

MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Report No. 57/2012

DOI: 10.4171/OWR/2012/57

Mini-Workshop: Geometries, Shapes and Topologies in PDE-based Applications

Organised by
Michael Hintermüller, Berlin
Günter Leugering, Erlangen
Jan Sokolowski, Nancy

25 November – 1 December 2012

ABSTRACT. The aim of the workshop was to study geometrical objects and their sensitivities in applications based on partial differential equations or differential variational inequalities. Focus topics comprised analytical investigations, numerical developments, issues in applications as well as new and future directions. Particular emphasis was put on: (i) combined shape and topological sensitivity; (ii) extended topological expansions and their numerical realization; (iii) level set based shape and topology optimization.

Mathematics Subject Classification (2000): 49Q10, 49Q20.

Introduction by the Organisers

The Mini-Workshop was jointly organised by Michael Hintermüller, Günter Leugering and Jan Sokolowski.

Shape and topological sensitivities are important tools in many applications in shape design, geometrical optimization and geometrical evolution. Typical applications include the topological optimization of structures, optimization of shapes, geometrical inverse problems e.g. in mathematical image processing, or geometric evolution (like mean curvature flow or other shape gradient related flows). In this context, shape sensitivity typically aims at perturbations of underlying geometrical objects, domains or manifolds, in a direction normal to the given geometry (while keeping the topology of the geometry unchanged), whereas the topological expansion allows to study the sensitivity of a solution of a partial differential equation (PDE) posed on a given domain or manifold and the sensitivity of a geometry

dependent objective function with respect to changes of the topology of the underlying geometry, respectively. Such objective functions, occurring for instance in shape optimization, may depend both, directly and implicitly, e.g. through the solution of a (system of) PDEs, on the geometry of interest.

Starting from early work in the field by Murat and Simon, in recent years significant progress has been achieved in the understanding of geometrical objects as variable structures which might be subject to optimization procedures or geometrical evolution. Here we refer to the monographs by Sokolowski and Zolesio as well as Delfour and Zolesio for a summary of the state-of-the-art and further references in shape sensitivity and to work by Sokolowski and Zochovski for basic analytical concepts in topological sensitivity; further see the work by Allaire and Jouve as well as Garreau, Guillaume and Masmoudi where also numerical realizations are presented. Concerning the numerical realization we also mention that level set methods, pioneered by Osher and Sethian, are widely used tools.

Despite the aforementioned progress many important theoretical and numerical questions in shape and topological sensitivity remain widely open. It was therefore the aim of the workshop to bring together a rather diverse group of scientists with all of them being internationally renown researchers in the field and excelling in different branches of the theme of the workshop. Their expertise ranges from analytical investigations, the design and analysis of numerical solution algorithms to the realization and further development of the subject within applications in shape and topology optimization, geometric evolution and geometric inverse problems.

The workshop was attended by 17 participants from 7 countries. In total 13 talks were scheduled in a flexible time frame to allow for ample discussion time, a special lecture (in two parts) by P. Plotnikov on "Compressible Navier-Stokes Equations. Theory and Shape Optimization" related to the recent monograph by P. Plotnikov and J. Sokolowski was scheduled, and a round table discussion on challenges and future topics (including a tutorial on constrained shape optimization) took place on Thursday afternoon.

The various talks of the workshop addressed the following major topics areas:

Combined shape and topological sensitivity. Applications in geometric inverse problems, such as inclusion detection in computerized tomography, for instance, require the combination of topological sensitivities (for an automatized detection of the correct number and topological properties of objects hidden in a given domain from boundary measurements) and shape sensitivity (for adjusting the shape of the detected objects). Currently, the computation of these sensitivities is typically done in separate resulting in two-phase approaches on the numerical level which first apply topological derivatives for detecting inclusions and then shape sensitivities for local shape adjustments. Subsequently, these two phases are repeated until "convergence", i.e., stationarity with respect to both, topology and shape.

Clearly, the separate application of topological and shape derivatives is sub-optimal only as one may get stuck at local minimizers possibly far from global optimizers. This behavior is in particular unwanted in the context of geometric inverse problems as the latter typically suffer from numerous (and spurious) local

minimizers. Moreover, on the numerical level the two-phase approach requires the separate implementation of the derivatives and their associated induced geometry changes and thus leads to inefficiencies.

A similar need for a combined application of both sensitivity concepts arises in topology optimization (minimal compliance minimization etc.), the design of band gaps in crystals, in Mumford-Shah based image segmentation, as well as in many other applied problems.

Moreover, on the analytical side typically perimeter constraints need to be taken into account in order to have a well-posed shape/topology optimization problem (and to avoid homogenization). From the topological sensitivity point of view this, however, yields singularities due to the difference of dimensionality of the space for the perimeter vs. the change in topology (in the domain). Again, this is a point where both communities need to combine their strengths in order to handle this situation properly on the analytical as well as on the numerical level.

Extended topological expansions and their numerical realization. The current literature almost exclusively considers first order topological expansions only. Indeed, in many applications and in minimal compliance problems in particular, the associated topological gradients yield satisfactory results. Algorithmically, these gradients are realized by "punching" a small hole at the location, where the topological derivative is most negative (if it would be non-negative on the entire domain, then the current shape would be topologically stationary). When creating, at a time, more than one (small) hole in a structure subject to topology optimization, interactions between these holes become important. Such interactions appear to be typically captured by higher order topological expansions only. Further, in the context of geometric inverse problems, there is evidence that extended (beyond first order) topological expansions are indispensable to provide correct information on the location of hidden inclusions. We mention that in this application rather than creating holes in domains, properties of coefficients in PDE-operators are changed in an infinitesimally small ball-shaped domain indicating a change in material properties. The latter obviously also constitute a topological change.

Analytically, such higher order expansions require an improved asymptotic analysis for the solutions of various types of PDEs relevant in associated applications such as the Navier-Lamé system in elasticity, or, in the context of tomography, the Neumann-to-Dirichlet map for second order linear elliptic problems in electrical impedance tomography or Maxwell's system in magnetic induction tomography. Here, higher order expansions of the PDE solution with respect to a characteristic quantity of the considered topological change (e.g., the radius of a hole (elasticity) or an inclusion (tomography)) are needed.

Level set based shape and topology optimization and applications. In many of the aforementioned topics, which were addressed within the workshop, the numerical realization of the shape and topological sensitivity based calculus plays an important role. It is well-known that the level set method, which was popularized by the work of S. Osher and J. Sethian, represents a versatile tool in the numerical realization of moving interface and free boundary problems. Over the years, highly

efficient algorithms for the numerical realization of the level set method (narrow band, fast marching method,...) have been invented, analyzed, implemented and used successfully in various applications.

Concerning the combined use of shape gradient related descent methods intertwined with topological sensitivity, level set based techniques are significantly less advanced. In contrast to moving boundary problems, in the context of shape and topology optimization the (pseudo)time marching through the level set equation, a PDE of Hamilton-Jacobi type, when equipped with appropriate descent criteria acts like a line search method well-known from numerical optimization. As a consequence, stability criteria such as the Courant-Friedrichs-Levy (CFL) condition for the discretization in time can be significantly relaxed and, thus, allow for larger geometry changes from one iteration to the next.

Mini-Workshop: Geometries, Shapes and Topologies in PDE-based Applications

Table of Contents

Pavel Plotnikov (joint with Jan Sokolowski)	
<i>Compressible Navier-Stokes Equations. Shape Optimization</i>	3381
Volker Schulz	
<i>Efficient Usage of the Shape Hessian in PDE Constrained Shape Optimization and a Riemannian Perspective</i>	3383
Antonio André Novotny (joint with Alfredo Canelas, Antoine Laurain)	
<i>A Non-Iterative Method for the Inverse Potential Problem Based on the Topological Derivative</i>	3383
James A. Sethian (joint with Robert I. Saye)	
<i>Applications of the Voronoi Implicit Interface Method</i>	3387
Dietmar Hömberg (joint with Michael Hintermüller, Kevin Sturm)	
<i>On a Phase Field Approach to Topology Optimization</i>	3390
Bojan Guzina	
<i>Bits and Pieces Put Together to Present a Semblance of a Whole</i>	3392
Samuel Amstutz	
<i>Techniques for Topology Optimization under Constraints</i>	3394
Harbir Antil (joint with Ricardo H. Nochetto, Patrick Sodr�)	
<i>Optimal Control of a Free Boundary Problem with Surface Tension Effects</i>	3397
Michael Stingl (joint with Bastian Schmidt)	
<i>Parametric Shape Optimization Revisited</i>	3400
Michel C. Delfour	
<i>Groups of Transformations for Geometrical Identification Problems: Metrics, Geodesics</i>	3403
Antoine Laurain (joint with Carlos Conca, Rajesh Mahadevan)	
<i>Minimization of the Ground State for Two Phase Conductors in Low Contrast Regime</i>	3407
Jan Friederich (joint with G�nter Leugering, Paul Steinmann)	
<i>Sensitivities for Graph Operations in Finite Element Meshes</i>	3411

Abstracts

Compressible Navier-Stokes Equations. Shape Optimization

PAVEL PLOTNIKOV

(joint work with Jan Sokolowski)

The talk is devoted to the study of boundary value problems for equations of viscous gas dynamics, named compressible Navier-Stokes equations. The principal significance of the mathematical theory of Navier-Stokes equations lies in the central role they now play in fluid dynamics. We focus on existence results for the inhomogeneous in/out flow problem, in particular the problem of the flow around a body placed in a finite domain, on the stability of solutions with respect to domain perturbations, on the domain dependence of solutions to compressible Navier-Stokes equations, and on the drag optimization problem.

Existence theory The problem of the flow of a viscous gas around a moving rigid body $S \in \mathbb{R}^d$, $d = 2, 3$, can be formulated as follows. Choose an arbitrary hold-all $B \subset \mathbb{R}^3$, for instance, a sufficiently large ball, such that $S \subset B$. Next, we transfer the boundary conditions from infinity to ∂B and arrive at the following boundary value problem for the velocity \mathbf{v} and the density ρ . Find functions (\mathbf{v}, ρ) satisfying

$$\begin{aligned} \partial_t(\rho \mathbf{v}) + \operatorname{div}(\rho \mathbf{v} \otimes \mathbf{v}) - \frac{1}{\operatorname{Re}} \operatorname{div} \mathbb{S}(\mathbf{v}) \\ + \frac{1}{\operatorname{Ma}^2} \nabla p(\rho) + \mathbb{C} \mathbf{v} = \rho \mathbf{f} \quad \text{in } \Omega \times (0, T), \end{aligned}$$

$$\partial_t \rho + \operatorname{div}(\rho \mathbf{v}) = 0 \quad \text{in } \Omega \times (0, T),$$

$$\mathbf{v} = 0 \quad \text{on } \partial S \times (0, T), \quad \mathbf{v} = \mathbf{V} \quad \text{on } \partial B \times (0, T),$$

$$\rho = \varrho_\infty \quad \text{on } \Sigma_{\text{in}},$$

$$\mathbf{v}(x, 0) = \mathbf{V}(x, 0) \quad \text{in } \Omega, \quad \rho(y, 0) = \varrho_\infty(y) \quad \text{in } \Omega,$$

where $\mathbf{V}, \mathbf{f} : \mathbb{R}^d \times [0, T]$ are given smooth vector fields, $\varrho_\infty : \mathbb{R}^d \rightarrow \mathbf{R}^+$ is a given nonnegative bounded function, \mathbb{C} is a skew-symmetric matrix,

$$\Omega = B \setminus S, \quad \Sigma_{\text{in}} = \{(x, t) \in \partial B \times (0, T) : \mathbf{V}(x, t) \cdot \mathbf{n}(y) > 0\},$$

$$\mathbb{S}(\mathbf{v}) = \nabla \mathbf{v} + (\nabla \mathbf{v})^\top + (\lambda - 1) \operatorname{div} \mathbf{v} \mathbb{I}.$$

The peculiarity of this problem is that we deal with the boundary value problem for the mass balance equations. We prove that for the adiabatic exponent $\gamma > d/2$, the problem has a renormalized solution. We follow the multilevel regularization scheme proposed by E. Feireisl, but with a different regularization technique. We show that the solution admits the energy estimate and the pressure $p(\rho)$ is locally integrable with some exponent greater than 1.

Stability of solutions with respect to nonsmooth data and domain perturbations. Propagation of rapid oscillations in compressible fluids. In compressible viscous

flows, any irregularities in the initial and boundary data are transferred inside the flow domain along fluid particle trajectories. We develop a new method for the study of the propagation of rapid oscillations of the density, which can be regarded as acoustic waves. The main idea is that any rapidly oscillating sequence is associated with a parametrized family μ_{xt} of probability measures on the real line named the Young measure. We establish that the distribution function $f(x, t, s) = \mu_{x,t}(-\infty, s]$ satisfies a differential relation named a kinetic equation. A remarkable property of compressible Navier-Stokes equations is that in this particular case the kinetic equation can be written in closed form as

$$\partial_t f + \operatorname{div} (f \mathbf{v}) - \partial_s \left(s f \operatorname{div} \mathbf{v} + \frac{s}{\lambda + 1} \int_{(-\infty, s]} (p(\tau) - \bar{p}) d_\tau f(x, t, \tau) \right) = 0.$$

The kinetic equation being combined with the momentum balance equations gives a closed system of integro-differential equations which describes the propagation of rapid oscillations in a compressible viscous flow. Notice that oscillations can be induced not only by oscillations of initial and boundary data, but also by irregularities of the boundary of the flow domain. We also prove that if the data are deterministic and the function f satisfies some integrability condition, then any solution to the kinetic equation satisfying some integrability conditions is deterministic.

Domain dependance of solutions to compressible Navier-Stokes equations We apply the kinetic equation method to the analysis of the domain dependence of solutions to compressible Navier-Stokes equations. We restrict our considerations to the problem of the flow around an obstacle placed in a fixed domain. Recall that in this problem, the flow domain $\Omega = B \setminus S$ is a condenser type domain, B is a fixed hold all domain and S is a compact obstacle. We introduce the notion of the Kuratowski-Mosco. To this end Denote by $C_S^\infty(B)$ the set of all smooth functions defined in B and vanishing on $S \subset B$. Let $W_S^{1,2}(B)$ be the closure of $C_S^\infty(B)$ in the $W^{1,2}(B)$ -norm. A sequence of compact sets $S_n \subset B$ is said to converge to S in the Kuratowski-Mosco sense if

- there is a compact set $B' \subset B$ such that $S_n, S \subset B'$;
- for any sequence $u_n \rightharpoonup u$ weakly convergent in $W^{1,2}(B)$ with $u_n \in W_{S_n}^{1,2}(B)$, the limit element u belongs to $W_S^{1,2}(B)$;
- whenever $u \in W_S^{1,2}(B)$, there is a sequence $u_n \in W_{S_n}^{1,2}(B)$ with $u_n \rightarrow u$ strongly in $W^{1,2}(B)$.

We show that if a sequence S_n of compact obstacles converges to a compact obstacle S in the Hausdorff and the Kuratowski-Mosco sense, then the sequence of corresponding solutions to the in/out flow problem contains a subsequence which converges to a solution to the in/out flow problem in the limiting domain. Moreover, we prove that the typical cost functionals, such as the work of hydrodynamical forces, are continuous with respect to \mathcal{S} -convergence. As a conclusion we establish the solvability of the problem of minimization of the work of hydrodynamical forces in the class of obstacles with a given fixed volume.

REFERENCES

- [1] P.I. Plotnikov, J. Sokolowski, *Compressible Navier-Stokes Equations. Theory and Shape Optimization*, Birkhäuser, Basel (2012).

Efficient Usage of the Shape Hessian in PDE Constrained Shape Optimization and a Riemannian Perspective

VOLKER SCHULZ

Shape optimization is an industrially highly important subject of research. The shape calculus is a very efficient way for the generation of shape derivatives circumventing computationally expensive mesh sensitivities. The resulting numerical methods can be greatly accelerated by approximations of the shape Hessian. This is demonstrated in practical applications from aerodynamics, thermoelastics and acoustics. On the other hand, this success raises the natural question about a theoretical framework for the explanation of this effect. The standard framework in shape calculus is not of much help since it lacks a Taylor series expansion and the standard shape Hessian is not symmetric. A novel approach via shape manifolds and the according Riemannian geometries is demonstrated based on the influential work of Peter Michor. As a result, a Taylor series expansion for smooth shapes is presented together with all results, one would like to have: quadratic Newton convergence, second order sufficiency conditions. It remains to bridge the gap between C^∞ for the shape manifold theory so far and the usual Sobolev spaces from PDE constrained optimization.

A Non-Iterative Method for the Inverse Potential Problem Based on the Topological Derivative

ANTONIO ANDRÉ NOVOTNY

(joint work with Alfredo Canelas, Antoine Laurain)

Problem Formulation. Let $\Omega \subset \mathbb{R}^2$ be an open and bounded domain, with smooth boundary $\partial\Omega$ or convex. Define

$$(1) \quad PC_\gamma(\Omega) := \{b \in L^\infty(\Omega), b = \gamma_0 \chi_{\Omega \setminus \omega} + \gamma_1 \chi_\omega | \omega \subset \Omega \text{ measurable}\},$$

where χ_ω denotes the indicator function of the set ω and $\gamma = (\gamma_0, \gamma_1) \in \mathbb{R}^2$ is given. The inverse potential problem reads: given $q^* \in H^{-1/2}(\partial\Omega)$ and $u^* \in H^{1/2}(\partial\Omega)$, find the source $b^* \in PC_\gamma(\Omega)$ such that there exists a solution to

$$(2) \quad \left\{ \begin{array}{l} -\Delta u = b^* \quad \text{in } \Omega \\ u = u^* \\ -\partial_n u = q^* \end{array} \right\} \text{ on } \partial\Omega \quad ,$$

Let $m > 0$ be a given integer, and $\mathcal{I} = \{1, \dots, m\}$. We also assume that the sets ω in $PC_\gamma(\Omega)$ are of the form:

$$(3) \quad \omega = \bigcup_{i \in \mathcal{I}} \omega_i \quad \text{with} \quad \omega_i \cap \omega_j = \emptyset \quad \text{for} \quad i \neq j.$$

with ω_i measurable, star-shaped and simply connected sets. The system of equations (2) is over-determined and may have no solutions for any b^* , so that the problem of reconstructing b^* is not well-posed in general, especially for noisy data q^* and u^* . We look for an approximate solution by reformulating the inverse problem as a minimization problem. The idea is to penalize one of the two boundary conditions on $\partial\Omega$. To this end, we minimize the so-called Kohn-Vogelius functional:

$$(4) \quad \min_{b \in PC_\gamma(\Omega)} J(b) := \frac{1}{2} \int_{\Omega} (u^D(b) - u^N(b))^2,$$

where $u^D(b)$ and $u^N(b)$ are solutions to the following auxiliary problems:

$$(5) \quad \left\{ \begin{array}{l} -\Delta u^D = b \quad \text{in} \quad \Omega, \\ u^D = u^* \quad \text{on} \quad \partial\Omega. \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{l} -\Delta u^N = b + c \quad \text{in} \quad \Omega, \\ -\partial_n u^N = q^* \quad \text{on} \quad \partial\Omega, \\ \int_{\Omega} u^N = \int_{\Omega} u^D. \end{array} \right.$$

The constant $c = c(b)$ is introduced in order to satisfy the compatibility condition for the Neumann problem. We obtain

$$c(b) = \frac{1}{|\Omega|} \left(\int_{\partial\Omega} q^* - \int_{\Omega} b \right)$$

We observe that if $b \in PC_\gamma(\Omega)$ satisfies $J(b) = 0$, then $u^D(b) = u^N(b)$ which implies $c(b) = 0$ and $u^D(b) = u^N(b)$ then solves the over-determined problem (2).

Topological Asymptotic Analysis. The topological derivative [2, 3, 7] is the first term of the asymptotic expansion of a given scalar-valued shape functional $\mathcal{J}(\Omega)$ with respect to a small parameter measuring the size of singular perturbations, such as holes, inclusions, or cracks. The topological derivative has been successfully applied in topology optimization, inverse problems and image processing; see for instance [1, 4, 5], respectively. In order to introduce these ideas, let us consider a non-smooth perturbation of Ω by removing a small set $\omega_{\varepsilon, \hat{x}}$ of size $\varepsilon > 0$ and center $\hat{x} \in \Omega$, or the union $\omega_{\mathbf{e}, \hat{\mathbf{x}}} := \cup_{i \in \mathcal{I}} \omega_{\varepsilon_i, \hat{x}_i}$ of such sets, where $\mathbf{e} := \{\varepsilon_i\}_{i \in \mathcal{I}}$, $\hat{\mathbf{x}} := \{\hat{x}_i\}_{i \in \mathcal{I}}$. Here, \hat{x}_i is an arbitrary point of Ω and $\varepsilon_i > 0$. Take $m = 1$ for simplicity and assume we have the following topological asymptotic expansion with respect to ε :

$$(6) \quad \mathcal{J}(\Omega \setminus \omega_{\varepsilon, \hat{x}}) = \mathcal{J}(\Omega) + f_1(\varepsilon) D_T^1 \mathcal{J}(\hat{x}) + f_2(\varepsilon) D_T^2 \mathcal{J}(\hat{x}) + \mathcal{R}(\varepsilon),$$

where $f_1(\varepsilon)$ and $f_2(\varepsilon)$ are positive functions such that

$$(7) \quad \lim_{\varepsilon \rightarrow 0} f_1(\varepsilon) = 0 \quad \text{and} \quad \lim_{\varepsilon \rightarrow 0} \frac{f_2(\varepsilon)}{f_1(\varepsilon)} = 0.$$

We assume that the remainder satisfies $\mathcal{R}(\varepsilon) = o(f_2(\varepsilon))$. The terms $D_T^1 \mathcal{J}(\hat{x})$ and $D_T^2 \mathcal{J}(\hat{x})$ are called first and second order topological derivatives of \mathcal{J} and are used to approximate $\mathcal{J}(\Omega \setminus \omega_{\mathbf{e}, \hat{x}})$. For our purposes, let us consider the particular case $\omega_{\mathbf{e}, \hat{x}} = \cup_{i \in \mathcal{I}} B(\varepsilon_i, \hat{x}_i)$, where $B(\varepsilon_i, \hat{x}_i)$ is a disk of radius ε_i and center $\hat{x}_i \in \Omega$. We consider a perturbed source term of the form

$$(8) \quad b_{\mathbf{e}, \hat{x}} = \gamma_0 \chi_{\Omega \setminus \omega_{\mathbf{e}, \hat{x}}} + \gamma_1 \sum_{i \in \mathcal{I}} \chi_{B(\varepsilon_i, \hat{x}_i)}, \quad B(\varepsilon_i, \hat{x}_i) \cap B(\varepsilon_j, \hat{x}_j) = \emptyset, \quad i \neq j.$$

The topological asymptotic expansion of the shape functional reads

$$(9) \quad \begin{aligned} \mathcal{J}(\Omega \setminus \omega_{\mathbf{e}, \hat{x}}) = J(b_{\mathbf{e}, \hat{x}}) &= \frac{1}{2} \int_{\Omega} (u^D(b) - u^N(b))^2 \\ &- \pi \int_{\Omega} (u^D(b) - u^N(b)) \sum_{i \in \mathcal{I}} \varepsilon_i^2 h_i + \frac{\pi^2}{2} \int_{\Omega} \left(\sum_{i \in \mathcal{I}} \varepsilon_i^2 h_i \right)^2, \end{aligned}$$

where the functions h_i are solutions of

$$(10) \quad \begin{cases} -\Delta h_i = \frac{\gamma_0 - \gamma_1}{|\Omega|} & \text{in } \Omega \\ -\partial_n h_i = g_i & \text{on } \partial\Omega, \\ \int_{\Omega} h_i = 0 \end{cases},$$

with $g_i := \partial_n v_i$ on $\partial\Omega$ and v_i is the solution of

$$(11) \quad \begin{cases} -\Delta v_i = (\gamma_1 - \gamma_0) \delta_i & \text{in } \Omega \\ v_i = 0 & \text{on } \partial\Omega, \end{cases},$$

where $\delta_i(x) = \delta(x - \hat{x}_i)$ is used to denote the Dirac mass concentrated at \hat{x}_i .

Numerical Experiments. We optimize $\mathcal{J}(\Omega \setminus \omega_{\mathbf{e}, \hat{x}})$ in (9) with respect to \mathbf{e}, \hat{x} . Differentiating (9), the first order optimality conditions with respect to the variables $a_i := \pi \varepsilon_i^2, i \in \mathcal{I}$ lead to the following linear system:

$$(12) \quad H_{ij} a_j = d_i \quad \text{for } i, j \in \mathcal{I},$$

where d_i and H_{ij} are given by

$$(13) \quad d_i = (\gamma_1 - \gamma_0) (p^D(\hat{x}_i) + p^N(\hat{x}_i)) \quad \text{and} \quad H_{ij} = \int_{\Omega} h_i h_j.$$

The adjoint states p^D and p^N satisfy similar equations as u^D and u^N , with $u^D - u^N$ as source terms. Once the above linear system is solved, we optimize with respect to the locations $\{\hat{x}_i\}_{i \in \mathcal{I}}$ of the objects. The problem is discretized using the finite element method. The resolution of (12) is combinatorial in the number of balls m so that m must stay small. In order to keep the computational cost tractable we solve (12) on a sub-grid of the grid where the partial differential equations are solved. In the examples we take $\Omega = (0, 1) \times (0, 1)$, $\gamma_0 = 1$ and $\gamma_1 = 10$. To obtain

noisy synthetic data, the true source term b^* is corrupted with white gaussian noise. The resulting level of noise in the boundary measurement is computed as

$$noise = \|q^* - q_n^*\|_{L^2(\partial\Omega)} / \|q^*\|_{L^2(\partial\Omega)} \times 100,$$

where q_n^* is the noisy boundary measurement used as the synthetic data. In Figures 1 to 3 some examples of reconstructions of b are plotted.

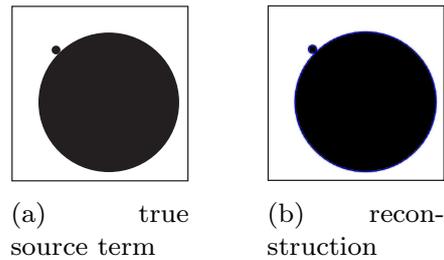


FIGURE 1. Two objects: true source term (left) and reconstruction using two balls (right) without noise in the data.

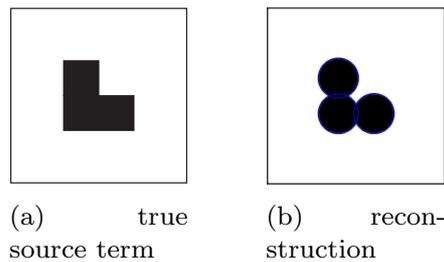


FIGURE 2. One object: true source term (left) and reconstruction using three balls (right) without noise in the data.

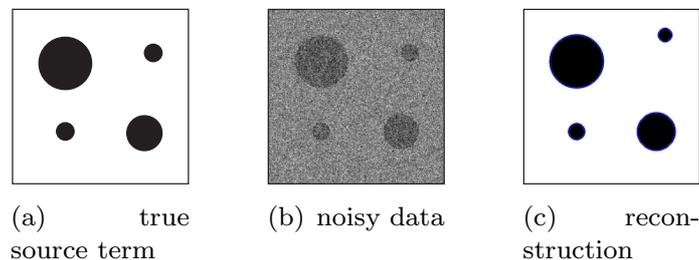


FIGURE 3. Four objects: true source term (left), noisy source term b^* (center) and obtained reconstruction using four balls with 4.04% of resulting noise on q^* (right).

Acknowledgements. We would like to thank Bojan Guzina for helpful comments on this paper.

REFERENCES

- [1] S. Amstutz, A.A. Novotny, and E. de Souza Neto. Topological derivative-based topology optimization of structures subject to Drucker-Prager stress constraints. *Comp. Meth. Appl. Mech. Engrg.* 233–236:123–136, 2012.
- [2] J. C ea, S. Garreau, P. Guillaume, and M. Masmoudi. The shape and topological optimizations connection. *Comp. Meth. Appl. Mech. Engrg.* 188(4):713–726, 2000.
- [3] H. Eschenauer, V. Kobelev, and A. Schumacher. Bubble method for topology and shape optimization of structures. *Structural Optimization*, 8(1):42–51, 1994.
- [4] M. Hinterm uller, A. Laurain, and A.A. Novotny. Second-order topological expansion for electrical impedance tomography. *Adv. Comp. Math.* 36(2):235–265, 2012.
- [5] M. Hinterm uller and A. Laurain. Multiphase image segmentation and modulation recovery based on shape and topological sensitivity. *J. Math. Im. Vis.* 35:1–22, 2009.
- [6] V. Isakov. *Inverse problems for partial differential equations*. Springer, New York, 1998.
- [7] J. Sokolowski and A. Zochowski. On the topological derivative in shape optimization. *SIAM J. Contr. Opt.* 37(4):1251–1272, 1999.

Applications of the Voronoi Implicit Interface Method

JAMES A. SETHIAN

(joint work with Robert I. Saye)

Many problems involve the physics of multiply-connected moving interfaces. Examples include liquid foams (e.g. soap bubbles, polyurethane and colloidal mixtures), and solid foams, such as wood and bone. Manufactured solid foams lead to lightweight cellular engineering materials, including crash absorbent aluminum foams, and controlling foams is critical in chemical processing.

These problems have multiple domains which share common walls meeting in multiple junctions. Boundaries move under forces which depend on both local and global geometric properties, such as surface tension and volume constraints, as well long-range physical forces, including incompressible flow, membrane permeability, and elastic forces.

Producing good mathematical models and numerical algorithms that capture the motion of these interfaces is challenging, especially at junctions where multiple interfaces meet, and when topological connections change. Methods have been proposed, including front tracking, volume of fluid, variational, and level set methods. It has remained a challenge to robustly and accurately handle the wide range of possible motions of an evolving, highly complex, multiply-connected interface separating a large number of phases under time-resolved physics.

We have recently developed [4, 5] a mathematical perspective and accompanying numerical methodology for tracking interfaces in general multiphase problems. Our “Voronoi Implicit Interface Method” (VIIM) has a variety of features, including:

- *Accuracy, consistency, efficiency*: The method works in any number of dimensions, using a fixed Eulerian mesh, and a single function plus an indicator function to track the entire multiphase system. Geometric quantities

and constraints are accurately computed, and phases are coupled together in a consistent fashion, with no gaps, overlaps, or ambiguities.

- *Multiple junctions and topological change:* Multiple junctions, such as triple points, are all handled naturally and automatically, as well as breakage, merger, creation, and disappearance of phases. No special attention is paid to discontinuous topological change.
- *Coupling with time-dependent physics:* The method uses a physical time step, which then allows coupling complex physics into the interface evolution. Feedback from the physics affects the interface, and changes to the interface affects the physics.

Briefly, these Voronoi Implicit Interface Methods work as follows. Given a collection of interfaces in an initial configuration, the unsigned distance function ϕ is constructed on a background mesh. Thus, the zero level set of the unsigned distance function corresponds to the interface. At each mesh point, both the distance (which is a non-negative real number) and an indicator function (an integer flag) are stored. Typical implementations have used a regular Cartesian mesh, though unstructured non-rectangular meshes may also be used. The central idea of the method is to then alternate between two steps:

- Advance this unsigned distance function on the background mesh, using the level set initial value PDE [3, 7] of the form

$$\phi_t + F|\nabla\phi| = 0,$$

where F is the velocity, defined throughout the domain and determined by solving the associated physics.

- Use the ϵ level sets of this advanced solution to reconstruct a new unsigned distance function. This is done by first computing the Voronoi interface from the ϵ level sets: this corresponds to the set of all points equidistant from at least two of the ϵ level sets from different phases. This Voronoi interface is then used to rebuild the unsigned distance function.

This is the most straightforward implementation of the method. More efficient and sophisticated techniques include the use of narrow banding [1] to limit computational labor to a small region near the interface, a fast Eikonal solver [6, 2] to find the new unsigned distance from the ϵ level sets without explicitly constructing the front, and careful data structures which allow any non-negative value for ϵ , including $\epsilon = 0^+$. For details, see [4, 5].

As application, Figure 1 illustrates the results for a three-dimensional simulation of a variable density fluid flow, computed on a 128^3 grid with slip boundary conditions, using $\epsilon = 0^+$. The simulation starts with 15 heavy phases and approximately 100 less dense phases. The incompressible Navier-Stokes equations are solved, using a second order projection method, and coupled to the Voronoi Implicit Interface Method. For all but the last snapshot in Figure 1, the heavier phase is dark, while the other phases have been rendered mostly transparent, together with the triple line junctions as a network of curves. In the last snapshot,

at time $t = 1.8$, we have rendered the bulk foam opaque, to make the structure of the foam more obvious.

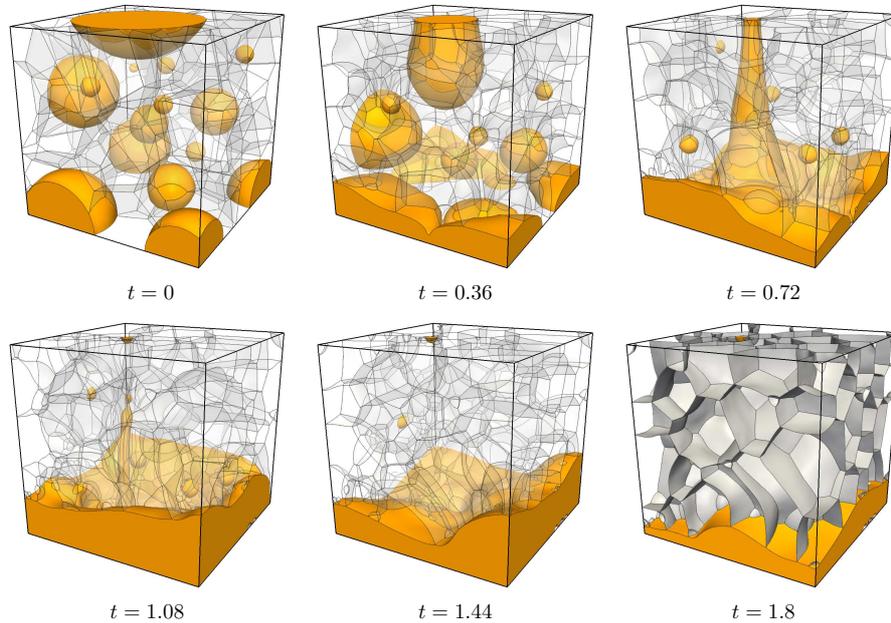


FIGURE 1. Results of a fluid flow simulation in three dimensions with gravity, in which the orange colored phase is more viscous and more dense than the other phases. The bulk foam is rendered mostly transparent except for the last frame, where it is rendered opaque to make the structure more prominent.

REFERENCES

- [1] Adalsteinsson, D., and Sethian, J.A., *A Fast Level Set Method for Propagating Interfaces*, J. Comp. Phys., 118, 2, pp. 269–277, 1995.
- [2] Chopp, D.L. *Some Improvements of the Fast Marching Method* SIAM Journal Scientific Computing, 23, 1, 2001.
- [3] Osher, S., and Sethian, J.A., *Fronts Propagating with Curvature-Dependent Speed: Algorithms based on Hamilton-Jacobi Formulations*, J. Comp. Phys., 79, pp.12-49, (1988).
- [4] Saye, R. and Sethian, J.A., *The Voronoi Implicit Interface Method for Computing Multiphase Physics*, Proceedings of the National Academy of Sciences, published on-line, Nov. 21, 2011.
- [5] Saye, R. and Sethian, J.A., *Analysis and Applications of the Voronoi Implicit Interface Method*, submitted for publication, Nov. 2011, Journal Computational Physics.
- [6] Sethian, J.A., *A Fast Marching Level Set Method for Monotonically Advancing Fronts*, Proc. Nat. Acad. Sci., 93, 4, pp.1591–1595, 1996.
- [7] Sethian, J.A., *Level Set Methods and Fast Marching Methods*, Cambridge Univ. Press, 1999.

On a Phase Field Approach to Topology Optimization

DIETMAR HÖMBERG

(joint work with Michael Hintermüller, Kevin Sturm)

By definition, distortion means undesired alterations in workpiece size and shape, which may happen as a side effect at some stage in the manufacturing chain. Assuming that no rate effects occur during the heat treatment, i.e., neglecting transformation-induced plasticity, one can tackle this problem mathematically in a hybrid approach. In the first step the optimal microstructure for distortion compensation is computed solving a shape design problem subject to a stationary mechanical equilibrium problem. In the second step an optimal cooling strategy is computed to realize this microstructure. While the latter has been studied extensively, the goal of this presentation was to explain a novel approach to compute an optimal microstructure or better phase mixture to compensate for distortion.

We assume that the workpiece domain $D \subset \mathbf{R}^3$ consists of a microstructure with two phases in the domains $\bar{\Omega} \subset D$ and $D \setminus \Omega$, separated by a sharp interface Γ . For instance one might think of these two phases as having been created from one parent phase during a heat treatment. To distinguish between the subdomains we introduce the characteristic function $\chi = \chi_\Omega$ of the set Ω , which is equal to 1 for $x \in \Omega$ and 0 otherwise.

Now, assume the workpiece to be in equilibrium. Then the stress tensor σ satisfies

$$\begin{aligned} (1) \quad & -\operatorname{div} \sigma = 0, \quad \text{in } D \\ (2) \quad & \sigma n = 0, \quad \text{in } \Gamma^N \\ (3) \quad & \mathbf{u} = 0, \quad \text{in } \Gamma_0 \end{aligned}$$

with $\bar{\Gamma}^N \cup \bar{\Gamma}_0 = \partial D$. According to Hooke's law only elastic strains contribute to the stress, so in the case of small deformations we obtain

$$(4) \quad \sigma = A(\varepsilon(\mathbf{u}) - \tilde{\varepsilon}),$$

with the stiffness tensor A , the internal strain $\tilde{\varepsilon}$ and the linearized overall strain

$$\varepsilon(\mathbf{u}) = \frac{1}{2}(\mathcal{D}\mathbf{u} + (\mathcal{D}\mathbf{u})^T).$$

In general, the stiffness might be different in both subdomains, hence we make the ansatz

$$(5) \quad A = A_\chi(x) := \chi(x)A_1 + (1 - \chi(x))A_2.$$

The main reason for the occurrence of internal stresses lies in the different densities of the two subdomains. Thus we make an analogous mixture ansatz, i.e.

$$\tilde{\varepsilon} = \tilde{\varepsilon}_\chi(x) := \chi(x)\tilde{\varepsilon}_1 + (1 - \chi(x))\tilde{\varepsilon}_2,$$

and assume in addition isotropy, i.e.

$$A_i \tilde{\varepsilon}_i = \beta_i(x)I,$$

where I is the identity matrix. Then the constitutive relation reads as

$$(6) \quad \sigma_\chi(x) = A_\chi \varepsilon(\mathbf{u}) - \beta_\chi I,$$

with

$$(7) \quad \beta_\chi(x) := \chi(x)\beta_1 + (1 - \chi(x))\beta_2.$$

As the phases have different densities, we may expect internal stresses along the interface Γ even if no external forces are performed, leading to a deformation of the outer shape. Our aim is utilize this effect by changing the fractions of the two phases or better by changing the interface Γ to achieve a desired outer shape. To this end, we choose a generic cost functional

$$J(u, \chi) = \int_{\Sigma_1} L(u) ds = \int_{\Sigma_1} |u - u^d|^2 ds + \alpha \mathcal{P}_D(\Omega)$$

with $\Sigma_1 \subset \Sigma_N$ and

$$\mathcal{P}_D(\Omega) = \|\nabla \chi_\Omega\|_{M^1(D)^n}.$$

In [3] we investigated the resulting optimal shape design problem and derived necessary optimality conditions. For the numerical computation of optimal subdomains we proceed as in [1] and employ a phase field relaxation to the problem. This means, we replace the perimeter term in the cost functional by a Ginzburg-Landau term, i.e.,

$$\int_D \left(\frac{\gamma\delta}{2} |\nabla \varphi|^2 + \frac{\gamma}{\delta} \psi(\varphi) \right) dx,$$

with double-well potential $\psi(\varphi) = c_1(1 - \varphi^2)^2$, $c_1 > 0$. We use an L^2 gradient flow dynamics for φ with an artificial time variable t . The resulting system, consisting of a parabolic equation for the phase field variable φ coupled to two elliptic equations for the state and its adjoint is studied in [2].

REFERENCES

- [1] L. Blank, et al., *Phase-field approaches to structural topology optimization*. Preprint No. 06/2010, Universität Regensburg Mathematik.
- [2] C. Chelminski, D. Hömberg, T. Petzold, *On a Phase Field Approach to Distortion Compensation*. In preparation.
- [3] D. Hömberg, M. Hintermüller, K. Sturm, *Shape Optimization for a Sharp Interface Model of Distortion Compensation*. In preparation.

Bits and Pieces Put Together to Present a Semblance of a Whole

BOJAN GUZINA

Abstract. This work examines the performance of topological sensitivity as a tool for tackling the inverse scattering of scalar waves in the high-frequency regime, when the wave length of the incident field is small relative to the remaining length scales in the problem. To provide a focus in the study, it is assumed that the obstacle is convex and impenetrable (of either Dirichlet or Neumann type), and that the full-waveform measurements of the scattered field are taken over a sphere whose radius is finite, yet large relative to the size of the sampling region. In this setting, the formula for topological sensitivity is expressed a pair of nested surface integrals – one taken the measurement sphere, and the other over the surface of a hidden obstacle. By way of multipole expansion, the inner integral (over the measurement surface) is reduced to a set of antilinear forms in terms of the Green’s function and its gradient. The remaining expression is distilled by evaluating the scattered field on the surface of the obstacle via Kirchhoff (physical optics) approximation, and deploying the method of stationary phase to evaluate the remaining integral. In this way the topological sensitivity is expressed as a sum of the closed-form expressions, signifying the contribution of critical points on the “illuminated” part of the surface of a hidden obstacle. Thus obtained result explicitly demonstrates the localizing nature of the topological sensitivity and, via numerical simulations, helps better understand some of the reconstruction patterns observed in earlier works.

Introduction. Since its inception within the context of shape optimization [1], the notion of topological sensitivity has been generalized and applied to deal with inverse scattering problems in acoustics [2,3], electromagnetism [4], and elastodynamics [5]. In the reconstruction approach the topological sensitivity, which quantifies the perturbation of a given cost functional due to the nucleation of an infinitesimal defect in the (reference) background medium, is used as an effective obstacle indicator through an assembly of sampling points where it attains extreme negative values. Typically, formulas for the topological sensitivity are amenable to an explicit representation in terms of the wavefields computed exclusively for the reference domain, which is the source of computational efficiency of this class of inverse scattering solutions. However, with the exception of the treatment of point-like scatterers [6], the justification for the performance of this class of inverse scattering solutions has been notably lacking. To help bridge the gap, this work aims to expose the essence of the topological sensitivity (TS) indicator in the high-frequency regime, when the scatterer extends many wavelengths of the incident wavefield.

Approach. Consider the scattering of time-harmonic scalar waves by a convex impenetrable obstacle $D \subset \mathcal{B}_1 \subset \mathbb{R}^3$ with smooth boundary $S = \partial D$ and outward normal \mathbf{n} , where \mathcal{B}_1 is an open ball of radius R_1 centered at the origin. On denoting by \tilde{u} the scattered field generated by the action of an incident field u^i on D , it is

assumed that the total field

$$u(\boldsymbol{\xi}) := u^i(\boldsymbol{\xi}) + \tilde{u}(\boldsymbol{\xi}), \quad \boldsymbol{\xi} \in \mathbb{R}^3 \setminus \bar{D}$$

is monitored over a closed measurement surface $\Gamma^{\text{obs}} = \partial\mathcal{B}_2$, where \mathcal{B}_2 is an open ball of radius $R_2 = \alpha^{-1}R_1$ ($\alpha \ll 1$) centered at the origin, see Fig. 1. The reference

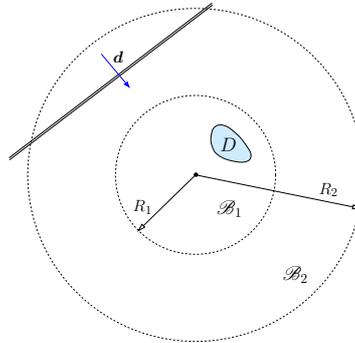


FIGURE 1. Obstacle $D \in \mathbb{R}^3$ illuminated by plane waves.

background medium is assumed to be homogeneous with wave speed c and mass density ρ . Writing the germane time dependence as $e^{i\omega t}$ where ω denotes the frequency of excitation, the incident field is for simplicity assumed in the form of a plane wave, $u^i = e^{-ik\boldsymbol{\xi} \cdot \mathbf{d}}$, where $k = \omega/c$.

On substituting the integral representation of the scattered field over Γ^{obs} into the adjoint-field formula [3] for TS and reversing the order of integration over S and Γ^{obs} , the expression for TS in the case of a sound-soft (Dirichlet) obstacle, taken here as an example, can be written as

$$(1) \quad \mathbb{T}(\mathbf{x}^\circ, \beta, \gamma) \\ = 2\text{Re} \left\{ (1 - \beta) \nabla u^i(\mathbf{x}^\circ) \cdot \mathbf{A} \cdot \int_S \bar{u}_{,n}^i(\boldsymbol{\zeta}) \int_{\Gamma^{\text{obs}}} \bar{G}(\boldsymbol{\xi}, \boldsymbol{\zeta}, k) \nabla G(\boldsymbol{\xi}, \mathbf{x}^\circ, k) d\Gamma_\xi dS_\zeta \right. \\ \left. - (1 - \beta\gamma^2) k^2 u^i(\mathbf{x}^\circ) \int_{S^f} \bar{u}_{,n}^i(\boldsymbol{\zeta}) \int_{\Gamma^{\text{obs}}} \bar{G}(\boldsymbol{\xi}, \boldsymbol{\zeta}, k) G(\boldsymbol{\xi}, \mathbf{x}^\circ, k) d\Gamma_\xi dS_\zeta \right\},$$

where G is the fundamental solution of the Helmholtz equation in \mathbb{R}^3 , while $\beta = \rho/\rho^*$ and $\gamma = c/c^*$ denote the material characteristics of a vanishing trial obstacle at \mathbf{x}° . When the latter is ball-shaped, $\mathbf{A} = 2/(3+\beta)\mathbf{I}$, where \mathbf{I} is the second-order identity tensor.

Representation (1) can further be reduced to a single surface integral with an *explicit* kernel by way of the Helmholtz-Kirchhoff identity

$$(2) \quad \int_{\Gamma^{\text{obs}}} \bar{G}(\boldsymbol{\xi}, \boldsymbol{\zeta}, k) G(\boldsymbol{\xi}, \mathbf{x}^\circ, k) d\Gamma_\xi \simeq -\frac{1}{k} \text{Im}(G(\mathbf{x}^\circ, \boldsymbol{\zeta}, k)), \quad \mathbf{x}^\circ, \boldsymbol{\zeta} \in \mathcal{B}_1, \quad \alpha \ll 1,$$

its extension in terms of $\bar{G} \nabla G$, and the Kirchhoff (high-frequency) approximation of the scattered field over S which states that

$$(3) \quad u = 0 \quad \text{on} \quad S = \partial D, \quad u_{,n} = \begin{cases} 2u_{,n}^i & \text{on} \quad S^f \\ 0 & \text{on} \quad S^b \end{cases},$$

when the obstacle is sound-soft. Here $S^f = \{\mathbf{x} \in S : \mathbf{n}(\mathbf{x}) \cdot \mathbf{d} < 0\}$ is the “front” (i.e. illuminated) part of S , and $S^b = \{\mathbf{x} \in S : \mathbf{n}(\mathbf{x}) \cdot \mathbf{d} \geq 0\}$ denotes its “back” side.

The remaining surface integral is next evaluated explicitly via the method of stationary phase [7] as a sum of contributions of the kernel in the neighborhood of *critical points* on S^f , namely those where i) the tangential gradient of the exponential part of the kernel vanishes, and ii) the kernel fails to be differentiable. In this way the TS indicator function is written in terms of basic transcendental functions combined with their specialized counterparts such as the Airy, Fresnel, and Pearcey integrals.

REFERENCES

- [1] H. A. Eschenauer, V. V. Kobelev, and A. Schumacher, *Bubble method for topology and shape optimization of structures*, Structural Optimization, **8** (1994), pp. 42–51.
- [2] G. R. Feijoo, *A new method in inverse scattering based on the topological derivative*, Inverse Problems, **20** (2004), pp. 1819–1840.
- [3] B. B. Guzina and M. Bonnet, *Small-inclusion asymptotic of misfit functionals for inverse problems in acoustics*, Inverse Problems, **22** (2006), pp. 1761–1785.
- [4] M. Masmoudi, J. Pommier, and B. Samet, *The topological asymptotic expansion for the Maxwell equations and some applications*, Inverse Problems, **21** (2005), 547–564.
- [5] B. B. Guzina and M. Bonnet, *Topological derivative for the inverse scattering of elastic waves*, Quart. J. Mech. Appl. Math., **57** (2004), pp. 161–179.
- [6] H. Ammari and H. Kang, *Reconstruction of the small inhomogeneities from boundary measurements*, Springer, Berlin, New York, 2004.
- [7] J. J. Stamnes, *Waves in Focal Regions: Propagation, Diffraction, and Focusing of Light, Sound, and Water Waves*, Taylor & Francis, New York, 1986.

Techniques for Topology Optimization under Constraints

SAMUEL AMSTUTZ

The aim of this presentation is to provide some methods to deal with shape and topology optimization problems of the form:

$$(1) \quad \min_{\Omega \in \mathcal{E}} \mathcal{J}(\Omega) \quad \text{subject to} \quad \mathcal{G}(\Omega) \in -K,$$

where \mathcal{E} is a set of admissible domains, K is a closed convex cone of a Banach space Y , and

- $\mathcal{J} : \mathcal{E} \rightarrow \mathbb{R}$ is the cost functional,
- $\mathcal{G} : \mathcal{E} \rightarrow Y$ is a given constraint functional.

In particular, problems with m scalar inequality constraints can be cast into this framework by taking $Y = \mathbb{R}^m$ and $K = \mathbb{R}_+^m$, but the infinite dimensional case is also of interest (structural optimization with infinitely many loads, pointwise constraints...). Most of the methods we will present rely on the concept of topological sensitivity, which was mathematically introduced in [15, 16] and subsequently developed by many authors.

1. TOPOLOGICAL SENSITIVITY

Let Ω be a domain of \mathbb{R}^d , $d = 2, 3$. Given a reference domain $\omega \subset \mathbb{R}^d$ (typically the unit ball), the topological derivative $\mathcal{J}'(\Omega)(z)$ of the functional $\mathcal{J}(\Omega)$ at a point $z \in \Omega$ is defined through the asymptotic expansion:

$$\mathcal{J}(\Omega \setminus \overline{(z + \rho\omega)}) - \mathcal{J}(\Omega) = f(\rho)\mathcal{J}'(\Omega)(z) + o(f(\rho)) \quad (\rho \rightarrow 0)$$

for an appropriate (nonnegative) scaling function $f(\rho)$.

From a numerical point of view, the topological derivative can be used as a descent direction to perform topology changes. It also provides optimality conditions. In the unconstrained case, the obvious necessary optimality condition $\mathcal{J}'(\Omega)(z) \geq 0 \forall z \in \Omega$ can be solved, for instance, by a fixed point method like in [4, 8, 10]. Alternatively, it is possible to design material interpolation schemes in order to reach the same optimality condition in the regions of extremal density, see [6].

2. OPTIMALITY CONDITIONS AND DUALITY-BASED ALGORITHMS

Suppose that Ω is optimal for (1) with respect to topological perturbations performed at points $z \in \mathcal{T}(\Omega) \subset \Omega$, and that for such perturbations the functionals $\mathcal{J}(\Omega)$ and $\mathcal{G}(\Omega)$ admit topological derivatives which are additive in the perturbations. We prove in [9] that, under the constraint qualification condition

$$\exists x_0 \in \mathcal{T}(\Omega), t \geq 0 \text{ s.t. } \mathcal{G}(\Omega) + t\mathcal{G}'(\Omega)(x_0) \in \text{int}(-K),$$

there exists $\mu \in K^+$ (the polar cone of K) such that:

$$\begin{aligned} \mathcal{J}'(\Omega)(z) + \langle \mu, \mathcal{G}'(\Omega)(z) \rangle_{Y', Y} &\geq 0 \quad \forall z \in \mathcal{T}(\Omega), \\ \langle \mu, \mathcal{G}(\Omega) \rangle_{Y', Y} &= 0. \end{aligned}$$

These conditions can be complemented by a geometrical optimality condition on $\partial\Omega$ based on the shape derivative, involving the same Lagrange multiplier μ . We further show [5] that optimal domains correspond to saddle points of the (possibly augmented) Lagrangian $\mathcal{L}(\Omega, \mu) = \mathcal{J}(\Omega) + \langle \mu, \mathcal{G}(\Omega) \rangle_{Y', Y}$. Uzawa-type algorithms may be used to find these saddle points.

3. POINTWISE STATE CONSTRAINTS

Let u_Ω be a state variable, solution to an elliptic PDE associated with Ω . It is often desired to impose a constraint of the form (for a symmetric positive definite matrix B):

$$\frac{1}{2}B\nabla u_\Omega \cdot \nabla u_\Omega \leq M \quad \text{a.e. in } \Omega.$$

In such cases duality-based algorithms are inappropriate due to the very low regularity of the Lagrange multiplier. A penalty method for this kind of problems is introduced in [1], and applied to particular damage criteria in structural mechanics in [13, 14].

4. PERIMETER CONSTRAINT

Perimeter constraints are of major interest in topology optimization due to their regularizing effect (leading generally to the existence of optimal domains). However, the perimeter is more sensitive to topological changes than the standard cost functionals, and therefore it does not admit a topological derivative in the usual sense. If $u \in L^\infty(D, [0, 1])$ we introduce the quantity

$$\tilde{F}_\varepsilon(u) = \inf_{v \in H^1(D)} \left\{ \frac{1}{2\varepsilon} \left(\|v\|_{L^2(D)}^2 + \langle u, 1 - 2v \rangle \right) + \frac{\varepsilon}{2} \|\nabla v\|_{L^2(D)}^2 \right\},$$

which is easily computable through the solution of a linear PDE. We prove in [11] the following Γ -convergence result when $\varepsilon \rightarrow 0$, which holds strongly in $L^1(D, [0, 1])$:

$$(2) \quad \tilde{F}_\varepsilon(u) \xrightarrow{\Gamma} \tilde{F}(u) := \begin{cases} \frac{1}{4}TV(u) = \frac{1}{4}\text{Per}_D(\Omega) & \text{if } u = \chi_\Omega \in BV(D, \{0, 1\}) \\ +\infty & \text{otherwise,} \end{cases}$$

where $\text{Per}_D(\Omega)$ is the relative perimeter of Ω in D . In addition, we show that the functionals \tilde{F}_ε are equicoercive for the same topology. This provides the ingredients for a proper approximation of shape functionals including a perimeter term.

It also stems from (2) that another benefit of the functionals \tilde{F}_ε is to penalize the intermediate values of u . This allows for the use of relaxation methods to solve the problem at ε fixed, while eventually retrieving a characteristic function when $\varepsilon \rightarrow 0$. This approach finds applications in compliance minimization by homogenization [11] and image classification [7].

When a relaxed formulation is not available, one can use instead the topological derivative, see [2], since \tilde{F}_ε is especially constructed so as to admit a topological derivative.

5. NEWTON TYPE METHODS

Consider the model problem:

$$(3) \quad \min_{u \in L^\infty(D, [0, 1])} j(u) = \frac{1}{2} \int_D (y_u - y^\dagger)^2 dx + \nu \int_D u dx \quad \text{with } -\Delta y_u = u.$$

In fact, under rather general assumptions, the solution u takes only 0 – 1 values. It is easily seen that a necessary and sufficient optimality condition for (3) can be written:

$$F(u) := u|g_u| + \min(0, g_u) = 0 \quad \text{with } g_u = \nabla j(u).$$

The idea is to solve this equation by the semismooth Newton method, however the generalized Jacobian of F is singular at the solution. Appropriate regularization techniques, leading to superlinear convergence, are analyzed in [3] for the unconstrained problem (3) and in [12] for a class of constrained problems.

REFERENCES

- [1] S. Amstutz. A penalty method for topology optimization subject to a pointwise state constraint. *ESAIM: Control, Optimisation and Calculus of Variations*, 16(03):523–544, 2010.
- [2] S. Amstutz. Regularized perimeter for topology optimization. Technical Report hal-00542854, 2010.
- [3] S. Amstutz. A semismooth Newton method for topology optimization. *Nonlinear Anal.*, 73(6):1585–1595, 2010.
- [4] S. Amstutz. Analysis of a level set method for topology optimization. *Optim. Methods Softw.*, 26(4-5):555–573, 2011.
- [5] S. Amstutz. Augmented Lagrangian for cone constrained topology optimization. *Comput. Optim. Appl.*, 49(1):101–122, 2011.
- [6] S. Amstutz. Connections between topological sensitivity analysis and material interpolation schemes in topology optimization. *Struct. Multidiscip. Optim.*, 43(6):755–765, 2011.
- [7] S. Amstutz. Minimal partitions and image classification using a gradient-free perimeter approximation. Technical Report hal-0069001175, 2012.
- [8] S. Amstutz and H. Andrä. A new algorithm for topology optimization using a level-set method. *Journal of Computational Physics*, 216(2):573–588, 2006.
- [9] S. Amstutz and M. Ciligot-Travain. Optimality conditions for shape and topology optimization subject to a cone constraint. *SIAM J. Control Optim.*, 48(6):4056–4077, 2010.
- [10] S. Amstutz, S.M. Giusti, A.A. Novotny, and E.A. de Souza Neto. Topological derivative for multi-scale linear elasticity models applied to the synthesis of microstructures. *International Journal for Numerical Methods in Engineering*, 84:733–756, 2010.
- [11] S. Amstutz and N. Van Goethem. Topology optimization methods with gradient-free perimeter approximation. *Interfaces and Free Boundaries*, 14:401–430, 2012.
- [12] S. Amstutz and A. Laurain. A semismooth Newton method for a class of semilinear optimal control problems with box and volume constraints. Technical Report hal-00636063, 2011.
- [13] S. Amstutz and A.A. Novotny. Topological optimization of structures subject to von Mises stress constraints. *Structural and Multidisciplinary Optimization*, 41(3):407–420, 2010.
- [14] S. Amstutz, A.A. Novotny, and E.A. de Souza Neto. Topological derivative-based topology optimization of structures subject to Drucker-Prager stress constraints. *Computer Methods in Applied Mechanics and Engineering*, 233–236:123–136, 2012.
- [15] S. Garreau, Ph. Guillaume, and M. Masmoudi. The topological asymptotic for PDE systems: the elasticity case. *SIAM Journal on Control and Optimization*, 39(6):1756–1778, 2001.
- [16] J. Sokółowski and A. Żochowski. On the topological derivative in shape optimization. *SIAM Journal on Control and Optimization*, 37(4):1251–1272, 1999.

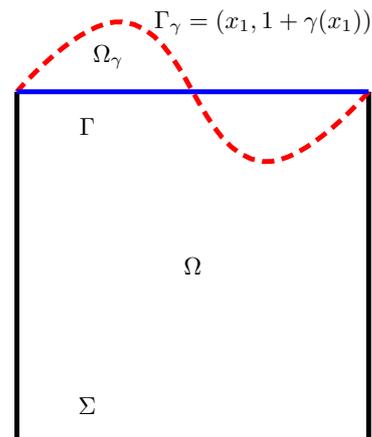
Optimal Control of a Free Boundary Problem with Surface Tension Effects

HARBIR ANTIL

(joint work with Ricardo H. Nochetto, Patrick Sodr e)

Free boundary problems (FBPs) are challenging due to their highly nonlinear nature. Besides the state variables, the domain is also an unknown. FBP find a wide range of applications from phase separation (Stefan problem, Cahn-Hilliard), shape optimization (minimal surface area), optimal control problems with state constraints, fluid dynamics (flow in porous media), crystal growth, biomembranes, electrowetting on dielectric, to finance. For many of these problems there is a close interplay between the surface tension and the curvature of the interface; see [1] and references therein.

Figure 1: Ω_γ denotes a physical domain with boundary $\partial\Omega_\gamma = \Sigma \cup \Gamma_\gamma$. Here Σ includes the lateral and the bottom boundary and is assumed to be fixed. Furthermore, the top boundary Γ_γ (dotted line) is “free” and is assumed to be a graph of the form $(x_1, 1 + \gamma(x_1))$, where $\gamma \in \dot{W}_\infty^1(0, 1)$ denotes a parametrization. Γ_γ is further mapped to a fixed boundary $\Gamma = (0, 1)$ and in turn the physical domain Ω_γ is mapped to a reference domain $\Omega = (0, 1)^2$, where all computations are carried out.



Of particular interest to us is the control of a model FBP previously studied by P. Saavedra and L. R. Scott in [9] and formulated in graph form; see Figure 1, where the free boundary Γ_γ is the dotted line. The state equations (2b) involve a Laplace equation in the bulk and a Young-Laplace equation on the free boundary to account for surface tension. This amounts to solving a second order system both in the bulk and on the interface. Below we give a detailed description of the problem.

Let $\gamma \in \dot{W}_\infty^1(0, 1)$ denote a parameterization of the top boundary (see Figure 1) of the physical domain $\Omega_\gamma \subset \Omega^* \subset \mathbb{R}^2$ with boundary $\partial\Omega_\gamma := \Gamma_\gamma \cup \Sigma$, defined as

$$\begin{aligned}\Omega^* &= (0, 1) \times (0, 2), \\ \Omega_\gamma &= \{(x_1, x_2) : 0 < x_1 < 1, 0 < x_2 < 1 + \gamma(x_1)\}, \\ \Gamma_\gamma &= \{(x_1, x_2) : 0 < x_1 < 1, x_2 = 1 + \gamma(x_1)\}, \\ \Sigma &= \partial\Omega_\gamma \setminus \Gamma_\gamma, \\ \Gamma &= \{(x_1, x_2) : 0 < x_1 < 1, x_2 = 1\}.\end{aligned}$$

Here, Ω^* and Σ are fixed while Ω_γ and Γ_γ deform according to γ .

We want to find an optimal control $u \in \mathcal{U}_{ad} \subset L^2(\Gamma)$ so that the solution pair (γ, y) of the FBP approximates a given boundary $\gamma_d : \Gamma \rightarrow \mathbb{R}$ and potential $y_d : \Omega^* \rightarrow \mathbb{R}$. This amounts to solving the minimization problem

$$(2a) \quad \min \mathcal{J}(\gamma, y, u) := \frac{1}{2} \|\gamma - \gamma_d\|_{L^2(\Gamma)}^2 + \frac{1}{2} \|y - y_d\|_{L^2(\Omega_\gamma)}^2 + \frac{\lambda_u}{2} \|u\|_{L^2(\Gamma)}^2,$$

subject to the state equations

$$(2b) \quad \begin{cases} -\Delta y = 0 & \text{in } \Omega_\gamma \\ y = v & \text{on } \partial\Omega_\gamma \\ -\kappa \mathcal{H}[\gamma] + \partial_\nu y = u & \text{on } \Gamma_\gamma \\ \gamma(0) = \gamma(1) = 0, \end{cases},$$

the state constraints

$$(2c) \quad |d_{x_1} \gamma(x_1)| \leq 1 \quad \text{a.e. } x_1 \in \Gamma,$$

with d_{x_1} being the total derivative with respect to x_1 , and the control constraint

$$(2d) \quad u \in \mathcal{U}_{ad}$$

dictated by \mathcal{U}_{ad} , a closed ball in $L^2(\Gamma)$. Here $\lambda_u > 0$ is the stabilization parameter; v is a given data which in principle could act as a Dirichlet boundary control;

$$\mathcal{H}[\gamma] := d_{x_1} \left(\frac{d_{x_1} \gamma}{\sqrt{1 + |d_{x_1} \gamma|^2}} \right)$$

is the *curvature* of γ ; and $\kappa > 0$ plays the role of surface tension coefficient.

Optimal control of partial differential equations (PDEs) allows us to achieve a specific goal (2a) with PDE (2b) and other constraints (2c)-(2d) being satisfied and can be highly beneficial in practice (see [12] for more details). For example using the reverse electrowetting i.e., by applying a control to change the shape of fluid droplets, one can generate enough power to charge a cellphone [7], by mere stroll in the park. There has been various attempts to solve optimal control problems with a FBP constraint. We refer to [5, 6] for control of a two phase Stefan problem in graph formulation and [2] for the same problem in level set formulation. Paper [8] discusses optimal control of a FBP with Stokes flow. Even though problem (2a)-(2d) is relatively simple, it captures the essential features associated with surface tension effects found in more complex systems, and allows us to develop a complete second order analysis in [1], based on [12]. Prior to [1], this analysis was absent in the literature on FBP.

There are several methodologies to formulate FBP depending on the role of the free boundary. We deal with a sharp interface method, written in graph form (see Figure 1), for which the interface Γ_γ is governed by the explicit elliptic PDE

$$-\kappa \mathcal{H}[\gamma] + \partial_\nu y = u.$$

A similar approach was used in [5, 6] for the optimal control of a Stefan problem, but without the full accompanying theory developed here. Alternative approaches to treat FBP are the level set method and the diffuse interface method [3, 2].

We use a fixed domain approach to solve the optimal control free boundary problem (OC-FBP). In fact, we transform Ω_γ to $\Omega = (0, 1)^2$ and Γ_γ to $\Gamma = (0, 1) \times \{1\}$ (see Figure 1), at the expense of having a governing PDE with rough coefficients. This avoids dealing with shape sensitivity analysis [10, 4]. We refer to [13] for a comparison between these approaches applied to a FBP. Using operator interpolation [11] we demonstrate how to improve the existing regularity of state variables derived earlier in [9], which turns out to be instrumental to derive the second order sufficient condition. One of the challenges of an OC-FBP is dealing with possible topological changes of the domain by introducing state constraints. Our analysis provides control constraints which always enforce the state constraints i.e., we can simply treat OC-FBP as a control constrained problem. We conclude by providing optimal a priori error estimates and a non trivial extension to Stokes equations.

REFERENCES

- [1] H. Antil, R. H. Nochetto, and P. Sodr . Optimal control of a free boundary problem: Analysis with second order sufficient conditions. *submitted*, 2012.
- [2] M. K. Bernauer and R. Herzog. Optimal control of the classical two-phase Stefan problem in level set formulation. *SIAM J. Sci. Comput.*, 33(1):342–363, 2011.
- [3] K. Deckelnick, G. Dziuk, and C. M. Elliott. Computation of geometric partial differential equations and mean curvature flow. *Acta Numerica*, 14:139–232, 2005.
- [4] M. C. Delfour and J.-P. Zol sio. *Shapes and geometries*, volume 22 of *Advances in Design and Control*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, second edition, 2011. Metrics, analysis, differential calculus, and optimization.
- [5] M. Hinze and S. Ziegenbalg. Optimal control of the free boundary in a two-phase Stefan problem. *J. Comput. Phys.*, 223(2):657–684, 2007.
- [6] M. Hinze and S. Ziegenbalg. Optimal control of the free boundary in a two-phase Stefan problem with flow driven by convection. *ZAMM Z. Angew. Math. Mech.*, 87(6):430–448, 2007.
- [7] T. Krupenkin and J.A. Taylor. Reverse electrowetting as a new approach to high-power energy harvesting. *Nat. Commun.*, 2:448, 2011.
- [8] S. Repke, N. Marheineke, and R. Pinnau. Two adjoint-based optimization approaches for a free surface Stokes flow. *SIAM J. Appl. Math.*, 71(6):2168–2184, 2011.
- [9] P. Saavedra and L. R. Scott. Variational formulation of a model free-boundary problem. *Math. Comp.*, 57(196):451–475, 1991.
- [10] J. Soko owski and J. P. Zol sio. *Introduction to shape optimization*, volume 16 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 1992. Shape sensitivity analysis.
- [11] L. Tartar. *An introduction to Sobolev spaces and interpolation spaces*, volume 3 of *Lecture Notes of the Unione Matematica Italiana*. Springer, Berlin, 2007.
- [12] F. Tr ltzsch. *Optimal control of partial differential equations*, volume 112 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2010. Theory, methods and applications, Translated from the 2005 German original by J rgen Sprekels.
- [13] KG van der Zee, EH van Brummelen, I. Akkerman, and R. de Borst. Goal-oriented error estimation and adaptivity for fluid-structure interaction using exact linearized adjoints. *Computer Meths. in Appl. Mech. and Eng.*, 2010.

Parametric Shape Optimization Revisited

MICHAEL STINGL

(joint work with Bastian Schmidt)

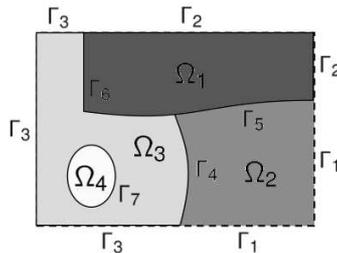
A new flexible shape optimization concept for the optimization for multiple-phase materials is described. Unlike in usual parametric shape optimization admissible deformations of a reference configuration are considered as design variables. We show existence for a wide class of cost functionals and convergence of an appropriate approximation scheme under standard assumptions.

BASIC SETTING AND EXISTENCE OF A SOLUTION

Let $\Omega \in \mathbb{R}^2$ be a domain. Let $\Gamma_k \in C([0, 1]; \mathbb{R}^2)$, $k = 1, \dots, K$ be curves describing the boundary of Ω (denoted by $\Gamma = \partial\Omega$) and partitioning of Ω into I subdomains Ω_i with $\bigcup_{i=1}^I \bar{\Omega}_i = \bar{\Omega}$, $\Omega_i \cap \Omega_j = \emptyset$, $i \neq j = 1, \dots, I$, see Figure 1. We require

$\Omega_i, i = 1, \dots, I$ to satisfy the uniform cone property[1] and additionally several properties on the curves Γ_k :

$$\begin{aligned} &\Gamma_k \text{ injective and Lipschitz, } k = 1, \dots, K \\ &\Gamma_{k_1}([0, 1[) \cap \Gamma_{k_2}([0, 1]) = \emptyset, k_1 \neq k_2 = 1, \dots, K \\ &\Gamma_k(\{0, 1\}) \subset \bigcup_{\substack{l=1 \\ l \neq k}}^K \Gamma_l(\{0, 1\}) \text{ or } \Gamma_k \text{ closed, } k = 1, \dots, K \end{aligned}$$



We choose $L \in (0, 1)$ and come to the following definition for the set of admissible deformations:

$$(1) \quad U_{\text{ad}} := \left\{ \varphi_1, \dots, \varphi_K \in C([0, 1], \mathbb{R}^2) \mid \|\varphi_{k_1}(t_1) - \varphi_{k_2}(t_2)\| \leq L \|\Gamma_{k_1}(t_1) - \Gamma_{k_2}(t_2)\| \forall k_1, k_2 = 1, \dots, K \forall t_1, t_2 \in [0, 1] \right\}.$$

Note that the condition

$$(2) \quad \|\varphi_{k_1}(t_1) - \varphi_{k_2}(t_2)\| \leq L \|\Gamma_{k_1}(t_1) - \Gamma_{k_2}(t_2)\| \forall k_1, k_2 = 1, \dots, K \forall t_1, t_2 \in [0, 1]$$

implies uniform Lipschitz continuity for each of the functions $\varphi_1, \dots, \varphi_K$. For simplicity we assume that $\partial\Omega$ is not allowed to deform, i.e. the associated φ_k are assumed to be 0. We now define the set $\tilde{\Gamma} := \bigcup_{k=1}^K \Gamma_k([0, 1])$ and associate with each tuple $\varphi_1, \dots, \varphi_K \in X$ a mapping

$$\varphi : \tilde{\Gamma} \rightarrow \mathbb{R}^2, x \mapsto \varphi_k(t), \text{ where } t \text{ and } k \text{ are defined by } \Gamma_k(t) = x.$$

Note φ is well-defined due to condition (2).

Theorem 1 *The transformation $\Phi : \tilde{\Gamma} \rightarrow \mathbb{R}^2, x \mapsto x + \varphi(x)$ is injective and therefore topology preserving.*

For a proof, we refer to [3].

For each $\varphi = (\varphi_1, \dots, \varphi_K) \in U_{\text{ad}}$ we consider an associated boundary value problem of linear elasticity in weak form:

$$\begin{aligned} (\mathcal{P}_\varphi) \quad &\text{find } u := u(\varphi) \in V \text{ s.t.} \\ &a_\varphi(u, v) = f(v) \forall v \in H^1(\Omega). \end{aligned}$$

Here $f \in H^1(\Omega)^*$ is given, $V := \{u \in H^1(\Omega) \mid u|_{\Gamma_0} = 0\}$ with $\Gamma_0 \subseteq \partial\Omega$ and $a_\varphi : H^1(\Omega) \times H^1(\Omega) \rightarrow \mathbb{R}, a_\varphi(u, v) \mapsto \int_\Omega \langle C_\varphi(x)e(u)(x), e(v)(x) \rangle dx$ is a uniformly elliptic, bounded and symmetric bilinear form. The material tensor $C_\varphi(x) :=$

$C_i \forall x \in \Omega_i(\varphi), i = 1, \dots, I$ represents a given material C_i on the subdomain $\Omega_i(\varphi)$ and $e_{i,j}(u) := \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ is the small strain tensor.

Using the state problem (\mathcal{P}_φ) , together with a lower semi-continuous objective function $J : V \times U_{\text{ad}} \rightarrow \mathbb{R}$, we can consider the optimization problem

$$(\mathcal{P}) \quad \begin{aligned} &\text{find } \varphi^* \in U_{\text{ad}} \text{ s.t.} \\ &J(u(\varphi^*), \varphi^*) \leq J(u(\varphi), \varphi) \forall \varphi \in U_{\text{ad}}. \end{aligned}$$

Theorem 2 *The problem (\mathcal{P}) admits a solution.*

Proof (sketch): In [3] compactness of U_{ad} is established. Using compactness, existence is shown precisely as in [2].

APPROXIMATION AND CONVERGENCE

In order to solve (\mathcal{P}) numerically, we have to discretize it. We begin by giving a discretization for the set of admissible deformations U_{ad} . This is done by approximating the curves φ_k by splines and applying condition (2) to control points only:

$$(3) \quad U_{\text{ad}}^d := \left\{ \varphi_1, \dots, \varphi_K \in C_{\text{spline}}^d([0, 1], \mathbb{R}^2) \mid \begin{aligned} &\|\varphi_{k_1}(t_1) - \varphi_{k_2}(t_2)\| \leq L \|\Gamma_{k_1}(t_1) - \Gamma_{k_2}(t_2)\| \forall k_1, k_2 = 1, \dots, K \\ &\forall t_1, t_2 \text{ a. w. control points of } \varphi_{k_1}, \varphi_{k_2} \end{aligned} \right\}$$

The parameter d denotes the number of control points per curve. For simplicity, we consider only piecewise linear splines here. As (3) is an outer approximation we cannot assume the resulting transformations to be topology preserving anymore. However we are able to show that for sufficiently large d_0 , where d_0 depends only on the cone constants of the reference configuration and the constant L , topology is again preserved and the uniform cone property for the resulting subdomains $\Omega_i(\varphi)$ remains valid with constants modified by L [3]. Using this discretization, we can prove the following theorem.

Theorem 3 *The system $\{U_{\text{ad}}^d\}_{d \rightarrow \infty}$ is compact in $\{U_{\text{ad}}\}$.*

Proof (sketch): It is easy to see that there exists a compact $\tilde{U} \supset U_{\text{ad}}^d \forall d > d_0$. Existence of a converging subsequence in \tilde{U} , Lipschitz continuity of the limit curves and preservation of condition (2) due to uniform convergence complete the proof.

Using a standard Galerkin approach for the linear elasticity problem (\mathcal{P}_φ) , we have the following discretized optimization problem:

$$(\mathcal{P}_{d,h}) \quad \begin{aligned} &\text{find } \varphi^{d,*} \in U_{\text{ad}}^d \text{ s.t.} \\ &J(u(\varphi^{d,*}), \varphi^{d,*}) \leq J(u(\varphi^d), \varphi^d) \forall \varphi^d \in U_{\text{ad}}^d. \end{aligned}$$

Assuming the usual non-degeneration conditions for the finite element mesh to hold, together with a continuous dependence of the mesh on the design parameters and $d \rightarrow \infty \Leftrightarrow h \searrow 0$ for the mesh size parameter h , we are able to show:

Theorem 4 Let \mathcal{T}_{h_n} be a sequence of regular triangulations with $h_n \searrow 0, d_n \rightarrow \infty$ and let $U_{ad}^{d_n} \ni \varphi^{d_n,*} =: \varphi_n^*$ and $u_n^* := u_{h_n}(\varphi_n^*)$ be optimal pairs of $(\mathcal{P}_{d,h})$. Then there exist subsequences with

$$\begin{aligned}\varphi_n^* &\rightarrow \varphi^* \\ u_n^* &\rightarrow u^*\end{aligned}$$

where (φ^*, u^*) is an optimal pair for (\mathcal{P}) .

The proof is similar as in [2] and presented in detail in [3].

REFERENCES

- [1] M. C. Delfour and J.-P. Zolésio, *Shapes and Geometries*, SIAM (2001).
- [2] J. Haslinger and R. Mäkinen, *Introduction to shape optimization*, SIAM (2003).
- [3] B. Schmidt and M. Stingl, *A new flexible parametric shape optimization approach: Existence and convergence theory*, COAP (2013), in preparation

Groups of Transformations for Geometrical Identification Problems: Metrics, Geodesics

MICHEL C. DELFOUR

INTRODUCTION. When modelling, optimizing, controlling, or identifying with respect to a family of subsets of an Euclidean space, say \mathbb{R}^N for convenience, the nice vector space structure of the calculus of variations and control theory is lost and definitions and tools have to be developed to effectively capture this reality. Among the many examples in pattern recognition or shape identification, the pattern matching in image analysis (cf., for instance, A. Trouvé [22]) and the surface matching problem from a cloud of points (cf., for instance, S. Osher and R. Fedkiw [19] and J. Barolet [4] for the follow up of face surgery by the 3D portable hand scanner).

GROUP STRUCTURE. The set of all subsets $\mathcal{P}(D)$ of a fixed set $D \subset \mathbb{R}^N$ (or *hold all*) has a group structure for the algebraic operation called *symmetric difference* of two sets. The family of the corresponding *characteristic functions* of measurable sets with finite measure forms a *complete metric group* where the metric is given by the L^p -norm of the difference of two characteristic functions. Hausdorff measures can be used to deal with objects of lower dimensions in \mathbb{R}^N . Other *set-parametrized functions* such as the *distance function*, the *oriented distance function*, or the *support function* can be used to construct such complete metric spaces (cf. Delfour and Zolésio [9]).

Another way to construct a family of variable domains is to consider the images of a fixed subset Ω_0 of \mathbb{R}^N by some family of transformations of \mathbb{R}^N . The natural algebraic structure for spaces of transformations is again a group structure with respect to *composition* \circ . It is then possible to construct a metric on the family of transformations that will serve as a metric or distance between two images of Ω_0 . There are many ways to do that, and specific constructions and choices are again very much problem dependent.

COURANT METRICS. In 1972 A.M. Micheletti [12] introduced what may be one of the first complete metric topologies on a family of domains of class C^k that are the images of a fixed open domain of class C^k through a family of C^k -diffeomorphisms of \mathbb{R}^N . The natural underlying algebraic structure is the *group structure* for the composition of transformations with the identity transformation as the neutral element. Her analysis culminates with the construction of a complete metric on the quotient of the group by the closed subgroup of transformations leaving the fixed subset Ω_0 unaltered. She called it the *Courant metric* because it is proved in the book of Courant and Hilbert [7] that the n -th eigenvalue of the Laplace operator depends continuously on the domain Ω , where $\Omega = (I + f)\Omega_0$ is the image of a fixed domain Ω_0 by $I + f$ and f is a smooth mapping. But there is no notion of a metric in that book. Her constructions naturally extend to other families of transformations of \mathbb{R}^N or of fixed holdalls D .

The next step in the construction is the choice of the closed subgroup of transformations of \mathbb{R}^N that is very much problem dependent. Originally, she chose the set of transformations that leave the underlying set or pattern unaltered. In some applications such a cavity filled with fluid, one might want to work in that subgroup and follow the paths of particles inside. One might think of the paper of V. I. Arnold [1]. In some applications, it might be interesting to look at the subgroup that leave the set unaltered up to a translation, a rotation, or a flip.

Going back to the set up of Micheletti, it is possible to show that the underlying set Ω_0 can be chosen *closed* or *open without cracks*. This includes *closed submanifolds of \mathbb{R}^N* . As long as the subgroup is closed, we get a complete Courant metric on the quotient group even if the group of Micheletti with its complete metric is not a metric group. Those groups with a complete metric have as tangent spaces a Banach space of smooth mappings from \mathbb{R}^N to \mathbb{R}^N and can be assimilated to infinite dimensional Finsler manifolds. By specializing the above constructions, it is possible to define a complete metric for all C^k -homeomorphisms or all diffeomorphisms of an open (but not necessarily bounded) subset of \mathbb{R}^N . With such larger spaces, it now becomes possible to consider subgroups involving not only translations but also isometries, symmetries, or flips in \mathbb{R}^N or D .

TRANSFORMATIONS GENERATED BY VELOCITY FIELDS. A convenient way to generate transformations of \mathbb{R}^N is to introduce a family of time-dependent velocity fields $V(t) : \mathbb{R}^N \rightarrow \mathbb{R}^N$. By solving the differential equation $x'(t) = V(t, x(t))$ over a fixed interval $[0, 1]$, we get a trajectory $t \mapsto T_t(V)$ of transformations. If Θ is a Banach space of mappings $\theta : \mathbb{R}^N \rightarrow \mathbb{R}^N$, say $\Theta \subset C^{0,1}(\overline{\mathbb{R}^N}; \mathbb{R}^N)$, choose the family of transformations given by $G_\Theta = \{T_1(V) : V \in L^1(0, 1; \Theta)\}$. This is a subgroup of the ones that can be obtained by the *generic* construction of Micheletti.

One advantage is the ability to construct $T_t(V)$ from the solution of an ordinary differential equation. The other advantage is that a simpler metric can be constructed from the norm of V . Yet, since there is no uniqueness of the velocity taking I to $T_1(V)$, one has to introduce an infimum over all admissible velocities.

But this is equivalent to introduce the *geodesic* between I to $T_1(V)$ in the subgroup G_Θ .

This Velocity Method was adopted by J.P. Zolésio [33], [34] as early as 1973 and considerably expanded in his *thèse d'état* in 1979. At that time most people were using a simple perturbation of the identity to compute shape derivatives. The first comprehensive book promoting the *velocity method* was published in 1992 by Sokolowski and Zolésio [20].

In 1994, at a congress in Cortona on imaging, R. Azencott [3] floated the idea of a *deformation distance* between two shapes constructed from *geodesics* in groups of diffeomorphisms generated by a velocity field. His student A. Trouvé [23] [22] wrote his thesis on this topic by integrating in infinite dimension ideas of differential geometry (infinite dimensional group action and pattern recognition) in 1995 [21]. In order to get the completeness of the subgroup for the metric, he had to go to a Hilbertian set-up and replace the L^1 -norm by an L^2 -norm and the Banach space $C^{0,1}(\overline{\mathbb{R}^N}; \mathbb{R}^N)$ by some Hilbertian subset $\mathcal{H} \subset C^{0,1}(\overline{\mathbb{R}^N}; \mathbb{R}^N)$. We explore the connections between the constructions of Azencott and Micheletti who implicitly uses a notion of *geodesic path with discontinuities*.

The reader is also referred to the *differential geometric approach* of P. W. Michor and D. Mumford [13], [14], [15], and L. Younes, P. W. Michor, and D. Mumford, [29].

Many issues and problems remain open and bridges have to be thrown between specialists of different horizons.

REFERENCES

- [1] V. I. Arnold, *Sur un principe variationnel pour les écoulements stationnaires des liquides parfaits et ses applications aux problèmes de stabilité non linéaires*, J. Méc. **5** (1966), 29–43.
- [2] V. I. Arnold, *Sur la géométrie des groupes de Lie de dimension infinie et ses applications à l'hydrodynamique des fluides parfaits*, Ann. Inst. Fourier Grenoble (1) **16** (1966), 319–361.
- [3] R. Azencott, *Geodesics in diffeomorphisms groups: Deformation distance between shapes*, Int. Conf. Stoch. Structures and Monte-Carlo Optim., Cortona, Italy, 1994.
- [4] J. C. Barolet, *Représentation et détection des images et des surfaces déformables*, Département de mathématiques et de statistique, Université de Montréal, 2011.
- [5] M. F. Beg, M. I. Miller, A. Trouvé and L. Younes, *Computing large deformation metric mapping via geodesic flows of diffeomorphisms*, Int. J. Comput. Vis. (2) **61** (2005), 139–157.
- [6] V. Caselles, R. Kimmel, and G. Sapiro, *Geodesic active contours*, Int.J. Comput.Vis. **22** (1997), 61–79.
- [7] R. Courant and D. Hilbert, *Methods of mathematical physics*, Interscience Publishers, New York, 1953–1962 (1st English ed.).
- [8] M. C. Delfour, *Representation of hypersurfaces and minimal smoothness of the midsurface in the theory of shells*, Control Cybernet. (4) **37** (2008), 879–911.
- [9] M. C. Delfour and J.-P. Zolésio, *Shapes and Geometries: metrics, analysis, differential calculus, and optimization*, deuxième édition, SIAM series on Advances in Design and Control, Society for Industrial and Applied Mathematics, Philadelphia, USA 2011.
- [10] P. Dupuis, U. Grenander, and M. Miller, *Variational problems on flows of diffeomorphisms for image matching*, Quart. Appl. Math. **56** (1998), 587–600.

- [11] J. Glaunès, A. Trouvé, and L. Younes, *Diffeomorphic matching of distributions: A new approach for unlabelled point-sets and sub-manifolds matching*, Proceedings CVPR '04, 2004 IEEE Computer Society Conference on Computer Vision and Pattern Recognition, 2004.
- [12] A. M. Micheletti, *Metrica per famiglie di domini limitati e proprietà generiche degli autovalori*, Ann. Scuola Norm. Sup. Pisa (3) **26** (1972), 683–694.
- [13] P. W. Michor and D. Mumford, *Vanishing geodesic distance on spaces of submanifolds and diffeomorphisms*, Doc. Math. **10** (2005), 217–245.
- [14] P. W. Michor and D. Mumford, *Riemannian geometries on spaces of plane curves*, J. Eur. Math. Soc. (JEMS) (1) **8** (2006), 1–48.
- [15] P. W. Michor and D. Mumford, *An overview of the Riemannian metrics on spaces of curves using the Hamiltonian approach*. Appl. Comput. Harmon. Anal. (1) **23** (2007), 74–113.
- [16] M. I. Miller, A. Trouvé, and L. Younes, *Computing large deformations via geodesic flows of diffeomorphisms*, Int. J. Comput. Vis. **61** (2) (2005), 139–157.
- [17] M. I. Miller, A. Trouvé, and L. Younes, *On the metrics and Euler-Lagrange equations of computational anatomy*, Annu. Rev. Biomed. Eng. **4** (2002), 375–405
- [18] M. I. Miller and L. Younes, *Group action, diffeomorphism and matching: a general framework*, Int. J. Comput. Vis. **41** (2001), 61–84.
- [19] S. Osher and R. Fedkiw, *Level Set Methods and Dynamic Implicit Surfaces*. Applied Mathematical Sciences Volume 153, Springer-Verlag New York, 2002.
- [20] J. Sokolowski and J.-P. Zolésio, *Introduction to shape optimization. Shape sensitivity analysis*, Springer Ser. Comput. Math., 16. Springer-Verlag, Berlin, 1992.
- [21] A. Trouvé, *Action de groupe de dimension infinie et reconnaissance de formes*, C. R. Acad. Sci. Paris Sér. I Math. (8) **321** (1995), 1031–1034.
- [22] A. Trouvé, *An approach of pattern recognition through infinite dimensional group actions*, Rapport de recherche du LMENS, France, 1995.
- [23] A. Trouvé, *Diffeomorphisms groups and pattern matching in image analysis*, Int. J. Comput. Vis. (3) **28** (1998), 213–221.
- [24] A. Trouvé and L. Younes, *On a class of diffeomorphic matching problems in one dimension*, SIAM J. Control Optim. (4) **39** (2000), 1112–1135.
- [25] L. Younes, *Computable elastic distances between shapes*, SIAM J. Appl. Math. (2) **58** (1998), 565–586.
- [26] L. Younes, *Optimal matching between shapes via elastic deformations*, Image Vision Comput. **17** (1999) 381–389.
- [27] L. Younes, *Invariance, déformations et reconnaissance de formes*, Mathématiques & Applications (Berlin) [Mathematics & Applications], 44, Springer-Verlag, Berlin, 2004.
- [28] L. Younes, *Shape and diffeomorphisms*, Applied Math. Sci., 171, Springer-Verlag, Berlin, 2010.
- [29] L. Younes, P. W. Michor, I. Shah, and D. Mumford, *A metric on shape space with explicit geodesics*, Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. Lincei (9) Mat. Appl. (1) **19** (2008), 25–57.
- [30] H. K. Zhao, S. Osher, B. Merriman, M. J. Kang, *Implicit and non-parametric shape reconstruction from unorganized data using a variational level-set method*, Computer vision and image understanding Volume 80 (2000), 295–314.
- [31] H. K. Zhao, S. Osher, R. Fedkiw, *Fast surface reconstruction using the level-set method*, Variational and Level-set Methods in Computer Vision, 2001, Proceedings, IEEE Workshop, 194–201.
- [32] H. K. Zhao, *A fast sweeping method for eikonal equations*, Mathematics of Computation **74**, no. 250 (2004), 603–627.
- [33] J.-P. Zolésio, *Sur la localisation d'un domaine*, Thèse de docteur de spécialité en mathématiques, Université de Nice, France, 1973.
- [34] J.-P. Zolésio, *Identification de domaines par déformation*, Thèse de doctorat d'état, Université de Nice, France, 1979.

Minimization of the Ground State for Two Phase Conductors in Low Contrast Regime

ANTOINE LAURAIN

(joint work with Carlos Conca, Rajesh Mahadevan)

Introduction. Let Ω be a bounded domain in \mathbb{R}^d called the design region. Let m be a given positive number, $0 < m < |\Omega|$, where $|\Omega|$ is the Lebesgue measure of the design region Ω . Two materials with conductivities α and β ($0 < \alpha < \beta$) are distributed in arbitrary disjoint measurable subsets A and B , respectively, of Ω so that $A \cup B = \Omega$ and $|B| = m$. Consider the two-phases eigenvalue problem:

$$(1) \quad -\operatorname{div}(\sigma \nabla u) = \lambda u \quad \text{in } \Omega,$$

$$(2) \quad u = 0 \quad \text{on } \partial\Omega,$$

with the conductivity $\sigma = \alpha\chi_A + \beta\chi_B$. Let λ be the first eigenvalue of (1)-(2) and u the associated eigenvector. The variational formulation for λ is

$$(3) \quad \lambda = \min_{u \in H_0^1(\Omega)} \frac{\int_{\Omega} \sigma |\nabla u|^2}{\int_{\Omega} u^2} = \min_{u \in H_0^1(\Omega), \|u\|_2=1} \int_{\Omega} \sigma |\nabla u|^2,$$

where $\|u\|_2$ denotes the L^2 -norm of u . Here Ω is fixed and we are interested in the dependence of λ on A and B . Since $A = \Omega \setminus B$ we write $\lambda = \lambda(B)$. We consider the problem of minimizing $\lambda(B)$ with the constraint that the two phases are to be distributed in fixed proportions; see [2]:

$$(4) \quad \text{minimize} \quad \lambda(B)$$

$$(5) \quad \text{subject to} \quad B \in \mathcal{B}$$

where

$$(6) \quad \mathcal{B} = \{B \subset \Omega, B \text{ measurable}, |B| = m\}$$

The existence of a solution to (4)-(6) remains an open question. In general, one may evidence microstructural patterns in relation to minimizing sequences and the original problem may have to be relaxed to include microstructural designs; see [5]. However, the original problem (4)-(6) may still have a solution for particular geometries as is the case when Ω is a ball. When $\Omega = \mathbb{B}(0, R)$ is a ball, the existence of a radially symmetric optimal set has been proved in [1, 3]. Even in this case an explicit solution to the problem is not known. It was conjectured in [3, 4], for higher dimensions, that the solution B^* to this problem is a ball $\mathbb{B}(0, R^*)$ as in dimension one [6]. We prove that the conjecture is not true in general. Indeed, the optimal domain B^* cannot be a ball when α and β are close to each other (low contrast regime) and m is sufficiently large. This result is provided by an asymptotic expansion of the eigenvalue with respect to $\beta - \alpha$ as $\beta \rightarrow \alpha$, which allows us to approximate (4)-(6) by a simpler optimization problem.

Optimal sets for small conductivity gap. We assume that $\beta = \beta^\varepsilon := \alpha + \varepsilon$ with $\varepsilon > 0$ converging eventually to zero. If the material with conductivity β^ε occupies the sub-domain B of Ω , the conductivity coefficient is, in this case,

$$(7) \quad \sigma = \sigma^\varepsilon(B) := \alpha\chi_A + \beta^\varepsilon\chi_B = \alpha + \varepsilon\chi_B.$$

Let $\lambda^\varepsilon(B)$ be the first eigenvalue in the problem

$$(8) \quad -\operatorname{div}(\sigma^\varepsilon(B)\nabla u^\varepsilon) = \lambda^\varepsilon(B) u^\varepsilon \quad \text{in } \Omega,$$

$$(9) \quad u^\varepsilon = 0 \quad \text{on } \partial\Omega$$

for the conductivity $\sigma^\varepsilon(B)$. It is well-known, from the Kreĭn-Rutman theorem [7], that the first eigenvalue of a linear elliptic operator is simple and the corresponding eigenfunction is of constant sign. We choose the eigenfunction $u^\varepsilon = u^\varepsilon(B)$ corresponding to $\lambda^\varepsilon(B)$ to be positive and normalize it using the condition

$$(10) \quad \int_{\Omega} (u^\varepsilon)^2 = 1,$$

For fixed B , $\lambda^\varepsilon(B)$ and $u^\varepsilon(B)$ depend analytically on the parameter ε ; see [8, Theorem 3, Chapter 2.5]. This justifies the ansätze

$$(11) \quad \lambda^\varepsilon(B) = \lambda_0(B) + \varepsilon\lambda_1(B) + \dots$$

$$(12) \quad u^\varepsilon(B) = v_0(B) + \varepsilon v_1(B) + \dots$$

The convergence of the series in (12) holds in $H_0^1(\Omega)$.

Proposition 1. *In ansätze (11) and (12), $\lambda_0(B)$ and $v_0(B)$ are independent of B . In fact, $\lambda_0(B) = \lambda_0$ is the first eigenvalue in the problem*

$$(13) \quad -\alpha\Delta v_0 = \lambda_0 v_0 \quad \text{in } \Omega,$$

$$(14) \quad v_0 = 0 \quad \text{on } \partial\Omega.$$

The function v_0 is the positive eigenfunction corresponding to λ_0 and satisfies the normalization $\int_{\Omega} v_0^2 = 1$.

Proposition 2. *In (11), $\lambda_1(B)$ is given explicitly as*

$$(15) \quad \lambda_1(B) = \int_B |\nabla v_0|^2 dx.$$

The following orthogonality relations hold true

$$(16) \quad \int_{\Omega} v_0 v_1(B) dx = 0 = \int_{\Omega} \nabla v_0 \cdot \nabla v_1(B) dx.$$

Introduce $\tilde{\lambda}^\varepsilon(B) = \lambda^\varepsilon(B) - \lambda_0 - \varepsilon\lambda_1(B)$, the remainder in the ansatz (11). We have the following uniform estimates with respect to B :

Theorem 1. *For $\varepsilon > 0$ sufficiently small, there exists a constant C independent of ε and B such that*

$$(17) \quad |\tilde{\lambda}^\varepsilon(B)| \leq C \varepsilon^{\frac{3}{2}} \quad \forall B \in \mathcal{B}.$$

Corollary 1. *If $B_\varepsilon^* \in \mathcal{B}$ is a minimizer of $\lambda^\varepsilon(\cdot)$ then we have the following estimate:*

$$(18) \quad \left| \lambda_1(B_\varepsilon^*) - \inf_{B \in \mathcal{B}} \lambda_1(B) \right| \leq 2 C \varepsilon^{\frac{1}{2}}$$

where the constant C is as in Theorem 1, independent of ε and $B \in \mathcal{B}$.

By the previous corollary we see that a minimizer for $\lambda^\varepsilon(\cdot)$ is approximately a minimizer for $\lambda_1(\cdot)$ when ε is small. Using a similar argument, we can show that if B^* is a minimizer of $\lambda_1(\cdot)$ then, for small $\varepsilon > 0$,

$$\left| \lambda^\varepsilon(B^*) - \inf_{B \in \mathcal{B}} \lambda^\varepsilon(B) \right| \leq 2 C \varepsilon^{\frac{3}{2}}.$$

Thus, minimizers for $\lambda_1(\cdot)$ are nearly optimal for $\lambda^\varepsilon(\cdot)$ in the above sense. The minimization of $\lambda_1(\cdot)$ follows from:

Theorem 2. *There exists $c^* \geq 0$ such that whenever B measurable satisfy*

$$\{x : |\nabla v_0(x)| < c^*\} \subset B \subset \{x : |\nabla v_0(x)| \leq c^*\}$$

and $|B| = m$, then B is an optimal solution for the problem of minimizing $\lambda_1(B)$ over $B \in \mathcal{B}$.

Disproving the disk conjecture. Consider the particular case $\Omega = \mathbb{B}(0, 1) \subset \mathbb{R}^d$. The solution v_0 of (13)-(14) is then radial and smooth. By setting $w_0(|x|) := v_0(x)$, equation (13)-(14) becomes, using the Laplacian in polar (r, θ) or spherical (r, θ, φ) coordinates, for $d = 2, 3$

$$(19) \quad r^2 w_0''(r) + (d - 1) r w_0'(r) + r^2 \frac{\lambda_0}{\alpha} w_0(r) = 0,$$

$$(20) \quad w_0'(0) = 0, \quad w_0(1) = 0.$$

where the boundary conditions (20) correspond to the continuity of the gradient at the origin and the Dirichlet condition on the boundary, respectively. The solution of this equation is

$$(21) \quad w_0(r) = J_0(\eta_d r) \quad \text{if } d = 2,$$

$$(22) \quad w_0(r) = j_0(\eta_d r) \quad \text{if } d = 3,$$

where J_0 and j_0 denote Bessel functions of the first and second kind, respectively and η_d , ($d = 2, 3$) are their respective zeros; see Figure 1. Let ω_d denote the volume of the unit ball, i.e. we have $\omega_d = \pi$ for $d = 2$ and $\omega_d = 4\pi/3$ for $d = 3$ and let r_d^0 and r_d^1 be as in Figure 1.

Proposition 3. *Assume $\Omega = \mathbb{B}(0, 1)$. The unique optimal domain B^* solution of the minimization problem for $\lambda_1(B)$ over $B \in \mathcal{B}$ is of two possible types*

- Type I: If $m \leq \omega_d (r_d^0)^d$ then $B^* = \mathbb{B}(0, (m/\omega_d)^{1/d})$ or,
- Type II: If $m > \omega_d (r_d^0)^d$ then there exists ξ^0 and ξ^1 with

$$(m/\omega_d)^{1/d} < \xi^0 < \xi^1 < 1$$

$$\text{and } B^* = \mathbb{B}(0, \xi^0) \cup \left(\mathbb{B}(0, 1) \setminus \overline{\mathbb{B}(0, \xi^1)} \right).$$

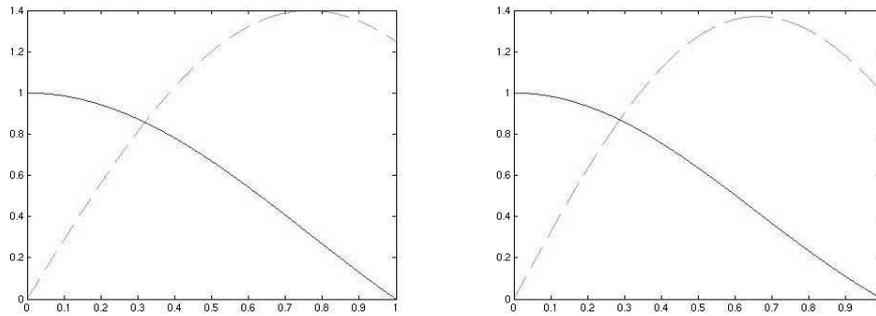


FIGURE 1. Functions $w_0(r)$ (plain), and $w_1(r) = -w_0'(r)$ (dashed) in dimensions $d = 2$ (left) and $d = 3$ (right). r_d^1 is such that w_1 is increasing on $[0, r_d^1]$ and decreasing on $[r_d^1, 1]$, and r_d^0 is such that $w_1(r_d^0) = w_1(1)$.

Finally we obtain

Theorem 3. *When $\Omega = B(0, 1)$, for $\beta = \alpha + \varepsilon$ sufficiently close to α and given an $m > \omega_d(r_d^0)^d$, the distribution of the materials wherein the material with the higher conductivity β is placed in a concentric disk in the center of the domain is not a solution of problem (4)-(5).*

REFERENCES

- [1] A. Alvino, G. Trombetti, and P.-L. Lions. On optimization problems with prescribed rearrangements. *Nonlinear Anal.*, 13(2):185–220, 1989.
- [2] C. Conca, A. Laurain, and R. Mahadevan. Minimization of the ground state for two phase conductors in low contrast regime. *SIAM Journal on Applied Mathematics*, 72(4):1238–1259, 2012.
- [3] C. Conca, R. Mahadevan, and L. Sanz. An extremal eigenvalue problem for a two-phase conductor in a ball. *Appl. Math. Optim.*, 60:173–184, 2009.
- [4] C. Conca, R. Mahadevan, and L. Sanz. Shape derivative for a two-phase eigenvalue problem and optimal configurations in a ball. In *CANUM 2008*, volume 27 of *ESAIM Proc.*, pages 311–321. EDP Sci., Les Ulis, 2009.
- [5] S. Cox and R. Lipton. Extremal eigenvalue problems for two-phase conductors. *Arch. Rational Mech. Anal.*, 136(2):101–117, 1996.
- [6] M. G. Krein. On certain problems on the maximum and minimum of characteristic values and on the Lyapunov zones of stability. *Amer. Math. Soc. Transl. (2)*, 1:163–187, 1955.
- [7] M. G. Krein and M. A. Rutman. Linear operators leaving invariant a cone in a banach space. *Amer. Math. Soc. Transl. (2)*, 26, 1950.
- [8] F. Rellich. *Perturbation Theory of Eigenvalue Problems*. Notes on mathematics and its applications. Gordon and Breach, New York, 1969.

Sensitivities for Graph Operations in Finite Element Meshes

JAN FRIEDERICH

(joint work with Günter Leugering, Paul Steinmann)

We consider h -refinement on finite element meshes based on sensitivities for continuous graph changes such as splitting nodes along edges. A possible scenario is depicted in figure 1(a), where the continuous process of inserting the new node \mathbf{x}_ϵ along edge $E = (\mathbf{x}_0, \mathbf{x}_+)$ is parametrized in the variable $\epsilon > 0$. As a model problem, we consider Poisson's equation $-\Delta u = f$, $u \in V := H_0^1(\Omega)$ with Galerkin solutions

$$\begin{aligned} u_h \in V_h : \quad & a(u_h, v_h) = (f, v_h)_\Omega \quad \forall v_h \in V_h, \\ u_h^\epsilon \in V_h^\epsilon : \quad & a(u_h^\epsilon, v_h^\epsilon) = (f, v_h^\epsilon)_\Omega \quad \forall v_h^\epsilon \in V_h^\epsilon \end{aligned}$$

for piecewise linear finite elements on the mesh \mathcal{T}_h and the refined mesh \mathcal{T}_h^ϵ , respectively. Then, we define the sensitivity for an objective functional $J : V \rightarrow \mathbb{R}$ for the topological mesh change by

$$D_E J(u_h) = \lim_{\epsilon \rightarrow 0} \frac{J(u_h^\epsilon) - J(u_h)}{\epsilon}.$$

For the computation of $D_E J(u_h)$ we rely on the analytical derivation of the first-order asymptotic expansion of u_h^ϵ with respect to $\epsilon > 0$. More precisely, one obtains

$$u_h^\epsilon = u_h + \epsilon(y_h + y_s) + o(\epsilon)$$

where $y_h \in V_h$ is the finite element solution of a dual equation and $y_s \in BV(\Omega)$ is a singular contribution that includes jumps over edges. Finally, $D_E J(u_h)$ can be calculated for an arbitrary edge E from given data, the current solution $u_h \in V_h$ and, typically, an adjoint solution $p_h \in V_h$.

In this context, a particular objective functional of interest is the total potential energy of the given variational problem

$$J(u) = \frac{1}{2}a(u, u) - (f, u)_\Omega,$$

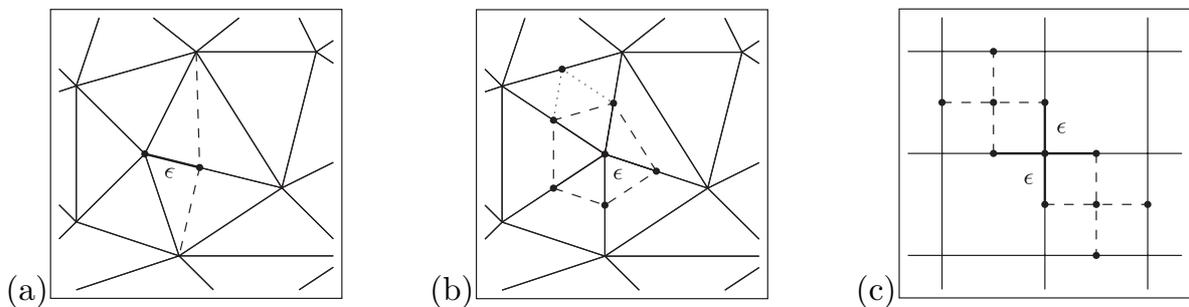


FIGURE 1. Mesh refinement scenarios: (a) Refinement of an edge. (b) Refinement around a node. (c) Refinement on quadrilateral elements with hanging nodes.

minimization of which can be shown to decrease the approximation error $\|u - u_h\|_a$ in the energy norm, cf. [1]. Hence, the corresponding sensitivities $D_E J(u_h)$ can be employed as edge-wise indicators for adaptive h -refinement. It turns out that in this case the sensitivities are related to the edge-wise residual-based refinement indicators η_E^2 , cf. [2, 3]. In particular, $|D_E J(u_h)|$ reveals the same orders of element and edge measures, residual terms and jumps over edges, and one easily obtains

$$|D_E J(u_h)| \leq C \eta_E^2.$$

A lower estimate seems to be more involved in general and remains the subject of further study. Note that $|D_E J(u_h)|$ delivers an approximation for the decrease of the error upon refinement rather than an upper estimate on the local error. However, numerical tests suggest that refinement based on our approach is as efficient as refinement based on residual-based error estimators, see figure 2 for an example in 2d. More general results are currently prepared for publication, for a study of our method in 1d we refer to [4].

Moreover, our concept is well-suited to be applied in goal-oriented refinement. Considering an output functional $J \in V'$, the sensitivities $D_E J(u_h)$ indicate the responsive behaviour of $J(u_h)$ with respect to refinement and may serve as an estimate for the decrease of the error $|J(u_h) - J(u)|$, i.e.

$$|D_E J(u_h)| \approx c |J(u_h^\epsilon) - J(u_h)| \geq c \left| |J(u_h^\epsilon) - J(u)| - |J(u_h) - J(u)| \right|$$

A more rigorous mathematical treatment involving higher-order asymptotic analysis is currently in development. However, our intuition is indeed confirmed by numerical experiments: As an example, we apply our concept to goal-oriented refinement with respect to a point-value error, i.e. we choose the regularized functional

$$J(u) := \frac{1}{|B_\delta(a)|} \int_{B_\delta(a)} u \, dx = u(a) + \mathcal{O}(\delta^2)$$

for a given point $a \in \Omega$, $\delta > 0$. The resulting sensitivity-based indicator is compared to the standard DWR-estimator from [5], see figure 3.

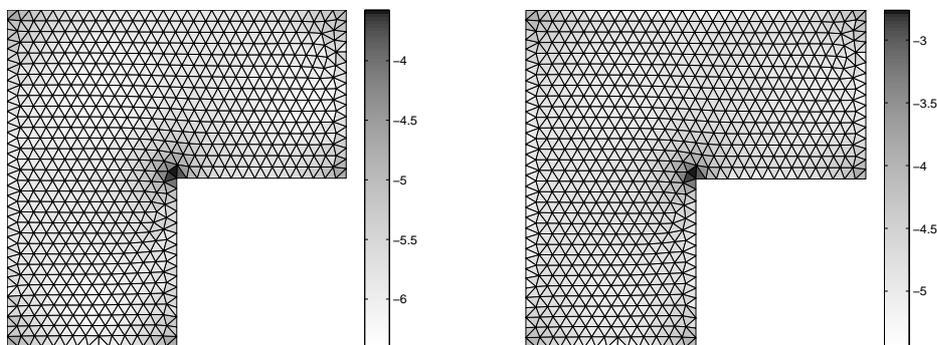


FIGURE 2. Refinement indicators for minimization of the energy error (logarithmic plot): $-\Delta u = 1$, $u|_{\partial\Omega} = 0$ on an L-shaped domain. (a) Indicator based on topological sensitivities $|D_E J(u_h)|$. (b) Residual-based error estimator η_E^2 .

Future research on this subject will include higher-order asymptotic analysis for graph changes, various applications in goal-oriented refinement and the extension to higher-order elements as well as non-linear equations.

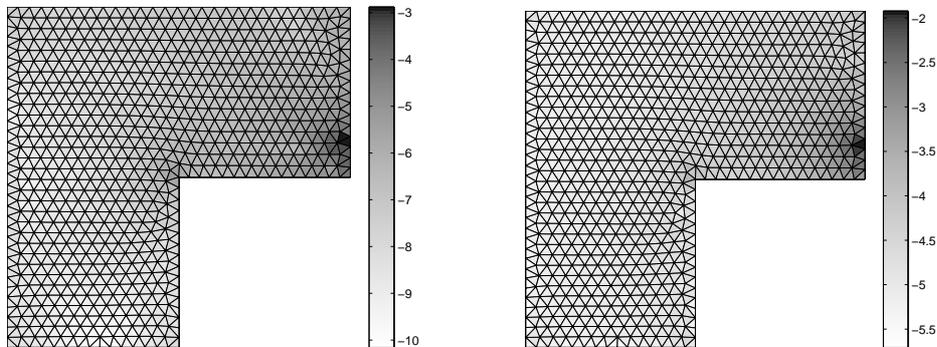


FIGURE 3. Refinement indicators for point evaluation at the right boundary (logarithmic plot): $-\Delta u = 1$, $u|_{\partial\Omega} = 0$ on an L-shaped domain. (a) Indicator based on topological sensitivities $|D_E J(u_h)|$. (b) DWR-based estimator η_{DWR} .

REFERENCES

- [1] M. Delfour, G. Payre, J.-P. Zolésio, *An optimal triangulation for second-order elliptic problems*, *Comput. Meth. Appl. Mech. Eng.* **50** (1985), 231–261.
- [2] S.C. Brenner, L.R. Scott, *The Mathematical Theory of Finite Element Methods*, 2nd ed., Springer, New York (2002).
- [3] R. Verfürth, *A review of a posteriori error estimation and adaptive mesh refinement techniques*, Wiley-Teubner, Chichester (1996).
- [4] J. Friederich, G. Leugering, P. Steinmann, *Adaptive refinement based on asymptotic expansions of finite element solutions for node insertion in 1d*, *GAMM-Mitt.* **35** (2012), 175–190.
- [5] W. Bangerth, R. Rannacher, *Adaptive Finite Element Methods for Differential Equations*, Birkhäuser, Basel (2003).

Participants

Prof. Dr. Samuel Amstutz
Université d'Avignon
U.F.R. Sciences et Technologies
Département de Mathématiques
74 rue Louis Pasteur
84029 Avignon
FRANCE

Harbir Antil
Department of Mathematics
George Mason University
MS3F2
4400 University Drive
Fairfax, VA 22030-4444
UNITED STATES

Prof. Dr. Michel Delfour
Centre de Recherches Mathématiques
Université de Montreal
C.P. 6128, Succ. Centre-Ville
Montreal P.Q. H3C 3J7
CANADA

Jan Friederich
Lehrstuhl für Technische Mechanik
Universität Erlangen
Egerlandstr. 5
91058 Erlangen
GERMANY

Prof. Dr. Bojan Guzina
University of Minnesota
Department of Civil Engineering
500 Pillsbury Drive S.E.
Minneapolis MN 55455
UNITED STATES

Prof. Dr. Michael Hintermüller
Fachbereich Mathematik
Humboldt-Universität Berlin
Unter den Linden 6
10117 Berlin
GERMANY

Prof. Dr. Dietmar Hömberg
Institut für Mathematik
Technische Universität Berlin
Sekt. MA 4-5
Strasse des 17. Juni 136
10623 Berlin
GERMANY

Martin Kanitsar
Institut für Mathematik und
wissenschaftliches Rechnen
Karl-Franzens-Universität Graz
Heinrichstr. 36
8010 Graz
AUSTRIA

Prof. Dr. Antoine Laurain
Institut für Mathematik
Sekt. MA 4-5
Technische Universität Berlin
Straße des 17. Juni 136
10623 Berlin
GERMANY

Prof. Dr. Günter Leugering
Department Mathematik
FAU Erlangen-Nürnberg
Cauerstraße 11
91058 Erlangen
GERMANY

Prof. Dr. Antonio Andre Novotny
Laboratorio Nacional de Computacao
Cientifica, MCT
Caixa Postal 95113
Av. Getulio Vargas 333
Petropolis RJ 25651-070
BRAZIL

Prof. Dr. Pavel I. Plotnikov

Lavryntyev Institute
Russian Academy of Sciences
Lavrentyev pr. 15
630 090 Novosibirsk
RUSSIAN FEDERATION

Prof. Dr. Jan Sokolowski

Département de Mathématiques
Université H. Poincaré (Nancy I)
Boite Postale 239
54506 Vandoeuvre-les-Nancy Cedex
FRANCE

Jennifer Rasch

Fachbereich Mathematik
Humboldt-Universität Berlin
Unter den Linden 6
10117 Berlin
GERMANY

Prof. Dr. Michael Stingl

Institut für Angewandte Mathematik
Universität Erlangen
Martensstr. 3
91058 Erlangen
GERMANY

Prof. Dr. Volker Schulz

Fachbereich IV - Mathematik
Numerik - Optimierung, partielle
Differentialgleichungen
Universität Trier
54286 Trier
GERMANY

Dr. Thomas M. Surowiec

Institut für Mathematik
Humboldt-Universität zu Berlin
Unter den Linden 6
10117 Berlin
GERMANY

Prof. Dr. James A. Sethian

Department of Mathematics
University of California
Berkeley CA 94720-3840
UNITED STATES

