} + t(\overline{n}\cdot\frac{\partial V}{\partial s})\cdot\overline{n} + o(t).\end{aligned} \tag{2.19}$$

We have also that

$$\overline{n}_t - \overline{n} = \big[(\overline{s}_t - \overline{s})\cdot\overline{n}\big]\overline{s} + \big[(\overline{s}_t - \overline{s})\cdot\overline{s}\big]\overline{n}. \tag{2.20}$$

But

$$(\overline{s}_t - \overline{s})\cdot\overline{s} = o(t) \text{ and } (\overline{s}_t - \overline{s})\cdot\overline{n} = t\ (\overline{n}\cdot\frac{\partial V}{\partial s}) + o(t). \tag{2.21}$$

Then

$$\overline{n}_t = \overline{n} - t\ (\overline{n}\cdot\frac{\partial V}{\partial s})\cdot\overline{s} + o(t).$$

Equality (2.17) can be achieved if we note that if $x_t \in \partial\omega_t$ then :

$$\mathcal{C}_t = \lim_{\substack{y_t\to x_t\\ y_t\in\partial\omega_t}} \frac{\overline{s}\cdot\overline{n}_t}{\delta s_t} = (\overline{s}_t\cdot\frac{\partial\overline{n}_t}{\partial s})\frac{\mathrm{d}s}{\mathrm{d}s_t}$$

and by substitution we obtain the result.

These technical lemmas allow us to compute the second derivative of the total energy with respect to the shape.

Theorem 2.4. *Let $\theta, \xi, \eta \in \overline{C}^2$. Assume that the derivatives $\varphi'(\theta)$ and $\varphi''(\theta)$ exist. Assume that the current density j is bounded in $\mathbb{R}^2$ with support in $\Omega(\theta)$. Then :*

$$\begin{aligned}L''(\theta,\Lambda)(\xi,\eta) = \frac{1}{2\mu_0}\int_{\partial\omega(\theta)} &\frac{\partial\varphi(\theta)}{\partial n}\big(V\cdot\nabla^2\varphi(\theta)\cdot W\\ &+ V\cdot\nabla\varphi'(\theta)(\eta) + W\cdot\nabla\varphi'(\theta)(\xi)\big)\\ &+ \sigma\int_{\partial\omega(\theta)}(\frac{\partial V}{\partial s}\cdot\overline{n})(\frac{\partial W}{\partial s}\cdot\overline{n}) + \Lambda\int_{\partial\omega(\theta)} V\cdot\frac{\partial W^\perp}{\partial s}\end{aligned} \tag{2.22}$$

where $W^\perp = (W_2, -W_1)$.

Proof.

We set:

$$L_1(\theta) = \frac{-1}{2\mu_0}\int_{\Omega(\theta)} |\nabla\varphi(\theta)|^2 \,\mathrm{d}x$$
$$L_2(\theta) = \sigma \int_{\partial\omega(\theta)} \mathrm{d}\gamma$$
$$L_3(\theta) = \text{ meas } (\omega) = \int_{\omega(\theta)} \mathrm{d}x = m(\omega(\theta)).$$

Let V and W be such that :

$$V(x,t) = \xi \circ \theta^{-1}\big((T_t^V)^{-1}(x)\big)$$
$$W(x,t) = \eta \circ \theta^{-1}\big((T_t^W)^{-1}(x)\big).$$

As :

$$\int_\Omega |\nabla\varphi(\theta)|^2 \,\mathrm{d}x = \mu_0 \int_\Omega \varphi(\theta)\cdot j \,\mathrm{d}x = \mu_0 \int_{spt(j)} \varphi(\theta)\cdot j \,\mathrm{d}x$$

and

$$\Big|\int_{spt(j)} \big(\varphi'(\theta)(\xi) - \frac{\varphi(\theta+t\xi)-\varphi(\theta)}{t}\big)\cdot j \,\mathrm{d}x\Big|$$
$$< |spt(j)|_\infty \,\big|\varphi'(\theta)(\xi) - \frac{\varphi(\theta+t\xi)-\varphi(\theta)}{t}\big|_\infty \xrightarrow{t\searrow 0} 0$$

we get:

$$L_1'(\theta)(\xi) = \frac{-1}{2}\int_{spt(j)} \varphi'(\theta)(\xi)(x) j(x)\,\mathrm{d}x.$$

By the same techniques we have

$$L_1''(\theta)(\xi,\eta) = \frac{-1}{2}\int_{spt(j)} \varphi''(\theta)(\xi,\eta)(x)\cdot j(x)\,\mathrm{d}x.$$

Moreover by Lemma 1.4 :

$$L_1(\theta)(\xi) = \frac{-1}{2}\int_{\Omega(\theta)} \varphi'(\theta)(\xi) j(x)\,\mathrm{d}x = \frac{1}{2\mu_0}\int_{\Omega(\theta)} \varphi'(\theta)(\xi)\Delta\varphi(\theta)\,\mathrm{d}x$$
$$= \frac{-1}{2\mu_0}\int_{\partial\omega} \frac{\partial\varphi(\theta)}{\partial n}\varphi'(\theta)(\xi)\,\mathrm{d}\gamma = \frac{1}{2\mu_0}\int_{\partial\omega} (\frac{\partial\varphi(\theta)}{\partial n})^2 (V\cdot\overline{n})\,\mathrm{d}\gamma$$

because the normal vector is oriented towards $\Omega(\theta)$, and in the same way we get:

$$L_1''(\theta)(\xi,\eta) = \frac{1}{2\mu_0}\int_{\partial\omega(\theta)} \frac{\partial\varphi(\theta)}{\partial n}\big(V(0)\nabla^2\varphi W(0) + V\nabla\varphi'(\theta)(\eta) + W\nabla\varphi'(\theta)(\xi)\big)\,\mathrm{d}\gamma$$

To compute $L_1''(\theta)(\xi,\eta)$ and $L_2''(\theta)(\xi,\eta)$, at first we find the expressions of $d^2L_1(\omega(\theta);V,W)$ and $d^2L_2(\omega(\theta);V,W)$ and using Theorem 1.3 we find the form of second derivatives L_2'' and L_3'' where V and W are given by (1.11) and (1.12).

Using the technical Lemmas 2.2, 2.3 and the definition 1.2 we can compute $L_2''(\theta)(\xi,\eta)$ and $L_3''(\theta)(\xi,\eta)$.

$$\mathrm{d}L_2\big(\omega(\theta);V\big) = \mathrm{d}L_2\big(\omega(\theta);V\big) = \sigma\int_{\partial\omega} \mathcal{C}(V\cdot\overline{n})\,\mathrm{d}\gamma$$
$$\mathrm{d}L_2\big(\omega(\theta+t\eta);V(t)\big) = \mathrm{d}L_2\big(T_t^W(\omega(\theta));V(t)\big) = \sigma\int_{\partial T_t^W(\omega(\theta))} \mathcal{C}_{tW}\big(V(t)\cdot\overline{n}\big)\,\mathrm{d}\gamma$$

and $\mathcal{C}_{tW}$ is the curvature of $\partial T_t^W(\omega(\theta))$. Then:

$$\begin{aligned}\mathrm{d}L_2\big(\omega(\theta+t\ \eta),V(t)\big) = \sigma\int_{\partial\omega}\big[\mathcal{C}-t\ \big(\mathcal{C}(\overline{s}\cdot\frac{\partial W(0)}{\partial s})+\frac{\partial}{\partial s}(\overline{n}\cdot\frac{\partial W(0)}{\partial s})\big]\\ \big[V(0)+t\ [DV(0)]\cdot W(0)+t\ \dot{V}(0)\big]\\ \big[\overline{n}-t\ (\overline{n}\frac{\partial W(0)}{\partial s})\overline{s}\big]\big[1+t\ (\overline{s}\cdot\frac{\partial W(0)}{\partial s})\big]\,\mathrm{d}\gamma+o(t)\end{aligned}$$

Then by definition 1.2 and Theorem 1.3 we have :

$$L_2''(\theta)(\xi,\eta)=\sigma\int_{\partial\omega}(\frac{\partial V}{\partial s}\cdot\overline{n})(\frac{\partial W}{\partial s}\cdot\overline{n})\,\mathrm{d}\gamma \tag{2.23}$$

In the same way we have

$$\mathrm{d}L_3\big(\omega(\theta);V\big)\ =\ \mathrm{d}L_3\big(\omega(\theta);V\big)\ =\int_{\partial\omega(\theta)}(V\cdot\overline{n})\,\mathrm{d}\gamma$$

and

$$\begin{aligned}\mathrm{d}L_3\big(\omega(\theta+t\eta);V(t)\big)\ =\ \mathrm{d}L_3\big(T_t^W(\omega(\theta));V\big)\ =\int_{\partial T_t^W(\omega(\theta))}\big(V(t)\cdot\overline{n}\big)\,\mathrm{d}\gamma\\ =\int_{\partial(\omega(\theta))}\big[V(0)+t[DV(0)]\cdot W(0)+t\,\dot{V}(0)\big]\cdot\big[\overline{n}-t(\overline{n}\cdot\frac{\partial W(0)}{\partial s})\overline{s}\big]\\ \big[1+t(\overline{s}\cdot\frac{\partial W(0)}{\partial s})\big]\,\mathrm{d}\gamma+o(t)\end{aligned}$$

Then

$$\begin{aligned}\mathrm{d}^2L_3\big(\omega(\theta);V,W\big)=\int_{\partial\omega}\big[\big([DV(0)]\cdot W(0)+\dot{V}(0)\big)\cdot\overline{n}+\big((\overline{s}\cdot\frac{\partial W(0)}{\partial s})\overline{n}\\ -(\overline{n}\cdot\frac{\partial W(0)}{\partial s})\overline{s}\big)V\big]\,\mathrm{d}\gamma\end{aligned}$$

By Theorem 1.3 we get :

$$\begin{aligned}L_3''(\theta)(\xi,\eta)=\int_{\partial\omega}\big((\overline{s}\cdot\frac{\partial W}{\partial s})\overline{n}-(\overline{n}\cdot\frac{\partial W}{\partial s})\overline{s}\big)\cdot V\,\mathrm{d}\gamma\\ =\int_{\partial\omega}(V\cdot\frac{\partial W^\perp}{\partial s})\,\mathrm{d}\gamma=\int_{\partial\omega}(W\cdot\frac{\partial V^\perp}{\partial s})\,\mathrm{d}\gamma\end{aligned}$$

We obtain the final result by addition :

$$\begin{aligned}L''(\theta,\Lambda)(\xi,\eta)=L_1''(\theta)(\xi,\eta)+L_2''(\theta)(\xi,\eta)+\Lambda\ L_3''(\theta)(\xi,\eta)\\ =\frac{1}{2\mu_0}\int_{\partial\omega(\theta)}\frac{\partial\varphi(\theta)}{\partial n}\big(V\cdot\nabla^2\varphi(\theta)\cdot W+V\cdot\nabla\varphi'(\theta)(\eta)+W\cdot\nabla\varphi'(\theta)(\xi)\\ +\sigma\int_{\partial\omega(\theta)}(\frac{\partial V}{\partial s}\cdot\overline{n})(\frac{\partial W}{\partial s}\cdot\overline{n})\,\mathrm{d}\gamma+\Lambda\ \int_{\partial\omega(\theta)}V\cdot\frac{\partial W^\perp}{\partial s}\,\mathrm{d}\gamma.\end{aligned}$$

3. Numerical Method

3.1 Introduction: the continuous Newton algorithm

Any minimun point $\theta^\star$ of energy functional $E(\omega(\theta))$ over $\overline{C}^2$ under constraint on the surface $m(\omega(\theta^\star))$ of $\omega(\theta^\star)$ satisfies the Kuhn and Tucker continuous equation, see [Fiacco & McCormick, 1968]. Thus, we consider the Lagrangian:

$$L(\theta,\Lambda) = E(\theta) + \Lambda\ (m(\omega(\theta)) - S_0) \tag{3.1}$$

where $\theta \in \overline{C}^2$ and $\Lambda \in \mathbb{R}$. A critical point of the energy $E(\omega(\theta))$ with the constraint $m(\omega(\theta)) - S_0 = 0$ is the first argument of the couple $(\theta^\star, \Lambda^\star)$ solution of the following first order necessary conditions:

$$D(\theta,\Lambda) = \begin{pmatrix} E'(\omega(\theta)) + \Lambda\ m'(\omega(\theta)) \\ m(\omega(\theta)) - S_0 \end{pmatrix} = \overline{0}. \tag{3.2}$$

Clearly the solutions of $D(\theta,\Lambda) = \overline{0}$ are not necessarily points which achieve a minimun; in general they are saddle points. To find a solution of the equation (3.2) we are going to apply a Newton method. The Newton method consists in computing a sequence of solutions (θ^k, Λ^k) of linearized form of (3.2). With the notations of section 1 this leads to the following algorithm:

$$\begin{cases} (\theta^\circ, \Lambda^\circ) \text{ given} \\ (\theta^{k+1}, \Lambda^{k+1}) = (\theta^k, \Lambda^k) + (\eta^k, \delta\Lambda^k), \quad (\eta^k, \delta\Lambda^k) \in \overline{C}^2 \times \mathbb{R} \ \text{ defined by :} \\ D(\theta^k, \Lambda^k) + D'(\theta^k, \Lambda^k)(\eta^k, \delta\Lambda^k) = 0 \ \text{ in } \ \mathcal{L}(\overline{C}^2, \mathbb{R}) \times \mathbb{R} \end{cases} \tag{3.3}$$

where $D'(\theta^k, \Lambda^k)$ is given by:
(3.4)

$$D'(\theta^k, \Lambda^k)(\eta^k, \delta\Lambda^k) = \begin{pmatrix} E''(\omega(\theta^k))(\eta^k) + \Lambda^k m''(\omega(\theta^k))(\eta^k) & \delta\Lambda^k m'(\omega(\theta^k)) \\ m'(\omega(\theta^k))(\eta^k) & 0 \end{pmatrix}$$

In the next subsection we apply this algorithm to the magneto-shaping problem in a discrete case.

3.2 - Discretization.

Numerically, we have to find a zero of an approximation of (3.1). For this we consider a discretized form of (3.3). We construct a sequence of domains $\omega(\theta^k)$, more precisely, we consider a sequence of domains determinated by its boundaries $\partial\omega(\theta^k)$.

In practice by $\partial\omega(\theta^k) = \Gamma^k$ we mean the piecewise closed Jordan curve with n edges $[x_i^k, x_{i+1}^k]$, $i = 1, \cdots, n$ and $x_{n+1}^k = x_1^k$.

At each iteration the sequence of boundaries $\partial\omega(\theta^k)$ is obtained by a local perturbation. To each vertex x_i^k of Γ^k is associated a direction $\hat{Z}_i^k \in \mathbb{R}^2$. We construct a continuous piecewise linear function $Z_i^k : \Gamma^k \to \mathbb{R}^2$ such that:

$$Z_i^k(x_j^k) = \hat{Z}_i^k \delta_{ij};\ i,j = 1, ...n, \tag{3.5}$$

δ_{ij} being the Kronecker symbol. The support of Z_i^k is equal to $[x_{i-1}^k, x_i^k] \cup [x_i^k, x_{i+1}^k]$. Then at each iteration we compute a field $Z^k(x) = (I + \sum_{i=1}^n u_i Z_i^k)(x)$ and the new surface Γ^{k+1} is constructed from Γ^k by:

$$\Gamma^{k+1} = \{X = x + \sum_{i=1}^n u_i Z_i^k(x) = (I + \sum_{i=1}^n u_i Z_i^k)(x); u_i \in \mathbb{R}, x \in \Gamma^k\} \tag{3.6}$$

where $\overline{u} = (u_1, ...u_n)$ are the unknowns which determine the evolution of the surface Γ^k. This procedure gives a family of domains ω^{k+1}, with a piecewise linear boundary Γ^{k+1} corresponding to $(u_1, ...u_n) \in \mathbb{R}^n$.

To better understand our algorithm we first consider an academic problem : minimizing the perimeter for a given area.

$$(3.7) \qquad \begin{cases} \min J(\omega) := \displaystyle\int_{\partial\omega} \mathrm{d}\gamma \\ \quad m(\omega) = \displaystyle\int_{\omega} \mathrm{d}x = S_0 \text{ given, } \omega \text{ regular enough.} \end{cases}$$

The solution is the circle with the prescribed area. As $J(\omega) = (\frac{1}{\sigma})L_2(\omega)$, the first and second order derivatives of the cost function and the constraint $S(\omega) = m(\omega) - S_0$ where calculated in section 2 Lemma 2.1, Theorem 2.4. Then the first order necessary conditions are given by:

$$(3.9) \qquad \begin{cases} \displaystyle\int_{\partial\omega} \mathcal{C}(V \cdot \overline{n})\,\mathrm{d}\gamma + \Lambda \int_{\partial\omega} (V \cdot \overline{n})\,\mathrm{d}\gamma = 0 \\ \qquad\qquad \displaystyle\int_{\omega} \mathrm{d}x - S_0 = 0 \end{cases}$$

where $\mathcal{C}$ is the curvature of $\partial\omega(\theta)$ and $V(x,t)$ is given by (1.11). The continuous second derivative (the Hessian) is the following:

$$(3.10) \qquad \begin{pmatrix} \int_{\partial\omega(\theta)} (\frac{\partial V}{\partial s} \cdot \overline{n})(\frac{\partial W}{\partial s} \cdot \overline{n})\,\mathrm{d}\gamma + \Lambda \int_{\partial\omega(\theta)} (V . \frac{\partial W^{\perp}}{\partial s})d\gamma & \int_{\partial\omega(\theta)} (V \cdot \overline{n})\,\mathrm{d}\gamma \\ \int_{\partial\omega(\theta)} (W \cdot \overline{n})\,\mathrm{d}\gamma & 0 \end{pmatrix}.$$

If we consider the discretization introduced in (3.4),(3.5) and implement the algorithm (3.3), at each iteration we have to solve the following equation:

$$(3.11) \qquad \begin{pmatrix} A_{ij}(u_1^k, ..., u_n^k, \Lambda^k) & S_i(u_1^k, ..., u_n^k) \\ S_j(u_1^k, ..., u_n^k) & 0 \end{pmatrix} \begin{pmatrix} (u_1, \ldots, u_N)^t \\ \delta\Lambda \end{pmatrix} = -\begin{pmatrix} D_i \\ m \end{pmatrix}$$

where:

$$(3.12) \qquad A_{ij}(u_1^k, ..., u_n^k, \Lambda^k) = \int_{\Gamma^k} (\frac{\partial Z_i^k}{\partial s} \cdot \overline{n})(\frac{\partial Z_j^k}{\partial s} \cdot \overline{n})\,\mathrm{d}\gamma + \Lambda \int_{\Gamma^k} (Z_i^k . \frac{\partial Z_j^{k\,\perp}}{\partial s})d\gamma$$

$$(3.13) \qquad S_i(u_1^k, ..., u_n^k) = \int_{\Gamma^k} (Z_i^k \cdot \overline{n})\,\mathrm{d}\gamma$$

$$(3.14) \qquad D_i = (\frac{(x_i^k - x_{i-1}^k)}{\|x_i^k - x_{i-1}^k\|} - \frac{(x_{i+1}^k - x_i^k)}{\|x_{i+1}^k - x_i^k\|}) \cdot \hat{Z}_i^k + \Lambda \int_{\Gamma^k} (Z_i^k \cdot \overline{n})\,\mathrm{d}\gamma$$

and

$$(3.15) \qquad m = \int_{\omega^k} \mathrm{d}x - S_0 \,.$$

Once the linear (3.11) system is solved we update the boundary by:

$$x_i^{k+1} = x_i^k + u_i Z_i^k \,. \tag{3.16}$$

In the next section we are going to give numerical results for this particular example.

The same algorithm is applied to the electromagnetic shaping problem described in section 2. Consider the following problem:

$$\begin{cases} \min\big(-\dfrac{1}{2\mu_0}\displaystyle\int_\Omega |\nabla\varphi|^2 \,\mathrm{d}x + \sigma \int_{\partial\omega} \mathrm{d}\gamma\big) \\ m(\omega) = \displaystyle\int_\omega \mathrm{d}x = S_0 \end{cases} \tag{3.17}$$

The Lagrangian of this problem has the following form:

$$L(\omega,\Lambda) = -\frac{1}{2\mu_0}\int_\Omega |\nabla\varphi|^2 \,\mathrm{d}x + \sigma\int_{\partial\omega}\mathrm{d}\gamma + \Lambda\big(\int_\omega \mathrm{d}x - S_0\big). \tag{3.18}$$

As it was proved in Lemma 2.1 we obtain the following first order necessary condition:

$$\begin{cases} \dfrac{1}{2\mu_0}\displaystyle\int_{\Gamma^k} |\nabla\varphi|^2\,(V\cdot\overline{n})\,\mathrm{d}\gamma + \sigma\int_\Gamma \mathcal{C}\,(V\cdot\overline{n})\,\mathrm{d}\gamma + \Lambda\int_\Gamma (V\cdot\overline{n})\,\mathrm{d}\gamma = 0 \\ \hfill i = 1,\ldots n \\ \hfill \displaystyle\int_\omega \mathrm{d}x - S_0 = 0 \end{cases} \tag{3.19}$$

The second order derivatives of the Lagrangian computed in Theorem 2.4 leads to the following Hessian:

$$H = \begin{pmatrix} A_{i,j,(i,j=1,\ldots,n)} & S_V \\ S_W & 0 \end{pmatrix} \tag{3.20}$$

where:

$$\begin{aligned} A_{i,j} = &\int_{\partial\omega} \frac{1}{2\mu_0}\frac{\partial\varphi}{\partial n}\big(V\cdot\nabla^2\varphi\cdot W + V\cdot\nabla\varphi'(\theta)(\eta) + W\cdot\nabla\varphi'(\theta)(\xi)\big) \\ &+ \int_{\partial\omega} \big((\frac{\partial V}{\partial s}\cdot\overline{n})(\frac{\partial W}{\partial s}\cdot\overline{n}) + \Lambda(V\cdot\frac{\partial W^\perp}{\partial s})\big)\,d\gamma \end{aligned}$$

$$S_V = \int_{\partial\omega} V\cdot\overline{n}\,\mathrm{d}\gamma \tag{3.21}$$

and

$$S_W = \int_{\partial\omega} W\cdot\overline{n}\,\mathrm{d}\gamma.$$

In practice we consider an approximation (not a discretization, because we need the solution of two exterior Dirichlet problems) of the Newton algorithm (3.3) which consists in constructing the sequence (Γ^k,Λ^k) :

$$(\Gamma^{k+1},\Lambda^{k+1}) = (\Gamma^k,\Lambda^k) + (Z^k(\Gamma^k),\delta\Lambda^k) \tag{3.22}$$

where $Z^k(x) = \sum_{i=1}^n u_i Z_i^k(x)$ and $(u_1^k, ..., u_n^k)$ is defined by the following system of equations :

$$(3.23) \qquad \begin{pmatrix} A_{ij}(u_1^k, ..., u_n^k, \Lambda^k) & S_i(u_1^k, ..., u_n^k) \\ S_j(u_1^k, ..., u_n^k) & 0 \end{pmatrix} \begin{pmatrix} (u_1, \dots, u_n)^t \\ \delta\Lambda \end{pmatrix} = -\begin{pmatrix} D_i \\ m \end{pmatrix}$$

where:
(3.24)

$$\begin{aligned} A_{ij}(u_1^k, ..., u_n^k, \Lambda^k) = & \int_{\partial\omega} \frac{1}{2\mu_o} \frac{\partial\varphi}{\partial n} (Z_i^k \cdot \nabla^2\varphi \cdot Z_j^k + Z_i^k \cdot \nabla\psi'_{Z_j^k} + Z_j^k \cdot \nabla\psi'_{Z_i^k})\, \mathrm{d}\gamma + \\ & + \int_{\Gamma^k} (\frac{\partial Z_i^k}{\partial s} \cdot \overline{n})(\frac{\partial Z_j^k}{\partial s} \cdot \overline{n})\, \mathrm{d}\gamma \\ & + \Lambda \int_{\Gamma^k} (Z_i^k \cdot \frac{\partial Z_j^{k\perp}}{\partial s}) d\gamma, \quad i,j = 1, ...n. \end{aligned}$$

$$(3.25) \qquad S_i(u_1^k, ..., u_n^k) = \int_{\Gamma^k} (Z_i^k \cdot \overline{n}) d\gamma, \; i = 1, ...n$$

$$(3.26) \qquad \begin{aligned} D_i = & \frac{1}{2\mu_0} \int_{\Gamma^k} |\nabla\varphi|^2 \, (Z_i^k \cdot \overline{n})\, \mathrm{d}\gamma + (\frac{(x_i^k - x_{i-1}^k)}{\|x_i^k - x_{i-1}^k\|} - \frac{(x_{i+1}^k - x_i^k)}{\|x_{i+1}^k - x_i^k\|}) \cdot \hat{Z}_i^k + \\ & \Lambda \int_{\Gamma^k} (Z_i \cdot \overline{n}) d\gamma \;, \quad i = 1, ...n \end{aligned}$$

and

$$(3.27) \qquad m = \int_{\omega^k} \mathrm{d}x - S_0$$

Then

$$(3.28) \qquad \begin{aligned} \Gamma^{k+1} & = (I + Z^k)(\Gamma^k) \\ & = \left\{ x : x = X + Z^k(X)\,;\, X \in \Gamma^k \right\} . \end{aligned}$$

3.3 - Quasi-Newton method.

In [Pierre&Roche,91,93] was implemented a numerical method to simulate the electromagnetic casting phenomenium without any evaluation of the second derivatives.

The algorithm consists to consider a penalized energy:

$$(3.29) \qquad E_r(\omega) = E(\omega) + \frac{r}{2}\big(\text{ meas } (\omega) - s_0\big)^2$$

where r is a real positive number going to infinity, in practice large enough.

For each r we solve by a Quasi-Newton method the unconstraint minimization problem :

$$(3.30) \qquad \begin{cases} \min E_r(\omega) \\ \omega \in \mathcal{O} \end{cases} .$$

The discrete version of the algorithm is similar to the Newton method. We construct a sequence Γ_r^k defined by:

$$
\begin{aligned}
\Gamma_r^{k+1} &= (I + Z^k)(\Gamma_r^k) \\
&= \left\{ x : x = X + Z^k(X) \,;\, X \in \Gamma_r^k \right\} \\
&= \left\{ x : x = X + \sum_{i=1}^{n} u_i Z_i^k(X) \right\}.
\end{aligned} \tag{3.31}
$$

with $u_1, \ldots, u_n$ given by:

$$
u_i = -\rho_k (H^k D E_r^k(\omega))_i. \tag{3.32}
$$

Here H^k is an approximation of the inverse of the Hessian E_r'' computed by the B.F.G.S (Broyden, Fletcher, Goldfarb and Shanno) method [Minoux, 1993], see also [Pierre & Roche, 1990] for more details about the application of Quasi-Newton method to electromagnetic casting. The computation of H^k requires only the gradient of the penalized cost function.

In fact at each iteration we compute an approximation of the continuous gradient $E_r'(\omega)$, we denote it $DE_r^k(\omega)$ and it is given by:

$$
\begin{aligned}
(DE_r^k(\omega))_i = \frac{1}{2\mu_o} \int_{\partial_\omega} (\nabla\varphi \cdot \overline{n})^2 (Z_i^k \cdot \overline{n}) \,\mathrm{d}\gamma + \sigma \int_{\partial\omega} \mathcal{C}(Z_i \cdot \overline{n}) \,\mathrm{d}\gamma \\
+ r(meas(\omega) - S_0) \int_{\partial_\omega} (Z_i \cdot \overline{n}) \,\mathrm{d}\gamma
\end{aligned} \tag{3.34}
$$

where φ^k is an approximation of φ and the integral of the term comming from the magnetic energy is computed by a numerical quadrature method.

The parameter $\rho_k \in]0,1]$ is given by a semi-arbitrary choice as we cannot evaluate the energy $E_r(\omega)$ at each iteration and so we can not implement any classical line search method , see [Hestenes, 1980].

3.4 Numerical solution of the exterior Dirichlet Problem.

We recall here that at each iteration it is necessary to solve the exterior problem (1.41),(1.42),(1.43) and (1.47).

In fact, we actually only need to know $\nabla\varphi$ at the boundary. Therefore, it is natural to choose a boundary integral representation for φ.

First of all we introduce the function :

$$
u(x) = \frac{-\mu_0}{2\pi} \int_{\mathbb{R}^2} ln\,|x - y| j_0(y) \,\mathrm{d}y + \frac{\mu_0}{2\pi} ln\,|x| \int_{\mathbb{R}^2} j_0(y) \,\mathrm{d}y. \tag{3.35}
$$

Since :

$$
-\Delta u = \mu_0 j_0 \text{ in } \mathbb{R}^2 \tag{3.36}
$$

$$
|u| = 0(|x|^{-1}) \text{ as } |x| \to \infty \tag{3.37}
$$

the problem (1.41),(1.42),(1.43) is equivalent to :

$$
\varphi = u + v \tag{3.38}
$$

where

$$-\Delta v(x) = 0 \text{ in } \Omega \tag{3.39}$$

$$v(x) = -u(x) \text{ on } \Gamma \tag{3.40}$$

$$|v(x)| = O(1) \text{ or } |x| \to \infty. \tag{3.41}$$

Next we introduce the integral single layer representation of the solution of the problem (3.39), (3.40) and (3.41) [G.C.Hsiao and W.L. Wendland, 1977], [Nedelec, 1977]

$$v(x) = \frac{-1}{2\pi} \int_\Gamma q(y) ln|x-y| \, \mathrm{d}\gamma(y) + c \tag{3.42}$$

where by Γ we have noted for simplicity the piecewise linear curve at step k, and the unknown function q is defined implicitly by the system (3.40), (3.42). The constant c must be chosen such that :

$$\int_\Gamma q(x) \, \mathrm{d}\gamma(x) = 0. \tag{3.43}$$

The system has been discretized using a finite element representation q^h of q. We introduce the basis $\{e_j\}_{j=1,\cdots,n}$ where $e_j(x)$ is piecewise constant on Γ and defined by :

$$e_j(x) = \begin{cases} 1 \text{ if } x \in [x_j, x_{j+1}] \\ 0 \text{ otherwise.} \end{cases} \tag{3.44}$$

Then, $q^h(x)$ is obtained as $q^h(x) = \sum_{j=1}^n \eta_j e_j(x)$ where $\{\eta_j\} \in \mathbb{R}^n$ is the solution of a discretized version of (3.40); (3.42), namely :

$$\begin{aligned} &\int_\Gamma e_i(x) \Big\{ \frac{1}{2\pi} \int_\Gamma q^h(y) ln|x-y| \, \mathrm{d}\gamma(y) \Big\} \, \mathrm{d}\gamma(x) + c \int_\Gamma e_i(x) \, \mathrm{d}\gamma(x) \\ &\qquad = \int_\Gamma e_i(x) v(x) \, \mathrm{d}\gamma(x), \qquad i = 1, \cdots, n. \end{aligned} \tag{3.45}$$

This is a $n \times n$ linear system with matrix $A = [A_{ij}]_{i,j=1,\cdots,n}$ where :

$$a_{ij} = \frac{1}{2\pi} \int_{\Gamma \times \Gamma} e_i(x) e_j(y) ln|x-y| \, \mathrm{d}\gamma(x) \, \mathrm{d}\gamma(y) \tag{3.46}$$

and

$$A\{\eta_i\} = \{b_i\} - c\{c_i\} \tag{3.47}$$

with

$$b_i = \int_\Gamma e_i(x) v(x) \, \mathrm{d}\gamma(x) \tag{3.48}$$

$$c_i = \int_{\Gamma_i} e_i(x) \, \mathrm{d}\gamma(x). \tag{3.49}$$

In fact we set $\{\eta_i\} = \{\eta_i^1\} + c\{\eta_i^2\}$ and we solve simultaneously

$$A\{\eta_i^1\} = \{b_i\} \text{ and } A\{\eta_i^2\} = \{c_i\}. \tag{3.50}$$

Once $\{\eta_i^1\}$ and $\{\eta_i^2\}$ are computed we evaluate c such that we have (3.43). Then

$$c = -\Big(\sum_{i=1}^{n} \int_\Gamma \eta_i^1 e_i(x)\,\mathrm{d}\gamma(x)\Big) \Big/ \Big(\sum_{i=1}^{n} \int_\Gamma \eta_i^2 e_i(x)\,\mathrm{d}\gamma\Big). \tag{3.51}$$

Once c is evaluated we can compute $\frac{\partial v}{\partial n}$ at every point in Γ, and in particular at quadrature nodes. For every $x \in \Gamma$ we have [Kress,1989] that :

$$\frac{\partial v(x)}{\partial n} = \frac{1}{2\pi} \int_\Gamma q^h(x) \frac{\partial}{\partial n}(ln|x-y|)\,\mathrm{d}\gamma(y) + \frac{1}{2}\, q^h(x) \tag{3.52}$$

and finally:

$$\frac{\partial \varphi}{\partial n} = \frac{\partial u}{\partial n} + \frac{\partial v}{\partial n}. \tag{3.53}$$

In the Newton method the computation of G'' needs $\varphi'(\theta)(\eta)$, (we note it φ') which in the discrete case is given by :

$$-\Delta\varphi' = 0 \text{ in } \Omega \tag{3.54}$$
$$\varphi' = -Z.\nabla\varphi \text{ on } \Gamma \tag{3.55}$$
$$|\varphi'(x)| = O(1) \text{ as } |x| \to \infty \tag{3.56}$$

where instead of W we have an approximation Z in the form $Z(x) = \sum_{i=1}^n u_i Z_i(x)$. Then we can compute an approximation of $\varphi' = \sum_{i=1}^n u_i \varphi_i'$ where φ_i' are the solutions of :

$$-\Delta\varphi_i' = 0 \text{ in } \omega \tag{3.57}$$
$$\varphi_i' = -Z_i\nabla\varphi \text{ on } \Gamma \tag{3.58}$$
$$|\varphi_i'(x)| = O(1) \text{ as } |x| \to \infty. \tag{3.59}$$

That means that we have to solve n exterior Dirichlet problems. In fact if we use the same numerical technique as in problem (3.39), (3.40) and (3.41), we obtain a linear system with the same matrix. As the LDL^t decomposition of this matrix is done, solving problem (3.57)(3.58) and (3.59) needs only n more solutions of a triangular system.

5. - Numerical Examples.

5.1 - Previous remarks, complexity.

Before making a numerical comparison between the two algorithms developed in the previous section we make some remarks.

In the case of the minimal perimeter problem we compute the second derivative of the discrete problem and then we consider two cases. In the first one when the directions of displacement are fixed we have an actual Newton method in a n-dimensional space and we reach a quadratic rate of convergence. In the second case, when changing the displacement directions we can have a better approximation of the continuous solution but we loose the quadratic rate of convergence.

When we apply Newton algorithm to the electromagnetic shaping problem we do not compute the second derivative of the Lagrangian but an approximation of it. Then we cannot have a quadratic rate of convergence. In the electromagnetic shaping problem we need to change the directions of local perturbations Z_i^k to reach a suitable approximation of the continuous solution.

To justify the use of a Newton method instead af a Quasi-Newton technique we give here an evaluation of the number of floating point operations(flops) needed for each iterations of both algorithms. In fact solving the state equations (3.39), (3.40) and (3.41) is the most important part of the computations. Computing the coefficients of the matrix A needs about $79n^2$ operations and $O(n^2)$ evaluations of the logarithmic function. The evaluation of the right hand side of the equation needs $O(n)$ flops.

The resolution of the linear system is done by a LDL^t decomposition, that means $O(\frac{n^3}{6})$ flops, and the resolution of the triangular system takes $O(\frac{n^2}{2})$ (flops), see [Golub,G.&Van Loan,Ch.F.,1983].

Once the solution of the state equation is known, the Quasi-Newton methods need $O(n^2)$ operations to compute an approximation of the Hessian matrix. Then the total number of operations is dominated by the numerical resolution of the state equation, more precily, if n is small, $n < 1000$, by the evaluation of the matrix of coefficients (3.46).

In the Newton method case we have to compute the Hessian matrix, that means n^2 evaluation of the second derivatives of E. The computation of coefficients $A_{i,j}(u_1^k, ..., u_n^k, \Lambda^k)$ of the Hessian imply the resolution of the state equation, as in the Quasi-Newton method, and the n extra exterior Dirichlet problems (3.57), (3.58) and (3.59).

In fact we use the same numerical technique as in state equation problem. Then the discretisation matrix A is the same, and also it's LDL^t decomposition. Then solving problem (3.57), (3.58) and (3.59) needs only n more solutions of a triangular system, that means $\frac{n^3}{2} + O(n^2)$ flops. The resolution of the Newton system (3.23) need $O(\frac{n^3}{3})$ flops. Then even in the Newton method case the number of operations is dominated by the evaluation of the coefficients of the matrix A if n is small. This is the key point that justifies the use of the Newton algorithm in our optimal shaping problem.

In conclusion each Newton iteration needs between 1.2 and 3. times more flops than a Quasi-Newton method iteration, 3 being the asymtotic limit when n tends to ∞. Obviously, the number of iterations needed is quite less.

5.2 - Numerical results.

First we study the case of the problem (3.7) and apply the Newton method described in the previous section. We consider the case of the unit circle of perimeter 2π. The initial point will be given by a piecewise perturbation of a circle of radius $1+\delta$. In Table 1 we present the results considering the domains with 128 nodes and using fixed displacement directions. We follow the evolution of $||G''||_2$ - the euclidean norm of the gradient, $||\theta^k - \theta^\star||_\infty$ - the distance between the approximation θ^k and the exact solution $\theta^\star$ (which is a circle), $||\theta^k - \tilde{\theta}^\star||_\infty$ - the distance between the θ^k and $\tilde{\theta}^\star$ (the solution in the set of polygons with 128 nodes) the area and difference of perimeters.

The error $||\theta^k - \theta^\star||_\infty$ and $|2\pi - \int_{\Gamma^k}|$ are almost-constant at the last iterations. This can be explained by the fact that θ^k converges to a polygon of 128 vertices and surface π and not to the unit circle. In this exemple we observe a quadratic rate of convergence of $||G'||_2$ to zero.

k	$\|2\pi - \int_{\Gamma^k}\|$	Surface	$\|\|G'\|\|_2$	$\|\|\theta^k - \theta^*\|\|_\infty$	$\|\|\theta^k - \tilde{\theta}^*\|\|_\infty$
1	0.1309E+00	2.998795359	0.2501E+00	0.50540E-01	0.5074E-01
2	0.2506E-02	3.143452027	0.7138E-02	0.10612E-02	0.8607E-03
3	0.6396E-03	3.141593681	0.7410E-05	0.21037E-03	0.4475E-06
4	0.6385E-03	3.141592653	0.5656E-11	0.21024E-03	0.4479E-12

Table 1: Newton method for minimization of the perimeter.

In Table 2 we consider the same problem but with evolutive displacement directions. In that case we observe a superlinear rate of convergence.

k	$\|2\pi - \int_{\Gamma^k}\|$	Surface	$\|\|G'\|\|_2$	$\|\|\theta^k - \theta^*\|\|_\infty$	$\|\|\theta^k - \tilde{\theta}^*\|\|_\infty$
1	0.13092E+00	2.9987953594	0.25012E+00	0.5054015E-01	0.50750E-01
2	0.25066E-02	3.1434520276	0.71597E-02	0.1061238E-02	0.86074E-03
3	0.63948E-03	3.1415935617	0.36902E-05	0.2105689E-03	0.39173E-06
4	0.63857E-03	3.1415926535	0.10649E-09	0.2105396E-03	0.31053E-10
5	0.63857E-03	3.1415926535	0.18185E-13	0.2105396E-03	0.65973E-13

Table 2: Newton method for minimization of the perimeter with variable displacement directions.

Now we apply both algorithms to the electromagnetic casting problem. In each case the surface tension σ and the surface of the liquid S_0 are given as well as the distribution of the current j_0 which is of the form:

$$j_0 = (\sum_{p=1}^{m} \alpha_p \delta_{x_p}) I \tag{5.1}$$

where I is a given intensity, $(\delta_{x_p})_{p=1\ldots n}$ are the Dirac masses at the points $(x_p)_{p=1\ldots m}$ in the plane and $(\alpha_p)_{p=1\ldots m}$ are coefficients which are indicated on the figures. Computations are made with the normalized cost functional:

$$\int_{\partial\Omega} |\nabla\widehat{\varphi}|^2 + \widehat{\sigma}P(\Omega) + \Lambda(m(\omega) - S_0) \tag{5.2}$$

for Newton method and :

$$\int_{\partial\Omega} |\nabla\widehat{\varphi}|^2 + \widehat{\sigma}P(\Omega) + r(m(\omega) - S_0)^2 \tag{5.2'}$$

for Quasi-Newton method, where $\widehat{\sigma} = 2\sigma/\mu_0 I^2$ and $\widehat{\varphi} = \varphi/\mu_0 I$.

We are going to present two cases of shaping examples. For the first example the number of nodes is 128, the number of masses is 4 and the prescribed surface S_0 is equal to π (see figure 1). The Table 3 allows to follow the evolution of the gradient of the cost function of intermediate domains computed with Newton algorithm and evolutive field displacement.

k	$\|\|\theta^k - \tilde{\theta}^*\|\|_\infty$	$\|\|G'\|\|_2$	Surface
1	0.2492771331769E+00	0.1419587660467E-02	3.14159265358979
2	0.5230303034182E-01	0.4395608328578E-01	3.18526797866267
3	0.5560099242130E-02	0.3375751466907E-02	3.14493039668217
4	0.1587645632387E-03	0.1772365599787E-04	3.14160885828425
5	0.2064952042143E-05	0.5100510205590E-07	3.14159266262547
6	0.8080172936524E-07	0.1343098030108E-08	3.14159265359339
7	0.2748245014916E-08	0.4468236354564E-10	3.14159265358981
8	0.9057617071558E-10	0.1548500725202E-11	3.14159265358979
9	0.2993352846718E-11	0.5740707232603E-13	3.14159265358979
10	0.1001025103677E-12	0.2573586822187E-14	3.14159265358979

Table 3

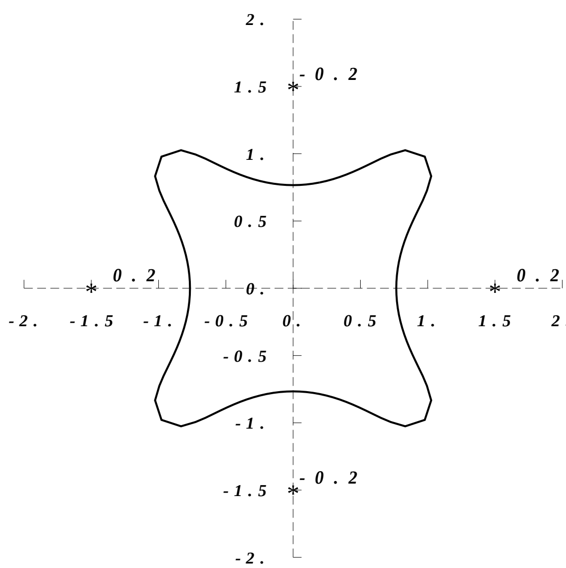

Figure 1.

In Table 4 we compare results computed with Newton and Quasi-Newton method for different values of $\hat{\sigma}$.

In the second exemple the number of nodes is 128, the number of masses is 12 and the prescribed surface S_0 is 4. The Table 5 gives the number of iterations of Newton and Quasi-Newton methods for different values of $\widehat{\sigma}$.

$\hat{\sigma}$	Newton error	Newton iterations	Surface	Q-Newton iterations
0.0003	6.2455802D-10	4	3.14159255	153
0.0002	7.9976834D-08	7	3.14159263	167
0.0001	1.1212912D-11	14	3.14159256	201

Table 4

$\hat{\sigma}$	Newton error	Newton iterations	Surface	Q-Newton iterations
0.05	0.134877E-06	5	4.0000001342	56
0.03	0.644887E-05	7	4.0000064433	73
0.01	0.713674E-08	10	4.0000000061	102
0.0075	0.740979E-07	12	4.0000000693	132
0.005	0.547113E-11	16	4.0000000000	148

Table 5

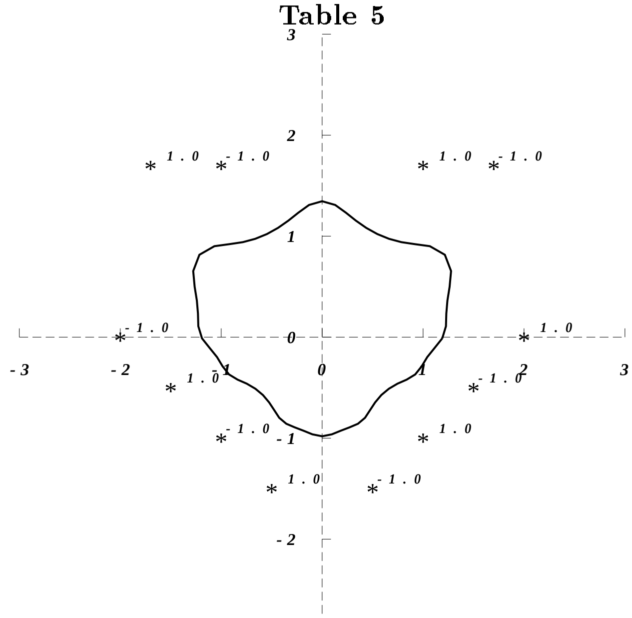

Figure 2.

Both electromagnetic shaping examples show the efficiency of the Newton method. As the cost of each Newton iteration is only between 1.2 and 3 times Quasi-Newton iteration cost, the use of Newton method is then clearly justified in electromagnetic casting problems.

Applications of the same technique in three dimensional electromagnetic casting problem is in progress. The difficultys in the 3-d case is that the state problem is now a Neumann exterior problem. The computation of the second order derivatives of the solution of the state equation solution need in that case the computation of singular integrals.

Acknowledgement. The authors are grateful to Prof. M. Pierre for helpful comments and inspiring discussions.

REFERENCES

BESSON O., BOURGEOIS J., CHEVALIER P.A, RAPPAZ J., TOUZANI R., 1991, Numerical modelling of electromagnetic casting processes, *Journal of Computational Physics* 92, n∘ 2, pp 482-507.

BRANCHER J.-P., ETAY J., SERO-GUILLAUME O., 1983, Formage d'une lame, *J. de Mécanique Théorique et Appliquée*, **2**, n° 6, 976–989.

BRANCHER J.-P., SERO-GUILLAUME O., 1983, Sur l'équilibre des liquides magnétiques, applications à la magnétostatique, *J. de Mécanique Théorique et Appliquée*, **2**, n° 2, 265–283.

COULAUD O., HENROT A., 1994, Numerical approximation of a free boundary problem arising in electromagnetic shape, *SIAM J. Numer. Anal.* 31, 4, pp. 1109-1127.

DELFOUR M.C., ZOLESIO J.P., 1991, Velocity method and lagrangian formulation for the computation of the shape Hessian, SIAM Control and Optimization , Vol 29, N. 6, pp. 1414-1442.

DESCLOUX J., 1990, On the two dimensional magnetic shaping problem without surface tension, Report n° 07. 90, Ecole Polytechnique Fédérale de Lausanne, Suisse.

ETAY J., 1982, Le formage électromagnétique des métaux liquides. Aspects expérimentaux et théoriques, Thèse Docteur-Ingénieur, U.S.M.G., I.N.P.G. Grenoble, France.

ETAY J., MESTEL A.J., MOFFATT H.K., 1988, Deflection of a stream of liquid metal by means of an alternating magnetic field, *J. Fluid Mech.*, **194**, 309–331.

GAGNOUD A., ETAY J., GARNIER M., 1986, Le problème de frontière libre en lévitation électromagnétique. *J de Mécanique Théorique et Appliquée*, **5**, n° 6, 911–925.

GAGNOUD A., SERO-GUILLAUME O., 1986, Le creuset froid de lévitation : modélisation électromagnétique et application. E.D.F. Bull. Etudes et Recherches, Série B; **1**, 41–51.

GOLUB G.,VAN LOAN Ch., 1983, Matrix Computations, The Johns Hopkins University Press.

GOTO Y,FUJII N., 1990, Second order numerical method for domain optimization problems,*Journal of Optimization Theory and Applications*, Vol. 67, pp. 533-550.

GRISVARD P., 1985, Elliptic problems in non smooth domains, Monograph and Studies in Math., **24**, Pitman.

HENROT A., PIERRE M., 1989, Un problème inverse en formage de métaux liquides,M^2AN,**23**, pp. 155–177.

HESTENES M., 1980, Conjugate Direction Methods in Optimization, Springer-Verlag , New York,USA.

HSIAO G.C., WENDLAND W.L., 1977, A finite element method for some integral equations of the first kind, *Journal of Mathematical Analysis and Applications* 58, 449-481.

KRESS R. 1989, Linear Integral Equations, *Springer-Verlag, 1989*

LI B.Q., EVANS J.W., 1989, Computation of shapes of electromagnetically supported menisci in electromagnetic casters. Part. I : Calculations in the two dimensions. *IEEE Trans. Magnetics*, **25**, n° 6, 4442.

MESTEL A.J., 1982, Magnetic levitation of liquid metals, *J. of Fluid Mech.* **117**, 27–43.

MINOUX M., 1983, Programmation mathématique ; théorie et algorithmes, tome 1, Dunod, 95–126.

MURAT F., SIMON J., 1976, Sur le contrôle par un domaine qéométrique, Rapport du Laboratoire d'Analyse Numérique, Université Paris VI.

NEDELEC J.C., 1977, Approximation des équations intégrales en mécanique et en physique, Rapport, Centre de Mathématiques Appliquées, Ecole Polytechnique, Palaiseau, France.

PIERRE M., ROCHE J.-R., 1990, Numerical computation of free boundaries in 2-d electromagnetic shaping, Rapport de Recherches, Institut National de Recherches en Informatique et en Automatique, France.

PIERRE M., ROCHE J.-R., 1993, Numerical simulation of tridimensional electromagnetic shaping of liquid metals, *Numer. Math.* 65, 203-217(1993).

SHERCLIFF J.A., 1981, Magnetic shaping of molten metal columns, *Proc. Royal. Soc. Lond.* **A 375**, 455–473.

SNEYD A.D., MOFFATT H.K., 1982, Fluid dynamical aspects of the levitation melting process, *J. of Fluid Mech.* , **117**, 45–70.

SERO-GUILLAUME O., 1983, Sur l'équilibre des ferrofluides et des métaux liquides, thèse, Institut Polytechnique de Lorraine, Nancy, France.

SIMON J., 1988, Optimum design for Neumann condition and for related boundary value conditions, *Boundary control and boundary variations*, Lecture Notes in Calcul and Informatics Sciences $n°100$, Springer Verlag.

SOKOLOWSKI J., ZOLESIO J.P.,1992 , Introduction to Shape Optimization, Shape Sensitivity Analysis, Springer-Verlag ,Berlin Heildelberg.

ZOLESIO J.P., 1984, Numerical algorithm and existence result for a Bernoulli-like problem steady free boundary problem, *Large Scale Systems, Th. & Appl.* **6**, n° 3, 263–278.

ZOLESIO J.P., 1990, Introduction to shape optimisation problems and free boundary problems, Séminaire de Mathématiques Supérieures, Université de Montréal, Montréal, Canada.