HAL
archives-ouvertes.fr

Adaptative Newton-like Method for Shape Optimization

Jean Rodolphe Roche

▶ **To cite this version:**

Jean Rodolphe Roche. Adaptative Newton-like Method for Shape Optimization. Control and Cybernetics, Polish Academy of Sciences, 2005, 34, pp.363-377. <hal-00095219>

HAL Id: hal-00095219

https://hal.archives-ouvertes.fr/hal-00095219

Submitted on 15 Sep 2006

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Adaptive Newton-like Method for Shape Optimization

Jean R. Roche

Laboratoire de Mathématiques (IECN) Université Henri Poincaré(Nancy I)
B.P. 238, 54506 Vandoeuvre lès Nancy Cédex, France,
e-mail: roche@iecn.u-nancy.fr

Summary The aim of this work is to introduce an adaptive strategy to monitor the rate of convergence of a Newton-like method in numerical shape optimization.

Such superlinear iterative algorithm are often computationally intensive and the rate of convergence depends on how accurate the numerical solution of the state equation is.

The model concerns a cost function depending on the unknown domain Ω, and the solution of an integral equation.

Key words Shape Optimization, Newton-like algorithm, a posteriori error, adaptability

1 Introduction

Shape optimization problems are characterized by a cost function and a partial differential equation (P.D.E.), the state equation, both depending on the geometrical domain.

Typically we want to compute a shape Ω^* such that

$$\Omega^* = \text{argmin}\{F(\Omega, \varphi_\Omega) : \Omega \in \mathcal{O}\} \tag{1}$$

The set of admissible domains $\mathcal{O}$ is characterized by geometrical and regularity constraints. For analytical calculus we consider domains of class $\mathcal{C}^2$.

The scalar potential φ_Ω is the solution in a Sobolev space $\mathcal{H}$ of an elliptic problem:

$$a(\varphi_\Omega, \psi) = (f, \psi) \quad \forall \psi \in \mathcal{H} \tag{2}$$

The function $F(\Omega, \varphi_\Omega) : \mathcal{O} \times \mathcal{H} \rightarrow I\!R$ is the cost function.

Numerical solution of this problem involves numerical representation of the domain, optimization methods and numerical solution of partial differential equations.

In the discretized finite dimensional shape optimization problem we consider an open and bounded domain $\Omega(u) \subset I\!R^m$ with boundary $\partial\Omega(u)$ parametrized by a function $u \in \mathcal{U}_{ad}$, usually a piecewise linear discretization of the $\Omega(u)$ boundary.

We are interested in solving the following problem, find $u^* \in \mathcal{U}_{ad}$ such that:

$$j(u^*) \leq j(u) \quad \forall\, u \in \mathcal{U}_{ad} \tag{3}$$

where $j(u) = F(\Omega(u), \varphi_{\Omega(u)})$ and $\varphi_{\Omega(u)}$ is the solution of the state equation (2) in the domain parametrized by u.

Clearly the solution of the discrete problem must be a good approximation of the continuous problem solution, that means a domain discretization adapted to the topological characteristic of the continuous solution and changing during the optimization procedure.

To obtain a superlinear rate of convergence of the shape optimization procedure we introduce Newton-like methods. As it is well known the rate of convergence depends on how accurate is the numerical solution of the state equation, see [2], [3] and [4]. More precisely let us denote e_n the error at iteration n in the optimization procedure, then in an appropriate norm we obtain:

$$||e_{n+1}|| \leq C_1(||e_n||^2 + \Delta_n||e_n|| + E_n) \tag{4}$$

The terms E_n and Δ_n are related to errors in approximation of the cost function j shape gradient and shape Hessian.

If φ_h is the numerical solution of the state problem (2) the term E_n is related to the error $||\varphi_{\Omega(u)} - \varphi_h||_{L^2}$. Thanks to a local a posteriori estimation of $||\varphi_{\Omega(u)} - \varphi_h||_{L^2}$ an adaptive algorithm to obtain mesh refinements of $\partial\Omega(u)$ is derived in order to have superlinear rate of convergence of the shape optimization Newton-like method.

The model problem concerns a cost function depending on the perimeter of $\Omega(u)$ and the solution of the exterior Dirichlet problem. The equilibrium shape is shown to be the stationary state of the total energy under the constraint that the area (the volume in 3-d) is prescribed.

Numerical results of the adaptive technique applied to the model problem are analyzed.

2 Numerical shape optimization

Let the boundary domain $\Omega(u) \subset I\!R^2$ with a boundary $\partial\Omega(u)$ parame -trized by a function $u \in \mathcal{U}_{ad}$.

The set of admissible solutions $\mathcal{U}_{ad}$ is in general a subset of a function space $\mathcal{U}$, in our case the piecewise linear representation of the boundary of Ω. The set $\mathcal{U}$ is characterized by its topological type and a constraint. In our case, the area of the domain $\Omega(u)$ is given.

The formulation of the numerical shape optimization problem considered in this paper is the following: find $u^* \in \mathcal{U}_{ad}$ such that it minimise the cost function $j(u) = F(\Omega(u), \varphi_{\Omega(u)})$.

The scalar potential $\varphi_{\Omega(u)}$ is the solution in a Sobolev space $\mathcal{H}$ of a elliptic P.D.E. problem in the domain $\Omega(u)$;

$$a(\varphi_{\Omega(u)}, \psi) = l(\psi) \quad \forall\, \psi \in \mathcal{H} \tag{5}$$

To introduce a Newton-like method we need to consider shape derivatives, that means the derivative of the cost function w.r.t. Ω.

2.1 Shape derivatives

To introduce shape optimization techniques we consider shape derivatives. For different approaches of first derivation techniques with respect to the shape, see [14], [15], [5] , [1].

Let V be a regular vector field (for instance $\mathcal{C}^1(I\!R^2, I\!R^2)$ with compact support in an open neighborhood of Ω). We consider domain deformations defined by the mapping:

$$T_t(V) : x \to x + t\,V(x) \tag{6}$$

and we set $\Omega_t = T_t(V)(\Omega)$. We verify that $\partial\Omega_t = T_t(V)(\partial\Omega)$ for t small enough (since $D_x T_t(x) = I + t\,DV(x)$ and thanks to the local inversion theorem).

Next we denote φ_{Ω_t} the solution of the elliptic problem (2) when we replace Ω by Ω_t. Then the shape derivative of φ_Ω is given by:

$$\varphi'_\Omega(V)(x) = \lim_{t\to 0} \frac{\varphi_{\Omega_t}(x) - \varphi_\Omega(x)}{t} \tag{7}$$

This derivative exist if Ω has a Lipchitz boundary.

In the same way we are going to consider the Eulerian shape derivative $F'(\Omega, \varphi_\Omega)(V)$:

$$F'(\Omega, \varphi_\Omega)(V) = \lim_{t\to 0} \frac{F(\Omega_t, \varphi_{\Omega_t}) - F(\Omega, \varphi_\Omega)}{t} \tag{8}$$

See [5] , definition 2.19, page 54 for a definition of the Eulerian shape derivative. See also [1] and [10] for an analysis of the second order shape derivative.

2.2 The Newton Lagrange method

To describe the Newton method studied in this paper, we introduce the Lagrangian, see [7], [8], [9], [11] and [12]:

$$L(\Omega, \Lambda) = F(\Omega, \varphi_\Omega) + \Lambda\Big(m(\Omega) - m_0\Big) \tag{9}$$

where $\Lambda \in I\!R$ and $\Omega \in \mathcal{O}$, the set of admissible domains. A critical point of the energy F with the assumption that $m(\Omega) - m_0 = 0$ is the first argument of the couple (Ω^*, Λ^*) solution of the following first order KKT necessary conditions:

$$D(\Omega, \Lambda) = \begin{pmatrix} L'(\Omega, \Lambda) \\ m(\Omega) - m_0 \end{pmatrix} = 0. \tag{10}$$

The Newton method to compute an approximation of (Ω^*, Λ^*) consists of computing a sequence of solutions (Ω^k, Λ^k) of a linear form of (10). This leads to the following algorithm:

$$\begin{cases} \Omega^\circ, \Lambda^\circ \text{ given} \\ (\Omega^{k+1}, \Lambda^{k+1}) = (\Omega^k, \Lambda^k) + (\delta\Omega^k, \delta\Lambda^k) \\ \text{ where } (\delta\Omega^k, \delta\Lambda^k) \in \mathcal{O} \times I\!R \text{ satisfies} \\ D(\Omega^k, \Lambda^k) + H(\Omega^k, \Lambda^k)(\delta\Omega^k, \delta\Lambda^k) = 0 \text{ in } \mathcal{L}(\mathcal{O}, I\!R) \times I\!R \end{cases} \tag{11}$$

where $H(\Omega^k, \Lambda^k)$ is given by:

$$H(\Omega^k, \Lambda^k) = \begin{pmatrix} L''(\Omega^k, \Lambda^k) & m'(\Omega^k) \\ m'(\Omega^k) & 0 \end{pmatrix} \tag{12}$$

The computations are carried out for the corresponding discrete formulation of problem (11). The domains Ω under consideration are characterised by the boundary $\partial\Omega = \Gamma$. In practice we consider domains with piecewise linear boundaries.

After discretization we have the following non-linear equation:

$$D(\Omega(\overline{u})) = 0 \quad \text{with } D : \mathcal{U}_h \in I\!R^N \to I\!R^N \tag{13}$$

Then the numerical optimization method construct a sequence $\{\overline{u}^k\}_k$ such that:

$$H(\Omega(\overline{u}^k), \Lambda_k)\, \delta\overline{u}^k = -D(\Omega(\overline{u}^k)) \tag{14}$$

$$\overline{u}^{k+1} = \overline{u}^k + \delta\overline{u}^k \tag{15}$$

where $H(\Omega(\overline{u}^k), \Lambda_k)$ is a discrete version of the Hessian $H(\Omega^k, \Lambda^k)$.

At this step of the procedure the fidelity of the corresponding approximative output is no assured. Approximation errors in $H(\Omega(\overline{u}^k), \Lambda_k)$ and $D(\Omega(\overline{u}^k))$ computation are cumulated with rounding errors and numerical errors in the resolution of the linear system (14).

2.3 Error analysis

Let $\overline{u}^*$ the solution of the non linear problem (10) , $\overline{u}^k$ the k-th theoretical iterate of the discrete optimisation algorithm and $e^k = \overline{u}^k - \overline{u}^*$ the theoretical numerical error.

Let $\tilde{\overline{u}}^k$ be the $\overline{u}^k$ iterate actually computed, including accumulated rounding errors, see [23]. Let $\tilde{e}^k = \tilde{\overline{u}}^k - \overline{u}^k$ the computation error.

Let $\tilde{D}_k(\overline{u}^k) = D(\Omega(\overline{u}^k)) + E(\overline{u}^k)$ the computed approximation of $D(\Omega(\overline{u}^k))$ and $E(\overline{u}^k)$ the error. Let $\tilde{D}_k(\tilde{\overline{u}}^k)$ be the actually computed approximation of $D(\Omega(\tilde{\overline{u}}^k))$, including cumulated rounding errors.

Let $\tilde{H}_k(\overline{u}^k) = H(\Omega(\overline{u}^k), \Lambda_k) + \Delta(\overline{u}^k)$ the computed approximation of the hessien $H(\Omega(\overline{u}^k), \Lambda_k)$ and $\Delta(\overline{u}^k)$ the error. Let $\tilde{H}_k(\tilde{\overline{u}}^k)$ be the computed approximation of $H(\Omega(\tilde{\overline{u}}^k), \Lambda_k)$, including cumulated rounding errors.

A first analyse of the error evolution [4] [18] gives:

$$||e^{k+1}||_2 \leq C_1(||e^k||_2^2 + \Delta_k||e^k||_2 + E_k) \tag{16}$$

where E_k and Δ_k are the euclidean norm of $E(\overline{u}^k)$ and $\Delta(\overline{u}^k)$.

This estimate shows that the rate of convergence of the Newton-like method are strongly related to the evolution of E_k and Δ_k which are related to the accuracy reached in the state equation numerical solution.

In fact $\tilde{\overline{u}}^k$ is the actually computed iterate at the k-th step. Then is crucial to estimate a relation between $||\, e^{k+1}\,||_2$ and $||\tilde{e}^{k+1}||_2$. Suppose that $H(\Omega(\tilde{\overline{u}}^k), \Lambda_k)$ and $\tilde{H}_k(\tilde{\overline{u}}^k)$ are regular in a neighborhood of the solution.

If we consider the rounding and numerical error accumulated during the (k+1)th step, using the Wilkinson[23] techniques we obtain:

$$||\tilde{e}^{k+1}||_2 \leq (\eta_k\, ||\, e^k\,||_2 + (1 + \eta_k)\, ||\, e^{k+1}\,||_2) \tag{17}$$

and

$$\eta_k = |||\, \tilde{H}_k(\tilde{\overline{u}}^k)^{-1}\, H(\, \Omega(\tilde{\overline{u}}^k), \Lambda_k) - I\,|||_2 \tag{18}$$

$$+ \frac{|| \tilde{H}_k (\tilde{\overline{u}}^k)^{-1} (\tilde{D}_k(\tilde{\overline{u}}^k) - D(\Omega(\tilde{\overline{u}}^k))) ||_2}{|| \tilde{H}_k (\tilde{\overline{u}}^k)^{-1} (D(\Omega(\tilde{\overline{u}}^k))) ||_2} \tag{19}$$

where $|||\,.\,|||_2$ is the matrix norm associated to the euclidean vector norm.

Bounds of the two errors:

$$||\tilde{D}(\tilde{\overline{u}}^k) - D(\tilde{\overline{u}}^k)||_2 \text{ and } ||| \tilde{H}_k (\tilde{\overline{u}}^k) - H(\Omega(\tilde{\overline{u}}^k), \Lambda_k) |||_2 \tag{20}$$

are related to how accurate is the numerical approximation φ_k of $\varphi_{\Omega(\tilde{\overline{u}}^k)}$ solution of the state equation (5) when $\Omega = \Omega(\overline{u}^k)$. Then the control of the error Δ_k and E_k are directly related to the knowlege of a posteriori bound of the error $||\varphi_k - \varphi_{\Omega(\tilde{\overline{u}}^k)}||$ in a suitable norm. This error bound is specific to each problem. We will give an example in next section.

To monitor the convergence of the algorithm we introduce the contraction factor [3]:

$$\theta_k = \frac{|| \tilde{D}(\tilde{\overline{u}}^{k+1}) ||_2}{|| \tilde{D}(\tilde{\overline{u}}^k) ||_2} \tag{21}$$

If the initial guess $\overline{u}^0$ is such that $\theta_0 < 1$ then, we consider that the rate of convergence of Newton-like iteration is not sufficiently if:

$$\theta_{k+1} \geq 2\, \theta_k^2 \tag{22}$$

The adaptative procedure consist in a monitoring step and in a mesh refinement step. If the inequality (22) is true then we compute an a posteriori error of the numerical solution of the state equation and we refine where is necessary.

3 Model Problem

The simplified model of the electro-magnetic shaping problem studied here concerns the case of a vertical column of liquid metal falling down into an electro-magnetic 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 electro-magnetic forces are reduced to the magnetic pressure acting on the interface.

Under suitable assumptions, [16], [17], the equilibrium configurations are given by a local critical point of the following total energy:

$$F(\Omega, \varphi_\Omega) = -\frac{1}{2\mu_0} \int_\Omega |\nabla \varphi_\Omega|^2 + \sigma P(\omega) \tag{23}$$

where $\omega = \Omega^c$ and ω is a bounded domain. $P(\omega)$ is the perimeter of ω, i.e. the length of $\partial\omega$ when $\partial\omega$ is regular enough (for instance of class C^1)

$$P(\omega) = \int_{\partial\omega} d\gamma, \qquad d\gamma = \text{ length measure on } \partial\omega. \tag{24}$$

In (23), σ is the boundary tension of the liquid and φ_Ω is solution of:

$$\begin{array}{l} -\Delta\varphi_\Omega = \mu_0 j_0 \quad \text{in } \Omega \\ \varphi_\Omega = 0 \qquad \text{on } \partial\omega \\ \varphi_\Omega(x) = O(1) \text{ as } |x| \to \infty \end{array} \tag{25}$$

where $\mathbf{j}_0 = (0, 0, j_0)$ denotes the density current vector and μ_0 is the vacuum permeability.

The variational formulation of (23), (24) and (25) consists in considering the equilibrium domain ω as a stationary point for the total energy (23), under the constraint that measure of ω is given by m_0.

4 Numerical Method

4.1 Discretisation of the problem

We want to evaluate numerically an approximation of the optimal domain Ω^* so that the discrete shape first order necessary condition vanishes for all admissible vector fields. To this end we build a sequence of domains ω^k, more precisely, we take a sequence of domains defined by their boundaries $\Gamma^k = \partial\omega^k$ that converge towards a critical point. By Γ^k, we mean a piecewise linear closed Jordan curve, that is, a union of finite element Γ_i, $i = 1, ..., n$. The nodes of the curve Γ^k are denoted by $x^{i,k}$, $i = 1, ..., n$.

At each iteration of the minimizing algoritm the boundary Γ^{k+1} is obtained by a local perturbation of Γ^k.

To each vertex $x^{i,k}$ of Γ^k is associated a direction $\hat{Z}^{i,k} \in I\!R^2$. The vector $\hat{Z}^{i,k}$ is a unitary vector of the same direction than the bisector of the normal vectors to Γ_{i-1} and Γ_i. We construct a continuous piecewise linear vector field $Z^{i,k}$ from $\Gamma^k \to I\!R^2$ such that $Z^{i,k}(x^{j,k}) = \delta_{i,j}\hat{Z}^{i,k}$.

The support of $Z^{i,k}$ is equal to the union of the finite element where $x^{i,k}$ is a node. At each iteration we compute the following vector field:

$$Z^{k+1}(x) = \sum_{i=1}^{n} u_i^{k+1} Z^{i,k}(x) \tag{26}$$

and the updated boundary Γ^{k+1} is then given by:

$$\Gamma^{k+1} = \{X = x + \sum_{i=1}^{n} u_i^{k+1} Z^{i,k}(x); u_i^{k+1} \in I\!R, x \in \Gamma^k\} \quad (27)$$

where $\bar{u}^{k+1} = (u_1^{k+1}, \cdots . u_n^{k+1})^t \in I\!R^n$ are the unknowns which determine the evolution of the curve Γ^k. Then in practice the continuous minimization problem is reduced to a n-dimensional optimization problem depending on the solution of the state problem. This method of evolution of the boundary has the important advantage that there is only one degree of freedom at each node.

4.2 The exterior Dirichlet problem

At each iteration we have to solve the following exterior problem

$$\begin{array}{lll} -\Delta v(x) = 0 & \text{in} & \Omega^k \\ v(x) = -r(x) & \text{on} & \partial\omega^k = \Gamma^k \\ |v(x)| = O(1) & \text{as} & |x| \to \infty \end{array} \quad (28)$$

Following [6] an integral single layer representation of the solution of (28) is given by:

$$v(x) = \frac{-1}{2\pi} \int_{\Gamma^k} q(y) ln|x - y| d\gamma + c \quad (29)$$

with $q(y) \in H^{-1/2}(\Gamma^k)$ and:

$$\int_{\Gamma^k} q(y) d\gamma = 0 \quad (30)$$

The constant $c = \lim_{|x|\to\infty} |v(x)|$. Then

$$\frac{\partial v}{\partial \nu_x}(x) = \frac{-1}{2\pi} \int_{\Gamma^k} q(y) \frac{\partial ln|x-y|}{\partial \nu_x} d\gamma + \frac{1}{2} q(x) \text{ if } x \in \Gamma \quad (31)$$

Here the unknown is the density $q(y)$ and we compute it using the boundary condition in a weak formulation. We seek $q(y) \in H^{-1/2}(\Gamma^k)$ solution of the following problem:

$$\begin{array}{l} \frac{-1}{2\pi} \int_{\Gamma^k} g(x) \int_{\Gamma^k} q(y) ln|x-y| d\gamma d\gamma + c \int_{\Gamma^k} g(x) d\gamma = \\ - \int_{\Gamma^k} r(x) g(x) d\gamma \end{array} \quad (32)$$

and

$$\int_{\Gamma^k} q(x) d\gamma = 0 \quad (33)$$

for all $g \in H^{-1/2}(\Gamma^k)$.
In numerical calculations we consider a piecewise constant approximation $q_h(x)$ of $q(x)$

$$q_h(x) = \sum_{i=1}^{n} q_i e_i(x) \tag{34}$$

where $e_i(x) = 1$ if $x \in \Gamma_i = [x^{i,k}, x^{i+1,k}]$ and zero elsewhere.

Then we obtain a linear system:

$$A\overline{q} = b \tag{35}$$

where

$$a_{i,j} = \frac{-1}{2\pi} \int_{\Gamma_i} \int_{\Gamma_j} ln|x - y| d\gamma d\gamma \qquad i, j = 1, ..., n \tag{36}$$

$$a_{i,j} = \int_{\Gamma_j} d\gamma \qquad j = 1, ..., n \text{ and } i = n + 1 \tag{37}$$

$$(\overline{q})_j = q_j \qquad j = 1, ..., n \qquad \text{and} \qquad q_{n+1} = c \tag{38}$$

Remark 1. The linear system (35) is symmetric and non sparse, then we use a LDL^t decomposition of A. The numerical approximation of the normal derivative in (31) is computed by Gauss quadrature.

Remark 2. The approximation of the normal derivative $\dfrac{\partial v}{\partial \nu_e}$ at $x_l \in \Gamma_l$ is given by:

$$\frac{\partial v_h}{\partial \nu_e}(x_l) = \frac{-1}{2\pi} \sum_{i=1, i\neq l}^{n} q_i \sum_{m=1}^{n} q_m \frac{\partial ln|x_l - x_i(s_m)|}{\partial \nu_e} + \frac{1}{2} q_l \tag{39}$$

Thus the computation of $\dfrac{\partial v_h}{\partial \nu_l}(x_l)$ needs $O(n)$ floating point operations.

Remark 3. If q is the solution of the system (32), (33) and $\overline{q}$ is solution of (35) with piecewise constant approximation we have the following error bounds, see [13]:

$$||q - q_h||_{H^{-1/2}(\Gamma)} \leq C_1 h ||q||_{H^1(\Gamma)} \tag{40}$$

and

$$||\frac{\partial v}{\partial \nu} - \frac{\partial v_h}{\partial \nu}||_{H^{-1/2}(\Gamma)} \leq C_2 h ||q||_{H^1(\Gamma)} \tag{41}$$

4.3 Adaptive method for the mesh refinement

In this subsection we introduce an a posteriori error estimate and an adaptive mesh-refinement procedure. Pioneer work of [19], [20], [21] and [22] gives a posteriori error estimate for finite element and boundary element methods.

Let h be the maximum of the local mesh size h_i of the finite element Γ_i, discretization of Γ. If q belongs to H^τ then for the Galerkin scheme(32) we have the a priori error estimate:

$$||q - q_h||_{H^{-\frac{1}{2}}(\Gamma)} \leq Ch^{l+\frac{1}{2}}||q||_{H^l(\Gamma)} \tag{42}$$

with $l = min\{\tau, \nu + 1\}$, $\nu = 0, 1$.

The residual R_h is given by :

$$\begin{aligned} R_h(x) &= r(x) - \frac{1}{2\pi}\int_\Gamma q_h(x)\, ln\,|x - y\,|\, d\gamma + c \\ &= r(x) - \frac{1}{2\pi}\sum_{i=1}^{n}\int_{\Gamma_i} q_h(x)\, ln\,|x - y\,|\, d\gamma + c \end{aligned} \tag{43}$$

then we have the following a posteriori error estimate:

$$||q - q_h||_{H^{-\frac{1}{2}}(\Gamma)} \leq C(\sum_{i=1}^{n} h_i||\frac{\partial R_h}{\partial s}||^2_{L^2(\Gamma_i)})^{\frac{1}{2}} \tag{44}$$

where $\frac{\partial}{\partial s}$ is the differentiation with respect to the arc length.

An adaptive method for mesh refinement of Γ is derived from a local interpretation of (44),see [20] and [22]. Given a uniform mesh after a few iterations, we compute the residual R_h and we refine the i-th path of the mesh if

$$h_i > \theta(h_{i+1} + h_{i-1}),\ \ 0.5 < \theta < 1 \tag{45}$$

or if

$$h_i||\frac{\partial R_h}{\partial s}||^2_{L^2(\Gamma_i)} \geq 0.5 \max_{k=1,n} h_k||\frac{\partial R_h}{\partial s}||^2_{L^2(\Gamma_k)} \tag{46}$$

The norm are computed by numerical integration of the analytical computed derivative of the residual using a Gaussian quadrature.

4.4 The discrete Newton-like method

The Lagrangian of problem (23), (24) has the following form:

$$L(\omega, \Lambda) = -\frac{1}{2\mu_0}\int_\Omega |\nabla\varphi_\Omega|^2 dx + \sigma\int_{\partial\omega} d\gamma + \Lambda(\int_\omega dx - m_0). \quad (47)$$

Let V and W be two regular vector field (for instance $\mathcal{C}^1(I\!R^2, I\!R^2)$ with compact support in an open neighborhood of Ω). Then we obtain the following first order necessary condition:

$$\frac{1}{2\mu_0}\int_{\partial\omega} |\nabla\varphi|^2 (V\cdot\overline{n})\, d\gamma + \sigma\int_{\partial\omega} \mathcal{C}\,(V\cdot\overline{n}) d\gamma + \Lambda\int_{\partial\omega}(V\cdot\overline{n}) d\gamma = 0 \quad (48)$$

$$\int_\omega dx - m_0 = 0 \quad (49)$$

The second order derivatives of the Lagrangian lead to the following Hessian:

$$H = \begin{pmatrix} A_{V,W} & S_V \\ S_W & 0 \end{pmatrix} \quad (50)$$

where:

$$A_{V,W} = \int_{\partial\omega} \frac{1}{2\mu_0}\frac{\partial\varphi_\Omega}{\partial n}(V\cdot\nabla^2\varphi_\Omega\cdot W + V\cdot\nabla\varphi'_\Omega(W) + W\cdot\nabla\varphi'_\Omega(V)) + \int_{\partial\omega}((\frac{\partial V}{\partial s}\cdot\overline{n})(\frac{\partial W}{\partial s}\cdot\overline{n}) + \Lambda(V\cdot\frac{\partial W^\perp}{\partial s}))d\gamma \quad (51)$$

$$S_V = \int_{\partial\omega} V\cdot\overline{n}\; d\gamma. \quad (52)$$

and

$$S_W = \int_{\partial\omega} W\cdot\overline{n}\; d\gamma. \quad (53)$$

In practice we consider an approximation (not a discretization, because we need the solution of two exterior Dirichlet problems) of the Newton algorithm (11). To this aim we consider a local perturbation given by the vectol field $Z^{k+1}(x) = \sum_{i=1}^n u_i^{k+1} Z^{i,k}(x)$ defined in section 4.1. Then the V and W discrete version are the vector field $Z^{i,k}$ and $Z^{j,k}$ defined in section 4.1.

The discrete version of the Hessian H if given by:

$$H(\Omega(\overline{u}^k), \Lambda^k) = \begin{pmatrix} A_{ij}(u_1^k, ..., u_n^k, \Lambda^k) & S_i(u_1^k, ..., u_n^k) \\ S_j(u_1^k, ..., u_n^k) & 0 \end{pmatrix} \quad (54)$$

where:

$$A_{ij}(u_1^k,....,u_n^k,\Lambda^k) = \int_{\partial\omega}\frac{1}{2\mu_o}\frac{\partial\varphi_h}{\partial n}(Z^{i,k}\cdot\nabla^2\varphi_h\cdot Z^{j,k}+Z^{i,k}\cdot\nabla\varphi_h'(Z^{j,k})+Z^{j,k}\cdot\nabla\varphi_h'(Z^{i,k})) + \int_{\Gamma^k}(\frac{\partial Z^{i,k}}{\partial s}\cdot\overline{n})(\frac{\partial Z^{j,k}}{\partial s}\cdot\overline{n})d\gamma + \Lambda^k\int_{\Gamma^k}(Z^{i,k}\cdot\frac{\partial Z^{j,k\perp}}{\partial s})d\gamma \tag{55}$$

for $i,j=1,...n$, and

$$S_i(u_1^k,....,u_n^k) = \int_{\Gamma^k}(Z^{i,k}\cdot\overline{n})d\gamma,\ \text{where}\quad i=1,...n \tag{56}$$

The vector $\overline{u}^{k+1} = (u_1^{k+1},....,u_n^{k+1})^t$ is defined by the following system of equations :

$$\begin{pmatrix} A_{ij}(u_1^k,....,u_n^k,\Lambda^k) & S_i(u_1^k,....,u_n^k) \\ S_j(u_1^k,....,u_n^k) & 0 \end{pmatrix}\begin{pmatrix}(u_1^{k+1},\ldots,u_n^{k+1})^t \\ \delta\Lambda\end{pmatrix} = -\begin{pmatrix}D_i\\ m\end{pmatrix} \tag{57}$$

where

$$D_i = \frac{1}{2\mu_0}\int_{\Gamma^k}|\nabla\varphi_h|^2\,(Z^{i,k}\cdot\overline{n})\,d\gamma + +(\frac{(x_i^k-x_{i-1}^k)}{\|x_i^k-x_{i-1}^k\|}-\frac{(x_{i+1}^k-x_i^k)}{\|x_{i+1}^k-x_i^k\|})\cdot\hat{Z}^{i,k}+ +\Lambda^k\int_{\Gamma^k}(Z^{i,k}\cdot\overline{n})\,d\gamma \tag{58}$$

for $i=1,...n$ and

$$m = \int_{\omega^k}dx - m_0 \tag{59}$$

Then the boundary Γ^{k+1} of $\Omega(\overline{u}^{k+1})$ is given by:

$$\Gamma^{k+1} = (I+Z^{k+1})(\Gamma^k) = \left\{x : x = X+Z^{k+1}(X)\,;\ X\in\Gamma^k\right\} \tag{60}$$

Remark 4. The computation of $A_{ij}(u_1^k,....,u_n^k,\Lambda^k), i,j=1,...n$ needs $\varphi_h'(Z^{i,k}), i=1,...,n$ which are given by:

$$\begin{array}{lll} -\Delta\varphi_h'(Z^{i,k}) = 0 & \text{in} & \Omega^k \\ \varphi_h'(Z^{i,k}) = -Z^{i,k}\cdot\nabla\varphi_h & \text{on} & \partial\omega^k=\Gamma^k \\ |\varphi_h'(Z^{i,k})(x)| = O(1) & \text{as} & |x|\to\infty \end{array} \tag{61}$$

That means that we have to solve n exterior Dirichlet problems. In fact if we use the same numerical technique as in problem (28), we obtain a linear system with the same matrix. As the $L\,D\,L^t$ decomposition of this matrix is done, solving problem (61) needs only n more solutions of a triangular system.

5 Numerical Results

The algorithm is applied to a test case. The boundary tension σ and the area m_0 of the liquid metal are given as well as the distribution of the current j_0 which is of the form:

$$j_0 = (\sum_{p=1}^{m} \alpha_p \delta_{x_p}) I \tag{62}$$

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

$$F(\Omega, \widehat{\varphi}) = -\int_{\Omega} |\nabla \widehat{\varphi}|^2 \, dx + \widehat{\sigma} P(\Omega) \tag{63}$$

and the Lagrangian:

$$L(\Omega, \Lambda) = -\int_{\Omega} |\nabla \widehat{\varphi}|^2 \, dx + \widehat{\sigma} P(\Omega) + \Lambda(m(\omega) - m_0) \tag{64}$$

First we consider the case without mesh refinement. The first guess is a uniform discretization of the circle with 128 nodes. The physical parameter are $m = 4$, $\alpha_p = \pm 0.2$ and $m_0 = \pi$. In figure 1 we observe the iteration rate of convergence: it becomes linear after a few iterations.

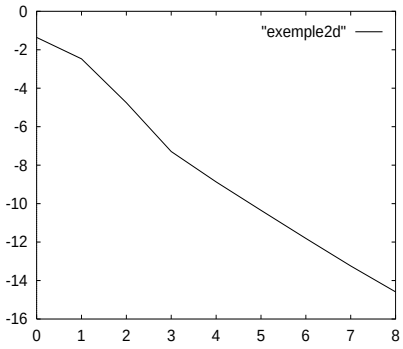

Figure 1: evolution of $||L'||_2$

In figure 2 we plot the last iterate. We observe that the uniformity of the mesh is destroyed by the optimization process. Afther 8 iterations the $||L'||_2$ norm is less than 10^{-14}.

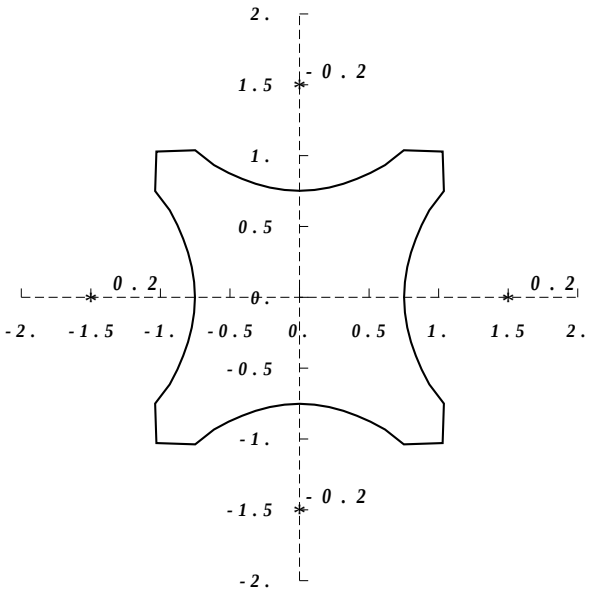

Figure 2: $N = 128$, area equal π and four masses

Now we consider the same case with mesh-refinement, at the end of iterations we have also 128 nodes. The first shape iteration is a circle discretized with 16 nodes. At the second iteration a mesh refinement is necessary to preserve the superlinear rate of convergence.Until iteration 6 and after two new mesh refinements we observe in figure 3 that the rate of convergence is superlinear. At this step, with 128 nodes, the $||L'||_2$ norm is of order 10^{-18} and we stop the processus.

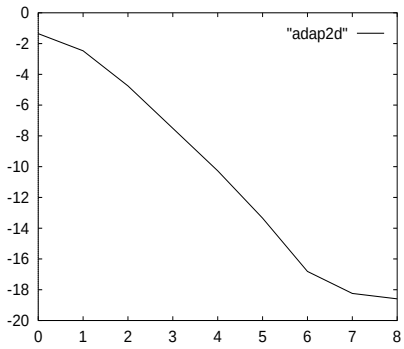

Figure 3: evolution of $||L'||_2$

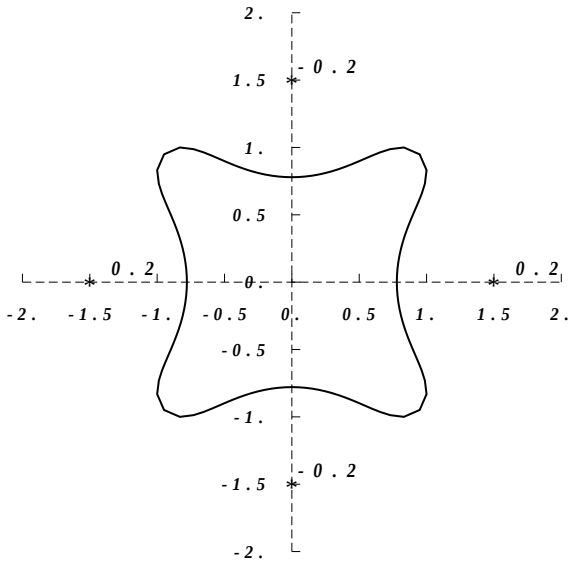

Figure 4: Final $N = 128$, area equal π and four masses

In figure 4 is clear that the adaptive mesh refinement gives a better distribution of nodes

The numerical results show that the rate of convergence monitoring with adaptive methods improves the performance of Newton-like methods in shape optimization. Adaptive mesh-refinement allows us to obtain a more accurate cost function critical point at a low cost.

References

1. M. C. Delfour and J. P. Zolesio, *Shapes and Geometries, Analysis, Differential Calculus, and Optimization* S.I.A.M., Advances in Design and Control, PhiladelPhia, (2001).
2. J.E. Dennis, JR. and R.B. Schnabel, *Numerical methods for Unconstrained Optimization and Nonlinear Equations*, Prentice Hall Series in Computational Mathematics' Prentice Hall,Inc., Englewood Cliffs, New Jersey 07632, (1983).
3. P. Deuflhard, *Newton Methods for Nonlinear Problems*, Springer Verlag, Berlin, Heilderberg, (2004).
4. C.T. Kelley, *Iterative Methods for Linear and Nonlinear Equations* SIAM. Philadelphia, (1995).
5. J. Sokolowski and J.P. Zolesio, *Introduction to Shape Optimization,Shape Sensitivity Analysis*, Springer Verlag, Berlin, Heilderberg, (1992).
6. R. Kress, *Linear Integral Equations*, Springer Verlag, Berlin, Heilderberg, (1989).
7. R. Fletcher, *Practical Methods of Optimization*, John Wiley & Sons, Chichester, (1987).
8. J. R. Roche *Algorithmes numériques en optimisation de formes et électromagnétisme.* Mémoire d'Habilitation à Diriger des Recherches, (1996).

9. A. Novruzi *Contribution en Optimisation de Formes et Applications.* Thèse de l'Université Henri Poincaré, Nancy 1, (1997).
10. A. Novruzi and M. Pierre "Structure of the shape derivatives" *Journal of Evolution Equations*, **2:3**, 365-382,(2002).
11. A. Novruzi and J.R. Roche, *Second Order Derivatives, Newton Method, Application to Shape Optimization*, Rapport INRIA, (1995).
12. A. Novruzi and J.R. Roche, " Newton Method in 3-dimensional Shape Optimization Problems. Application to electromagnetic casting", *BIT*, **40:1**, 102-120, (2000).
13. J.-C. Nedelec, *Approximation des équations intégrales en mécanique et en physique*, Rapport Interne, Ecole Polytechnique, (1977).
14. S. Murat and J. Simon, *Sur le contrôle par un domaine géométrique*, Rapport du Laboratoire d'Analyse Numérique, Université de Paris , (1976).
15. J. Simon, "Differentation with respect to the domain in boundary value problems", *Numer.Funct.Anal.And.Opt*, **2**, 649 -687, (1980).
16. A. Henrot and M. Pierre, "Un probléme inverse en formage de métaux liquides", M^2AN, **23**, 155-177, (1989).
17. M. Pierre and J.R. Roche, "Numerical simulation of tridimensional electromagnetic shaping of liquid metals", *Numer. Math*, **65**, 203-217, (1993).
18. T.J. Ypma, "The effect of rounding errors on Newton-like methods", *IMA J. Numer. Anal.*, **3**, 109-118, (1983).
19. I. Babuska and A. Miller, "A feedback finite element method with a posteriori error estimation", *Comp. Methods Appl. Mech. Engrg.*, **61**, 1-40, (1987).
20. K. Eriksson and C. Johnson, "An adaptive finite element method for linear elliptic problems", *Math. Comp.*, **50**, 361 - 383, (1988).
21. M. Costabel and E.P. Stephan, "Boundary integral equations for mixed boundary value problems in polygonal domains and Galerkin approximation", *Banach Center Publ.*, **15**, 175-251, (1985).
22. C. Carstensen and E.P. Stephan, "A posteriori error estimates for Boundary element methods", *Math. Comp.*, **64**, 483-500, (1995).
23. J. H. Wilkinson, *Rounding Errors in Algebraic Processes* Her Majesty's Stationery Office, London, (1963).