Geometric Aspects of Shape Optimization

Jan Sokolowski

9 stycznia 2023

Geometric Aspects

1. Introduction
2. Model Problem

Geometric Aspects

Shape Optimization

1. Direct method of calculus of variations: regularization and shape calculus;
2. State equation, cost functional, numerical method of solution: finite elements;
3. Phase field method for problems depending on characteristic functions: a possibility to use the homogenization method;
4. Level set method based on the shape gradent and/or on the topological derivative concept.

Shape Optimization

1. The convergence of simple gradient method for numerical solution of shape optimization problems is still not known.
2. We have a result on the convergence in two spatial dimensions for a model problem.
   - The regularization of the cost is required in order to assure the existence of an optimal shape.
   - The regularization term can be considered as a cost of manufacturing so the parameter is not small.
   - in numerical methods of shape optimization the discretization of the continuous gradient is exclusively used, the exact gradient is expensive.

Shape optimization is useful in structural mechanics. **Numerical** shapes obtained by *some computations* are used for design of cars, aircrafts, ships and other structures. Shape optimization is also a domain of Mathematics in the fields of Calculus of Variations, Free Boundary Problems or more generally Theory of Partial Differential Equations. The main applications are solids, fluids, gases, or new materials. The starting points in mathematical analysis were the monographs by O. Pironneau (Optimal Shape Design for Elliptic Systems, Springer, 1984), J.S. and J.-P. Zolesio (Introduction to Shape Optimization, Springer, 1992), M. Delfour and J.-P. Zolesio (Shapes and Geometries, SIAM, 2001, 2011). The case of compressible Navier-Stokes equations is studied in great details in the monograph by J.S. and P.I. Plotnikov (Compressible Navier-Stokes equations. Theory and shape optimization. Birkhauser, 2012).

The presentation is based on two papers. The first is a review prepared on the invitation from the journal. The second is a companion paper with some proofs of new results presented for the first time in [1].

1. Pavel I. Plotnikov, J.S.
Geometric Aspects of Shape Optimization
J. Geometric Analysis
Special issue on Shape Optimization, 54 pages
2. Pavel I. Plotnikov, J. S.
Gradient flow for Kohn-Vogelius functional.
https://hal.archives-ouvertes.fr/hal-03896975
HAL INRIA-CNRS, (2022) 72 pages.

The methods used in shape optimization which require mathematical analysis:

1. Shape calculus (also *Topological derivatives*);
2. Phase fields models: the characteristic function of unknown domain is replaced by a phase field;
3. Level set method: for given functional the shape gradient or the topological derivative is used in the Hamilton-Jacobi equation without mathematical justification;
4. *Our Model Problem*:
   Gradient flow for Kohn-Vogelius functional.

We restrict the analysis to $\mathbb{R}^2$. We need the state equation and the shape functional to be minimized. We use the notation.

1. $\Omega = \Omega_i \cup \Gamma \cup \Omega_e$
2. $J(\Omega_i) = J(\Gamma)$
3. regularization term $\mathcal{E}(\Gamma)$
4. the shape optimization problem

$$\min_{\Gamma} \{J(\Gamma) + \mathcal{E}(\Gamma)\}$$

$J(\Gamma)$ is the shape functional and $\mathcal{E}(\Gamma)$ governs the regularity of the curve Γ or the cost of manufacturing.

Let us assume that a material occupy the a bounded region Ω in the space of points $x \in \mathbb{R}^d$, $d = 2, 3$. Without loss of generality, we can assume that the boundary of Ω is infinitely differentiable. Furthermore, we will assume there are two disjoint open arcs $\Gamma_N, \Gamma_D \subset \partial\Omega$ such that $\mathrm{cl}\, \Gamma_N \cup \Gamma_D = \partial\Omega$. The inclusion, which is unknown and must be determined together with the solution, occupies the subdomain $\Omega_i \Subset \Omega$ with the boundary Γ. The equilibrium equations for the electric field potential $u : \Omega \to \mathbb{R}$ in the simplest case can be written as

$$\begin{aligned} \operatorname{div}(a\nabla u) = 0 \;\text{ in }\; \Omega, \\ a\nabla u \cdot n = h_n \;\text{ on }\; \Gamma_N, \quad u = h_d \;\text{ on }\; \Gamma_D. \end{aligned} \tag{1}$$

Here n is the outward normal vector to $\partial\Omega$, h_n is a given voltage, and h_d is a given distribution of the electric potential.

The conductivity a is defined by the equalites

$$a = 1 \text{ in } \Omega_e, \quad a = a_0 \text{ in } \Omega_i, \tag{2}$$

where a_0 is a given positive constant. If $\Gamma_D \neq \emptyset$, then problem (1) has a unique solution $u \in W^{1,2}(\Omega)$. If in addition, the arcs Γ_N, Γ_D belong to different connected components of $\partial\Omega$, $h_n, h_d \in C^\infty(\partial\Omega)$, and $\partial\Omega$ belongs to the class C^∞, then $u \in C^\infty(\Omega)$. The problem on the identification of the inclusion Ω_i is formulated as follows. For a given function $g : \Gamma_D \to \mathbb{R}$ it is necessary to find an inclusion Ω_i such that the solution to problem (1) satisfies the extra boundary condition

$$a\nabla u \cdot n = g \text{ on } \Gamma_D. \tag{3}$$

It is assumed that g satisfies the orthogonality condition

$$\int_{\Gamma_D} g\,ds + \int_{\Gamma_N} h_n\,ds = 0.$$

More generally, the problem of identification is to determine the shape of the inclusion by the additional boundary condition. This inverse problem is ill-posed and in general case has no solution. In practice, its approximate solution can be found by solving the variational problem

$$\min_{\Omega_i \in \mathcal{A}} J(\Omega_i), \tag{4}$$

where the objective functional $J(\Omega_i)$ is a positive function that vanishes if and only if a solution to problem (1) satisfies the condition (3), $\mathcal{A}$ is some class of admissible inclusions.

The most successful choice of the objective functional is the Kohn-Vogelius energy functional, which is defined as follows,

$$J(\Omega_i) = \int_\Omega a\nabla(v - w) \cdot \nabla(v - w)\, dx. \tag{5}$$

Here $v, w : \Omega \to \mathbb{R}$ satisfy the equations and boundary conditions

$$\begin{aligned}
\text{div } a\nabla v &= 0 & \text{div } a\nabla w &= 0 & &\text{in } \Omega, & (6)\\
a\nabla v \cdot n &= g & w &= h_d & &\text{on } \Gamma_D, & (7)\\
a\nabla v \cdot n &= h_n & a\nabla w \cdot n &= h_n & &\text{on } \Gamma_N. & (8)
\end{aligned}$$

In order to solve the Shape Optimization Problem from mathematical point of view we need:

1. Propose a regularization of the cost in order to assure the existence of an optimal shape;
   - weak regularization: perimeter $\mathcal{L}$;
   - strong regularization: the Willmore functional of the mean curvature of Γ;
2. Show the shape differentiablity of the cost and of the regularization part;
3. Find the Hessian of the cost;
4. Define the nonlinear PDE of parabolic type which governs the minimization process;
5. Prove the well posedness of the nonlinear, degenerate PDE which gives an optimal shape for the regularized minimization process.

Our approach to assure the existence of an optimal domain is to penalize the shape perimeter by adding a regularizing term to the objective functional:

$$\epsilon_p \mathcal{L} + J \tag{9}$$

Here $\mathcal{L}$ is the perimeter of Ω_i, $\epsilon_p > 0$ is the regularization parameter. If $\Gamma = \partial\Omega_i$ is a regular manifold, then $\mathcal{L}$ is the area of Γ in $3D$ case and the length of Γ in $2D$ case.
However, an optimal domain may be irregular, thus impossible to manufacture.

The stronger regularization is obtained if we impose constraints on the curvatures of Γ. This approach also was motivated by the theory of image processing. The only possible conformally and geometrically invariant penalization functional depending on curvatures is the Willmore functional defined by the equality

$$\mathcal{E}_e(\Gamma) = \int_\Gamma |H|^2 \, ds, \tag{10}$$

where H is the mean curvature of Γ. In $2D$ case $\mathcal{E}_e$ coincides with the famous Euler elastica functional. Therefore, we can define the strong regularization of an objective function as follows

$$\mathcal{E} + J, \quad \text{where} \quad \mathcal{E} = \epsilon_e \, \mathcal{E}_e + \epsilon_p \, \mathcal{L}. \tag{11}$$

The most important question of the theory is the construction of a robust algorithm for the numerical study of shape optimization problems. The standard approach is to use the steepest descent method based on the shape calculus developed by Sokolowski and Zolesio (1992), see also Delfour and Zolesio (2001). The shape calculus works for inclusions Ω_i with the regular boundary $\Gamma = \partial\Omega_i$. In this setting, the objective function J is considered as a functional defined on the totality of smooth curves Γ. This assumption is natural from the practical point of view. Without loss of generality we may restrict our considerations by the class of twice differentiable immersions (parametrized surfaces, curves) $f : \mathbb{S}^{d-1} \to \mathbb{R}^d$ with $\Gamma = f(\mathbb{S}^{d-1})$ diffeomorphic to the sphere $\mathbb{S}^{d-1}$. In this framework, we will use the denotation $J(f)$ along with the denotation $J(\Gamma)$. The main goal of the shape calculus is to develop the method of differentiation of objective functions with respect to shapes of geometrical objects.

Following the general method of the shape calculus, we define the shape derivative of an objective function. To this end, choose an arbitrary vector field $X : \mathbb{S}^{d-1} \to \mathbb{R}^d$ and consider the immersion

$$f^t(\theta) = f(\theta) + tX(\theta), \quad t \in (-1,1), \quad \theta \in \mathbb{S}^{d-1}.$$

The manifolds $\Gamma^t = f^t(\mathbb{S}^{d-1})$, $t \in (-1,1)$, define the one-parametric family of perturbations of Γ. The shape derivative $\dot{J}$ of J in the direction X is defined by the equality

$$\dot{J}(\Gamma)\,[X] \;=\; \frac{d}{dt}\,J(\Gamma^t)\Big|_{t=0}. \tag{12}$$

If it admits the Hadamard representation

$$\dot{J}(\Gamma)\,[X] \;=\; \int_\Gamma \phi\,\mathbf{n}\cdot X\,ds,\;\phi\in L^1(\Gamma), \tag{13}$$

where $\mathbf{n}$ is the inward normal to $\Gamma = \partial\Omega_i$, then the vector field

$$dJ(\theta) := \phi(\theta)\mathbf{n}(\theta), \quad \theta\in\mathbb{S}^{d-1}, \tag{14}$$

is said to be the gradient of J at the point f. The same definition holds for the geometric energy functional $\mathcal{E}$

The steepest descent method and the gradient flow. It follows from the definition that the shape gradient dJ can be regarded as a normal vector field on Γ. If f is sufficiently smooth, for example $f \in C^{2+\alpha}$, then the mapping $f + \delta\, dJ\,(f)$ defines an immersion of $\mathbb{S}^{d-1}$ into $\mathbb{R}^d$ for all sufficiently small $\delta > 0$. In the steepest descent method, the optimal immersion f and the corresponding shape $\Gamma = f(\mathbb{S}^{d-1})$ are determined as a limit of the sequence of immersions

$$f_{n+1} = f_n - \delta\,\big(\,d\mathcal{E}(f_n) + dJ(f_n)\,\big), \quad n \geqslant 0, \tag{15}$$

and the corresponding sequence of surfaces $\Gamma_n = f_n(\mathbb{S}^{d-1})$. Here the energy $\mathcal{E}$ is defined (11), δ is a fixed positive number, usually small, f_0 is an arbitrary admissible initial shape.

Relation (15) can be considered as the time discretization of the Cauchy problem

$$\partial_t f(t) = -\big(d\mathcal{E}(f(t)) + dJ(f(t)) \big), \quad f(0) = f_0 \tag{16}$$

Since $\mathcal{E}(f(t)) + J(f(t))$ is a decreasing function of t, solution to problem (16) can be considered as approximate solution to the penalized variational problem

$$\min \ (\mathcal{E} + J)$$

Hence the existence of a solution to Cauchy problem (16) guarantees the well-posedness of the steepest descent method. In its turn, the existence of the limit $\lim_{t\to\infty} f(t)$ guarantees the convergence of the method.

The shape gradient of the Kohn-Vogelius functional

Assume that

$$\partial\Omega, \Gamma \in C^{2+\alpha}, \quad h \in C^{2+\alpha}(\partial\Omega), \quad g \in C^{1+\alpha}(\partial\Omega)), \quad \alpha \in (0,1).$$

Denote by v^-, w^- the restrictions of v, w on Ω_e and by v^+, w^+ the restrictions of v, w on Ω_i. For every function Φ with Φ^- and Φ^+ continuous in $\overline{\Omega}_e$ and $\overline{\Omega}_i$, the denotation $\left[\Phi\right]$, stands for the jump of Φ across Γ,

$$\left[\Phi\right](x) = \lim_{\Omega_e \ni y \to x} \Phi^-(y) - \lim_{\Omega_i \ni y \to x} \Phi^+(y) \ \text{ for all } x \in \Gamma.$$

For strong solutions to transmission problem we have

$$\left[a\partial_n v\right] \equiv \left[a\nabla v\right]\cdot n = 0, \quad \left[a\partial_n w\right] \equiv \left[a\nabla w\right]\cdot n = 0, \quad \left[v\right] = \left[w\right] = 0.$$

With this notation the gradient dJ of the Kohn-Vogelius objective function is defined as follows,

$$dJ = 2\big(a\partial_n v\,[\partial_n v] - a\partial_n w\,[\partial_n w]\big)\,\mathbf{n} - \big[a\nabla v\cdot\nabla v - a\nabla w\cdot\nabla w\big]\,\mathbf{n},$$

Geometric functionals.

The standard formulation of the geometric flow equations deals parametrized curves (surfaces). Further we will assume that the interface admits the representation $\Gamma = f(\mathbb{S}^1)$ where the immersion $f : \mathbb{S}^1 \to \mathbb{R}$ is unknown and should be defined along with the solution to the geometric flow problem. $f(\mathbb{S}^1)$. Note that f a 2π periodic function of the angle variable $\theta \in \mathbb{R}/2\pi\mathbb{Z}$. the element of the length of Γ equals

$$ds = \sqrt{\mathbf{g}(\theta)}\, d\theta,$$

where $\mathbf{g}$ is the only nontrivial coefficient of the first fundamental form of the curve Γ.

In this setting, the derivative with respect to the arc-length variable s

$$\partial_s = \frac{1}{\sqrt{g}} \partial_\theta$$

becomes the nonlinear differential operator depending on f. Hereinafter we assume that the point $f(\theta)$ is going around Γ in the positive counterclockwise direction while the parameter θ increases. The tangent vector

$$\tau(\theta) = \partial_s f(\theta) := |\partial_\theta f|^{-1} \partial_\theta f(\theta),$$

and the normal vector

$$n(\theta) = \tau^\perp(\theta) = (-\tau_2, \tau_1),$$

form the positive oriented moving frame on Γ. Notice that n is the unit inward normal vector to $\partial\Omega_i = \Gamma$

The curvature vector k is defined by the equalities

$$k(\theta) = \partial_s \tau(\theta) = \partial_s^2 f(\theta). \tag{17}$$

Notice that the curvature vector field k is orthogonal to τ and is directed along the normal vector n.
The Euler elastic energy $\mathcal{E}_e$ and the perimeter $\mathcal{L}$ are defined by the equalities

$$\mathcal{E}_e = \int_\Gamma \frac{k^2}{2}\, ds, \quad \mathcal{L} = \int_\Gamma ds = \int_0^{2\pi} \sqrt{\mathbf{g}}\, d\theta \tag{18}$$

Without loss of generality we can take the penalization energy in the form

$$\mathcal{E} = \mathcal{E}_e + \mathcal{L} = \int_\Gamma \Big(\frac{k^2}{2} + 1 \Big)\, ds, \tag{19}$$

The gradient of $\mathcal{E}$ is given by the following lemma.

Lemma

Under the above assumptions, we have

$$d\mathcal{E}_e(f) = \nabla_s \nabla_s k + \frac{1}{2}|k|^2 k, \quad d\mathcal{L} = -k, \tag{20}$$

$$d\mathcal{E}(f) = \nabla_s \nabla_s k + \frac{1}{2}|k|^2 k - k. \tag{21}$$

Here the connection ∇_s for every vector field $\Phi : \Gamma \to \mathbb{R}^2$, is defined by the equality

$$\nabla_s \Phi = \partial_s \Phi - (\partial_s \Phi \cdot \tau)\,\tau. \tag{22}$$

Gradient flow equations

We are now in a position to specify the gradient flow equation

$$\partial_t f + d\mathcal{E} + dJ = 0, \quad f(0) = f_0. \tag{23}$$

for the penalized Kohn-Vogelius functional. Applying Lemma 1 we can rewrite equation (23) in the form

$$\partial_t f + \nabla_s \nabla_s k + \frac{1}{2}|k|^2 k - k + dJ = 0 \text{ for } t > 0, \ \ f(0) = f_0. \tag{24}$$

Here the gradient dJ is defined by relation (3) and can be regarded as nonlinear nonlocal operator acting on Γ. Hence (24) is a nonlinear operator equation. It may be considered as a nonlocal perturbation of the elastic flow equation

$$\partial_t f + \nabla_s \nabla_s k + \frac{1}{2}|k|^2 k - k = 0 \text{ for } t > 0, \ \ f(0) = f_0.$$

In the literature, this equation is also named as straightening equation and, $1D$-Willmore flow equation. Now we have almost complete theory of this equation in the literature, we use the methods developed in the papers on such an equation in our analysis.

H.1 The Jordan curve $\Gamma \subset \Omega$ satisfies the energy condition

$$\frac{1}{2}\int_{\Gamma} |k^2| ds + \mathcal{L} \leqslant E_0.$$

H.2 There is $\nu > 0$ with the property

$$\text{dist}\left(\Gamma \setminus \Gamma_{3\kappa}, \Gamma_{2\kappa}\right) \geqslant \nu,$$

where κ, depending only on E_0, is given.

H.3 There is $\rho > 0$ such that dist $(\Gamma, \partial\Omega) > \rho$.

Every curve Γ satisfying Conditions **H.1**-**H.3** is a Jordan curve of the class $C^{1+\alpha}$, $0 < \alpha < 1/2$. It splits the domain Ω into two parts. The first $\Omega_i \Subset \Omega$ (inclusion)is the one-connected domain with boundary Γ. The second is the curvilinear annulus $\Omega_e = \Omega \setminus \overline{\Omega_i}$ bounded by Γ and $\partial\Omega$. For simplicity, we will assume that $\partial\Omega$ is a Jordan curve of the class C^∞.

Existence theory Assume that the initial data satisfy the following conditions:

I.1 The even integer number $m \geqslant 10$

I.2 The initial curve $\Gamma_0 = f_0$ satisfies conditions **H.1-H.3.**

I.3 There is a constant E_m such that

$$\int_{\Gamma_0} |\nabla_s^r k_0|^2 \, ds \leqslant E_m \ \text{ for all } \ 0 \leqslant r \leqslant m. \tag{25}$$

I.4 The length element $\sqrt{\mathbf{g}_0} = |\partial_\theta f_0|$ satisfies the condition

$$\|\sqrt{\mathbf{g}_0}\|_{C^{m-5}(\mathbb{S}^1)} \leqslant c_g < \infty.. \tag{26}$$

Theorem

Assume that the initial data satisfy Conditions **I.1-I.4**. Then there is a maximal $T \in (0, \infty]$ with the following properties. Problem (23) has a solution f such that

$$f \in C(0, T; C^{m-5}(\mathbb{S}^1)), \quad \partial_t f \in C(0, T; C^{m-9}(\mathbb{S}^1)). \tag{27}$$

Moreover, the Jordan curves $\Gamma(t) = f(t, \mathbb{S}^1)$, $t \in [0, T)$, are separated from $\partial\Omega$. If $T < \infty$, then there is a sequence $f(t_j)$, $t_j \to T$ as $j \to \infty$, such that $\operatorname{dist}(\Gamma(t_j), \partial\Omega) \to 0$, or (and) $f(t_j)$ converge in $C^1(\mathbb{S}^1)$ as $j \to \infty$ to some immersion f_∞ such that the limiting curve Γ_∞ has a self-intersection.