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METODY NEWTONOWSKIE I QUASI-NEWTONOWSKIE W
OBLICZENIACH NUMERYCZNYCH POWIERZCHNI SWOBODNYCH
PRZY KSZTAŁTOWANIU ELEKTROMAGNETYCZNYM METALI
CIEKŁYCH

Streszczenie. Przedstawiono zastosowanie metody Newtona do obliczenia powierzchni swobodnych przy kształtowaniu elektromagnetycznym metali ciekłych i porównano ją z algorytmami quasi-newtonowskimi wprowadzonymi w pozycji [Roche i Pierr, 1991, 93]. W obydwu przypadkach kształt optymalny jest punktem krytycznym odpowiedniej energii. Każdy krok algorytmu wymaga rozwiązania dwóch eliptycznych problemów brzegowych, które sformułowano w postaci całkowej.

NEWTON AND QUASI-NEWTON METHODS IN NUMERICAL
COMPUTATION OF FREE SURFACES IN THE ELECTROMAGNETIC
SHAPING OF LIQUID METALS

Summary. We describe the Newton method to compute free surfaces in electromagnetic shaping of liquid metals and we compare it to Quasi-Newton algorithms implemented in [Roche & Pierre, 1991,93]. In both cases the optimal shape is a critical point of an appropriate energy. Each step of the algorithm requires solving two exterior elliptic boundary value problems. This is done by using an integral representation of solutions on these surfaces.

NEWTONSCHE UND QUASI-NEWTONSCHE METHODEN IN
NUMERISCHEN BERECHNUNGEN DER FREIEN OBERLÄCHEN BEI
ELEKTROMAGNETISCHER FORMUNG DER SCHMELZEN

Zusammenfassung. Wir beschreiben die Newtonsche Methode für die Berechnung der freien Oberflächen bei elektromagnetischer Formung der Schmelzen und vergleichen sie mit der Quasi-Newtonschen Algorithmus, der in [Roche, Pierre, 1991, 93] eingeführt ist. In beiden Fällen ist die optimale Form der Kritische Punkt der entsprechenden Energie. Die unbekannte Oberfläche wird durch teilweise lineare endliche Elemente dargestellt. Jeder Schritt das Algorithmus verlangt die Lösung von zwei äußeren Problemen der elliptischen Randwertes. Dies wird unter Verwendung der Integraldarstellung von Lösungen auf diesen Oberflächen durchgeführt.

1. INTRODUCTION

In several engineering processes the possibility of shaping surfaces of molten metal by electromagnetic forces can be studied, see [Sero-Guillaume,1983]. One point of view is to consider models where the computation of the free boundary amounts to solve a shape optimization problem where the functional to be minimized is the total energy of the phenomenon under consideration.

Our interest is to develop numerical algorithms to compute the free surface for an electromagnetic shaping problem by optimization methods. Significant examples are:

- In two- dimensions: determine the stationary section of a vertical column of liquid metals falling down in an electromagnetic field.

- In three-dimensions: determine the form of a bubble of liquid metal levitating under the action of a magnetic field.

Under convenient assumptions, the equilibrium configurations are described by a set of equations containing an equilibrium relation at the boundary between electromagnetic, gravitational and superficial tension forces. It involves, in particular, the mean curvature of the boundary.

This equilibrium is shown to be a stationary state of the total energy under the constraint that the volume (or the surface of the section in 2-d) is prescribed.

Our purpose is to describe and to compare the performances of Quasi-Newton and Newton algorithms to compute the free boundary Γ . Here the domain is unknown, then first and second derivatives of the shape functional in the form of energy must be computed with respect to the geometrical domain, [Zolesio,86], [Zolesio & Delfour,1991], [Sokolowski & Zolesio,1992] and [Goto & Fujii,1990].

This is the main difficulty in the algorithm since it requires solving two elliptic boundary value problems in an exterior domain at each iteration. This is done using an integral representation of the solution and solving an integral equation by boundary Galerkin method. This is possible since only knowledge of the solution and its derivatives at the boundary is necessary on the algorithm, [Pierre & Roche,91,93], [Novruzi & Roche,1993]. Numerical computations of shapes in particular situations and with different methods can also be found in [Shercliff,1981], [Gagnoud & Sero-Guillaume, 1986], [Coulaud & Henrot, 1990], [Etay,1982], and [Li & Evans, 1989].

2. PROBLEM FORMULATION

The 2-dimensional model concerns the case of a vertical column of liquid metal falling down in an electromagnetic field created 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 and the electromagnetic forces are reduced to the magnetic pressure acting on the interface.

We assume that a stationary horizontal section is reached so that the following simple 2-dimensional model is valid. We denote by Ω the exterior in the plane of the closed and simply connected domain Ω^c occupied by the metal. We deal with the mean square values of the relevant quantities: $\vec{j}_0 = (0, 0, j_0)$ denotes the density current vector, $\vec{B} = (B_1, B_2, 0)$ is the total magnetic field. We have the following system of equilibrium.

$$\nabla \wedge \vec{B} = \mu_0 \vec{j}_0 \text{ in } \Omega, \tag{1}$$

$$\nabla \cdot \vec{B} = 0 \text{ in } \Omega, \tag{2}$$

$$\vec{B} \cdot \vec{n} = 0 \text{ on } \Gamma = \partial\Omega^c, \tag{3}$$

$$|\vec{B}|^2 / 2\mu_0 + \sigma\mathcal{C} = \text{constant on } \Gamma, \tag{4}$$

$$|\vec{B}| = O(|x|^{-2}) \text{ as } |x| \rightarrow \infty \text{ in } \Omega, \tag{5}$$

where μ_0 is the vacuum permeability, \vec{n} the unit normal vector to the boundary Γ , \mathcal{C} the curvature of Γ (seen from the metal), σ the surface tension of the liquid and $|\cdot|$ denotes the euclidian norm. The constant in (4) and the boundary Γ are the unknowns of the problem.

This problem or very similar ones have been considered in several places in the literature. We refer the reader to the following papers and to references given there for the physical analysis of the simplifying assumptions used to justify the model: see [Shercloff, 1981], [Sero-Guillaume, 1983], [Brancher & Sero-Guillaume, 1983], [Sneyd & Moffatt, 1982], [Brancher et al. 1983], [Gagnoud et al. 1986], [Mestel, 1982], [Etay et al., 1988].

According to (2), (3), there exist $\varphi : \Omega \rightarrow \mathbf{R}$ such that

$$\frac{1}{2\mu_0} \vec{B} = (\varphi_y, -\varphi_x, 0). \tag{6}$$

By (3) φ is constant on $\Gamma = \partial\Omega$. φ can be chosen to be zero on Γ . Then the system (1)-(5) can be rewritten

$$-\Delta\varphi = \mu_0 j_0 \text{ in } \Omega, \tag{7}$$

$$\varphi = 0 \text{ on } \Gamma, \tag{8}$$

$$\frac{1}{2} |\nabla\varphi|^2 + \tau\mathcal{C} = P \text{ on } \Gamma, \tag{9}$$

with $\tau = \sigma/\mu_0$ and P is an unknown constant. If there is no current at infinity and \vec{j}_0 is compactly supported, we can add the condition following:

$$\varphi(x) = O(|x|^{-1}) \text{ as } |x| \rightarrow \infty. \tag{10}$$

The total energy can be written in terms of φ and Ω .

$$E(\Omega) = -\frac{1}{2\mu_0} \int_{\Omega} |\nabla\varphi|^2 + \sigma P(\Omega^c), \tag{11}$$

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

$$P(\Omega) = \int_{\partial\Omega^c} d\Gamma, \quad d\Gamma = \text{length measure on } \Gamma = \partial\Omega^c$$

and φ is solution of (7), (8), (10). The variational formulation of (1)-(5) consists in considering the equilibrium domain Ω as a stationary point for the functional (11), where Ω is the variable, under the constraint that $meas(\Omega^c)$ is given.

The relation (9) is similar to the Bernoulli conditions for potentials which is studied in hydrodynamic problems. It is classical that it correspond to a variational formulation likes (11).

3. VARIATIONAL FORMULATION

Let Ω be the complement of a compact subset of \mathbf{R}^2 and let $V \in C_c^2(\mathbf{R}^2; \mathbf{R}^2)$. We consider the transformation of \mathbf{R}^2 given by:

$$\forall x \in \mathbf{R}^2, \forall t \in [0, \tau], \tau > 0 \quad T_t^V(x) = x + tV(x) \tag{12}$$

Then we note $\Omega_t = T_t^V(\Omega)$ and we verify that $\Gamma_t = T_t^V(\Gamma) = T_t^V(\partial\Omega)$ for t small enough (since $D_x T_t^V = I + tD_x V(x)$ we can use the local inversion theorem).

Proposition 1 Let j_0 be a square integrable function Ω with compact support in Ω . Then for t small enough there exists $\varphi(\cdot, t)$, unique solution of:

$$-\Delta_x \varphi(x, t) = \mu_0 j_0 \quad \text{in } \Omega_t, \tag{13}$$

$$\varphi(x, t) = 0 \quad \text{on } \partial\Omega_t, \tag{14}$$

$$\varphi(x) = O(|x|^{-1}) \text{ as } |x| \rightarrow \infty. \tag{15}$$

Moreover, if $P_0 \in \mathbf{R}$ and

$$E(\Omega_t) = -\frac{1}{2\mu_0} \int_{\Omega_t} |\nabla \varphi|^2 dx + \sigma P(\Omega_t^c) - P_0 m(\Omega_t^c), \tag{16}$$

where $P(\Omega_t)$ and $m(\Omega_t)$ are the perimeter and the measure of Ω_t , then for any $V \in C_c^2(\mathbf{R}^2; \mathbf{R}^2)$ there exists $E'(\Omega; V)$ defined as follows:

$$E'(\Omega; V) = \lim_{t \rightarrow 0^+} (E(T_t^V(\Omega)) - E(\Omega))/t \tag{17}$$

of the form:

$$E'(\Omega; V) = \int_{\partial\Omega} \left(\frac{1}{2\mu_0} |\nabla \varphi|^2 + \sigma \mathcal{C} - P_0 \right) (V \bullet \vec{n}) d\partial\Omega, \tag{18}$$

where \vec{n} is the unit normal vector in $\partial\Omega$ oriented towards Ω and \mathcal{C} is the curvature of $\partial\Omega$ defined as:

$$\mathcal{C} = \vec{s} \bullet \frac{\partial \vec{n}}{\partial s} \tag{19}$$

where $\frac{\partial}{\partial s}$ is the partial derivative in $\partial\Omega$ relative to the length and \vec{s} is the unitary tangential vector such that the pair (\vec{s}, \vec{n}) is right•

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

According to (18) the variational formulation of the continuous problem (1)-(5) consists in finding a (Ω, P_0) such that:

$$E'(\Omega; V) = 0, \quad \forall V \in C_c^2(\mathbf{R}^2; \mathbf{R}^2). \tag{20}$$

Note that computing of this derivative for a given Ω requires to solve an exterior boundary value problem.

To realize a Newton method we need to compute the second derivative with respect to transformations like (12).

Theorem 2 Let us make the same assumptions as in the Proposition 1. Moreover, let be $W(x) \in C^2(\mathbf{R}^2; \mathbf{R}^2)$ and φ'_W the solution of the following problem:

$$-\Delta \varphi'_W = 0 \quad \text{in } \Omega, \tag{21}$$

$$\varphi'_W = -W \nabla \phi \quad \text{on } \partial \Omega. \tag{22}$$

If $d^2E(\Omega; V, W)$ is defined as in [Delfour, Zolesio, 1991] we introduce:

$$E''(\Omega; V, W) = d^2E(\Omega; V, W) - E'(\Omega; [DV]W), \tag{23}$$

where [DV] is the Jacobian matrix of V.

Then:

$$E''(\Omega; V; W) = \frac{1}{\mu_0} \int_{\partial \Omega} \{ (V \bullet \bar{n}) (\nabla \varphi \bullet \nabla \varphi'_W) + (W \bullet \nabla^2 \varphi) \bullet \nabla \varphi + \tag{24}$$

$$-\frac{1}{2} (V \bullet \frac{\partial W^r}{\partial s}) |\nabla \varphi|^2 \} + \sigma \int_{\partial \Omega} (\frac{\partial V}{\partial s} \bullet \bar{n}) (\frac{\partial W}{\partial s} \bullet \bar{n}) + P_0 \int_{\partial \Omega} (V \bullet \frac{\partial W^r}{\partial s})$$

where \bar{n}, \bar{s} are the unitary normal and tangent vector and $W^r = (W_2, -W_1) \bullet$

The second derivative E'' defined in this manner, is symmetric for any V, W in $C_c^2(\mathbf{R}^2; \mathbf{R}^2)$. It depends only on the values of V, W at the boundary of the domain and one can use a Newton method for finding the zeros of E' . For more details in this subject and a complete proof of Theorem 2, see [Novruzı & Roche, 1993].

Remark Computing first derivative with respect to the domain is classical in the literature. Definitions and results can be found in [Zolesio, 1984], [Descloux, 1990], [Sokolowski & Zolesio, 1992]. The second derivative problem is highly non trivial and its computation is not obvious, see for example [Delfour & Zolesio, 1991], [Pierre & Henrot, 1989], [Goto & Fujii, 1990] and [Novruzı & Roche, 1993].

4. THE NUMERICAL METHOD

4.1. The Newton algorithm

The algorithm for the continuous problem consists in constructing a sequence $(\varphi^k, \psi^k, W^k, \Omega^k)$ where:

- φ^k is the solution of (13)-(15) in Ω^{k-1}
- ψ^k is the solution of (21)-(22) in Ω^{k-1}
- W^k and Ω^k are defined by the following equations:

$$E'(\Omega^{k-1}; V) + E''(\Omega^{k-1}; V, W^k) = 0, \quad \forall V \in C_c^2(\mathbf{R}^2; \mathbf{R}^2), \tag{25}$$

$$\Omega^k = (I + W^k)(\Omega^{k-1}), \tag{26}$$

where I is the identity on \mathbf{R}^2 and Ω^0 is a given initial domain.

We consider an approximate version of the continuous Newton algorithm which consists in constructing the sequence $(\varphi^k, \psi^k, W^k, \Omega^k)$ defined by:

- φ^k is an approximation of φ , solution of:

$$-\Delta\varphi = \mu_0 j_0 \quad \text{in } \Omega^{k-1}, \tag{27}$$

$$\varphi = 0 \quad \text{on } \partial\Omega^{k-1}, \tag{28}$$

- ψ^k is an approximation of ψ , solution of:

$$-\Delta\psi = 0 \quad \text{in } \Omega^{k-1}, \tag{29}$$

$$\psi = -W^k \nabla\varphi \quad \text{on } \partial\Omega^{k-1}, \tag{30}$$

- $W^k = \sum_{i=1}^N w_i Z_i$, a piecewise linear Jordan curve, Ω^k are defined by:

$$E'(\Omega^{k-1}; V) + E''(\Omega^{k-1}; V, W^k) = 0, \quad \forall V = \sum_{i=1}^N v_i Z_i, \tag{31}$$

$$\Omega^k = (I + W^k)(\Omega^{k-1}), \tag{32}$$

where Ω^0 is given such that $\partial\Omega^0$ be a piecewise closed Jordan curve.

In the discretized version, instead of functional E , we have applied the Newton method for the penalized functional E_μ given by:

$$\Omega \rightarrow E_\mu(\Omega) = -\frac{1}{2\mu_0} \int_{\partial\Omega} |\nabla\varphi|^2 + \sigma P(\Omega) + \mu(m(\Omega) - S_0)^2, \tag{33}$$

where S_0 is a given area and μ is a positive real number large enough so that Ω satisfies the constraint: $m(\Omega) = S_0$ as well as possible.

4.2. The Quasi-Newton algorithm

We recall here the method used in [Pierre & Roche,1991,1993], namely the B.F.G.S, (Broyden, Fletcher, Goldfarb and Shano), Quasi-Newton technique which requires only the gradient of the cost functional (33), see [Minoux,1983]. Then now we compute a sequence $(\Gamma^k, \varphi^k, V^k)$ defined as in section (4.1). At each iteration we update the nodes of the boundary Γ^k in such a way that $\Gamma^{k+1} = (I + V^k)(\Gamma^k)$ where $(V^k = \sum_{i=1}^N v_i Z_i)$. The parameters v_i are computed in the following way:

$$v_i = -\rho_k H^k E'_\mu(\Omega^k), \tag{34}$$

where H^k is an approximation of the Hessian E'' , computed by the BFGS method.

The parameter $\rho_k \in]0, 1]$ and it must be computed by a line search method. In fact we can not evaluate the energy E'_μ at each iteration; then we take a arbitrary choise of ρ_k , but it becomes equal to one very quickly, see [Hestenes,1980].

To compare Quasi-Newton method performances with Newton one's, we can examine two characteristics: first,the rate of convergence and second,the total number of floating point operations.

Theorically the Newton method, when convergen, converges at a quadratic rate. For the B.F.G.S method the rate is superlinear. In fact, practice in our problem shows that the performance of both methods are perturbed by the fact that we compute only the approximate solutions of the exterior (27),(28) problem and the (29),(30) problem. Then we compute only an approximation of the gradient and Hessian of the cost function. But when the Newton's method converges, the rate of convergence is greater than this B.F.G.S's method.

About the number of floating point operations, solving the state equation is the most important part of the calculations .Each coefficient of the matrix associate to the discretized state problem is a double integral.This that means a total number of $O(kn^2)$ floating point operations with k greater than n if n is small.The resolution of the linear system is done by Cholesky decomposition, that is about $O(n^3/6)$. Once the solution of the state equation is known, the Quasi-Newton method needs $O(n^2)$ 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.

In the Newton method we have to compute the inverse of the Hessian matrix, that means n^2 evaluations of the second derivative of E_μ and we also have to solve numerically the problem (29),(30). In fact the matrix associated to the numerical solution of problem (29),(30) is the same as the matrix associated to the approximation of the state equation.Then the matrix and the Cholesky decomposition are computed only one time by iteration as in the Quasi-Newton method.

In conclusion we have verified that in practice we have twice as many operations for the Newton method than for the Quasi-Newton method.

4.3. Numerical example

We present here some examples computed with algorithms described in the previous section. In each case the surface tension σ and the surface S_0 of the liquid are given as well as the distribution of the current j_0 which is of the form:

$$j_0 = \left(\sum_{p=1}^m \alpha_p \delta_{x_p} \right) I, \tag{35}$$

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

$$\int_{\partial\Omega} |\nabla\widehat{\varphi}|^2 + \tau P(\Omega) + \mu(m(\Omega) - S_0)^2, \tag{36}$$

where $\tau = 2\sigma/\mu I^2$ and $\widehat{\varphi} = \varphi/\mu I$.

We are going to present two cases of shaping exemples. For the first example the number of nodes is 128, the number of masses is 4 and the prescribed surface S_0 is equivalent to π . The Table 1 allows to compare results computed with Newton and Quasi-Newton method for different values of τ .

Table 1

τ	Newton iterations	Q-Newton iterations
$3 \cdot 10^{-4}$	7	120
$2 \cdot 10^{-4}$	12	159
$1.8 \cdot 10^{-4}$	13	161
$1.4 \cdot 10^{-4}$	20	165
$1.13 \cdot 10^{-4}$	25	198

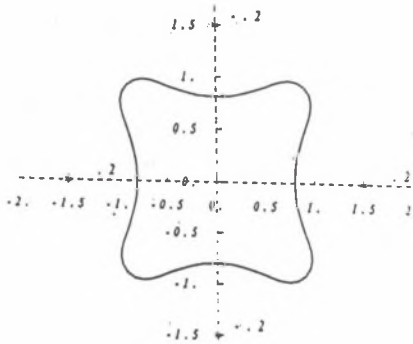


Fig. 1.
Rys. 1.

In the second example the number of nodes is 128, the number of masses is 12 and the prescribed surface S_0 is 4. The Table 2 gives the number of iterations of Newton and Quasi-Newton methods for different values of τ .

Table 2

τ	Newton iterations	Q-Newton iterations
$5.0 \cdot 10^{-2}$	7	72
$3.0 \cdot 10^{-2}$	9	95
$0.5 \cdot 10^{-2}$	14	163
$0.2 \cdot 10^{-2}$	18	196
$0.1 \cdot 10^{-2}$	20	228

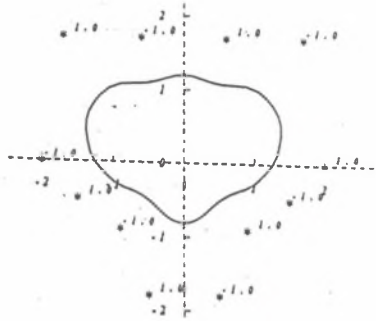


Fig. 2.
Rys. 2.

The two examples show the advantages of the Newton method. One explanation is that in the Quasi-Newton method we should solve a problem of line search to obtain good ρ_k results. In our case it would be too costly since it would require the evaluation of the total energy at each iteration.

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Streszczenie

W pracy przedstawiono zastosowanie algorytmów numerycznych optymalizacji do obliczania kształtu powierzchni swobodnej ciekłego metalu. Stan równowagi opisano układem równań przedstawiających równowagę między siłami grawitacyjnymi, elektromagnetycznymi i siłami powierzchniowymi na brzegu. Wykazano, że stan równowagi równoważny jest punktowi stacjonarnemu całkowitej energii przy ograniczeniu nałożonym na objętość. Tak sformułowane zadanie rozwiązano za pomocą metody Newtona i quasi-Newtona. W każdej iteracji pierwszą i drugą pochodną funkcjonalu energii obliczono rozwiązując dwa eliptyczne zagadnienie brzegowe. Zagadnienie sprowadzono do postaci całkowitej rozwiązując równanie całkowite metodą Galerkiną. Wskazano na zalety i wady metody Newtona i quasi-Newtona w rozważanym zagadnieniu.