Pointe-à-Pitre, December 04

INTRODUCTION TO OPTIMAL DESIGN: PROBLEMS, THEORY AND NUMERICS

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INTRODUCTION

Optimal design is a broad field of research in Applied Mathematics. It refers to a large class of problems in which, roughly speaking, one controls a system by means of a control variable which is the shape of the domain itself, rather than an external or boundary force applied to the system.

Optimal shape design may also be viewed as a pasive control mechanism introduced in a system at the manufacturing level. Choosing an optimal shape once forever one optimizes the behavior of the system for all its time duration.

Of course, in practice, one combines often optimal shape design with feedback controllers: pasive + active control, to guarantee an optimal behavior.

The number of applications is hughe:

- * Aeronautics.
- * Design of flexible structures.
- * Location of pollutants.
- * Optical fibers, wave guides.
- * Medicine, Biology,...

Optimal shape design is also very closely related to the field of Inverse Problems in which one wishes to determine some unkown shape from partial measurements: natural resources, the dammage in a structure after an earthquake, the size and form of a tumor, or of the region dammaged by some pollutant, ...

One of the intrinsic difficulties of the field lies on the fact that, we are obliged to manipulate "shapes" (open sets, for instance) and not functions. Obviously, shapes, when they are "regular enough" they can be represented by functions: the graph of a function determines a hypersurface in \mathbb{R}^N , the local charts for the parametrization of the boundary of a domain,... But, often in practice, the shapes appearing in nature or in manufactured systems are rather "complex": fractal domains, reticulated structures, perforated domains, domains with

fractures and cracks, ... and consequently, they are hard to represent as graphs of smooth functions,...

Moreover, when the domains under consideration are complex, the solutions of the underlying PDE's (the heat equation if a diffusion process is optimized or a wave equation in the case of flexible structures or acustic waves in noise reduction) develop singularities, thus making the analysis more difficult.

There are several different approaches to the mathematical theory of optimal design in the context of Continuum Mechanics and/or PDE. Different topics are also often addressed. Their relevance and mathematical complexity may differ significantly. Often in practice "simple" ideas and results are those that are more frequently implemented. The most sophisticated part of the theory, based on the deep theory pf PDE and/or Geometric Measure Theory, is rarely applied in real problems.

The following topics/approaches may be investigated:

* **Numerical issues**: To develop efficient numerical algorithms for improving shape in a reasonable manner for relevant engineering problems: elasticity/structures, fluid flows/aeronautics,...

This is the "optimization" point of view.

Here we do not look for sophisticated theorems but rather methods whose efficiency has to be tested/proved in the real mechanism. Very often a very subtle improvement of the shape may produce hughe economical succes.

Normally the methods that are developed in this setting are based on some minimization algorithm (conjugate gradient method, steepest descent,...).

The main difficulty is: what is the right descent direction? In which direction the shape should be modified in order to guarantee the best decrease of the functional under consideration?

Lagrange multipliers give the answer in the context of the minimization of a function in a set of the euclidean space represented as the level set of a smooth function.

But in the context of PDE's we are neither in the euclidean space (we work with functions, solutions of PDE's, that, of course, do cover infinite-dimensional spaces) and the contrainsts on the feasible domains may be not be written easily as the level set of a smooth function.

Of course, at this level, the natural and implicit constraints of the problem can not be ignored.

For instance, we do not want the wing of the plane to have a fractal shape....

Very often, in real applications, this has to be done on models for which we do not still have a good existence and uniqueness theory: nonlinear elaticity, turbulent 3 - d flows,... Thus, we can not expect to have a clear and rigorous notion of the "derivative of the functional with respect to the domain". But still mathematics may be of great help.

Some of the most relevant progresses in this field have been done precisely in situations in which the theory is not completely justified. The works by Jameson on Optimal Design in aeronautics and the mathematical counterpart that can be found in the books by Pironneau and Glowinski, for instance, is a good example of this. The same can be said about the application of the "level-set" method by Osher-Shetian in the context of optimal design in elasticity as applied by Allaire.

Mathematics are indeed needed even in the formal setting. One has to compute "linearizations", "adjoints", "gradients", "numerical discretizations", "discrete gradients",...

All known receipts are thus welcome: characterization of gradients by means of the adjoint state, the need of numerical viscosity for a better stability of numerical schemes,....

* **Theoretical issues:** This time one looks for rigourous theorems on the existence of optimal shapes.

One needs to work in the context of PDE's for which one disposes of a good theory for existence and uniqueness. But even in those cases the problem may become very complex if the class of shapes under consideration is not restricted enough.

In fact, there is a beatiful theory on these topics very much based in the ideas by De Giorgi, combining Γ -convergence and Geometric measure theory. The interested reader may find an introduction to this topic in the books by Dal Maso, Buttazzo, Pironneau, and the forthcoming ones by Bucur-Buttazzo and Henrot-Pierre.

The difficulty is easy to understand. Consider the Dirichlet laplacian. It is well-kown that, if the domain under consideration is of class C^2 and the right hand size is in L^2 , then solutions belong to H^2 . Moreover, this result is robust in the sense that estimates are uniform, when one works with classes of domains which are uniformly bounded in C^2 , or a family of right hand side terms which are uniformly bounded in L^2 .

Thus, it is not hard to guess that, when working in such restricted classes of admissible domains, the existence of an optimal shape is guaranteed by some compactness argument.

But, what happens if the requirements of the real problem impose considering general shapes which are not smooth?

For instance, the space $H_0^1(\Omega)$ and therefore the solution of the Dirichlet problem is well-defined for all open set Ω . Why then imposing so restrictive regularity conditions in the domain Ω ?

Then the following type of questions arises naturally: What is the minimal convergence notion of domains Ω so that the solutions of the Dirichlet laplacian converge in H_0^1 ?

Note that, in this particular case, we do not need to face the problem that each solution is defined in a different domain. We can simply extend all solutions by zero to the exterior of its domain of definition, and view all of them as elements of $H^1(\mathbf{R}^N)$.

Important efforst have been done in order to unify the two different approaches: the more theoretical and the more applied one. But there is still a lot to be done.

Here we mention some of the issues that arise and that are still the object of intensive research:

* The optimal shapes are not computed in the context of PDE's but rather for suitable numerical approximations.

Even in those cases in which an optimal shape is known to exist and in which one is able to write a reasonable descent algorithm, it has to be implemented in the computer. Thus, one has to apply the same ideas for a numerical model in which the PDE has been replaced by a numerical scheme.

Is it true that the optimal discrete shape for the numerical model converges to the optimal shape for the continuous one?

By now we know well that this is often not true in the simpler problem of boundary control of waves!

Later in the ocurse we will however prove a positive result in this sense in the context of the optimal shape design of the Dirichlet laplacian in \mathbf{R}^2 .

* When the domain under consideration are smooth perturbations of a reference smooth domain, one can develop the analysis initiated

by Hadamard (whose rigorous development for PDE's was done by Murat and Simon (see the Lecture Notes by Jacques Simon in the University of Sevilla)). **But what happens if there are topological changes of the domains?**

At this respect we should refer to the works by Guillaume and Masmoudi (Toulouse) in which the notion of topological derivative is introduced and developed. Roughly pseaking, one analyzes the sensitivity of the solution of a PDE with repect to an infinitesimal hole. The leading term of the asymptotic development is viewed as a topological derivative an it indicates whether the functional under consideration diminishes when perforating the domain or rather eliminating an existing hole. Note that, normally, one has to limit the class of domains under consideration to only have a finite number of holes. Otherwise, homogenization phenomena may occur, and the PDE may change in the limit process as the number of holes tends to infinity (the "term étrange" by Cioranescu and Murat).

* Recently the "level set approach" has been applied to the problem of optimal design. The point of view is rather natural: Manipulating domains is complex. But one can view a domain as the support of a characteristic function or, even better, as the level set of a regular version of it. One can then try to optimize the functional by improving the function whose level set provides the domain. In this way we do not need to deal with shapes but rather with functions. This method is very felxible and can be easily implemented. In particular it allows

holes to be created or to disappear. But, as far as we know, there is no rigorous analysis of the convergence of the method.

* Generic properties of PDE's. Optimal design and/or derivatives with respect to domains appear also naturally when addressing fine properties of solutions of PDE's. One of the most classical example is related with the spectrum of the Dirichlet Laplacian.

It is well known that the spectrum of the Dirichlet laplacian is not simple in the case of a square domain.

But is this an exceptional situation or rather a general property?

Using differentiation with respect to the domain and Baire's Theorem (together with unique continuation properties of eigenfunctions) one

can show that generically with respect to the domain the Dirichlet spectrum of the laplacian is simple. That means that multiplicity of the spectrum only occurs in very particular and exceptional situations.

This kind of ideas arise also for control problems. Consider for instance the heat equation with Neumann boundary control. In the absence of control the average of the solution is constant in time. It is then natural to raise the question of whether one may control the trajectories by keeping the average constant in time. In the context of approximate controllability this issue has been addressed by Ortega anz Zuazua. It has been proved that the answer to the question is negative for the ball, but generically positive.

The problem has not been addressed in the context of null-control but we think that a combination of the work mentioned above with the

recent developments by Nakoulima et al. in the context of null control with partial boundary observations in which a finite-dimensional projection is dropped, may solve the problem.

Another interesting problem in this setting is that of the generic simpliicity of the spectrum of the Stokes operator. Ortega-Zuazua have proved that to be the case in 2 - d. But the problem is open in 3 - d. An important to fact to always keep in mind is that

THE LINEZARIZATION OF AN OPTIMAL SHAPE DESIGN PROB-LEM IS A PROBLEM OF BOUNDARY CONTROL.

To make this statement rigorous let us consider the simplest problem, that of the Dirichlet laplacian in 1-d in a interval (0, L) whose lenght L is to be determined to fulfill some optimality condition:

$$-u'' = f, 0 < x < L; \quad u(0) = u(L) = 0.$$

Here f is given and the solution not only depends on x, as usual, but also on the length of the interval L. Thus, u = u(x, L). We want to determine L so that the solution is optimal in some sense. For instance, so that the functional

$$J(L) = \int_0^L |u(x, L) - u_d(x)|^2 dx,$$

achieves its minimum.

This is a very natural and frequently arising problem in which L is searched so that the solution is as close as possible from the given desired state u_d .

This is an optimization problem. Note that the controllability problem does not make sense in this context. Indeed, all solutions are confined to satisfy the condition -u'' = f and therefore, necessarily, they lie in an affine subspace of the space of all functions.

To minimize the functional J one has to be able to compute the derivative of J with respect to L, the "shape parameter in this simple problem". In this case we have:

$$J'(L) = |u(L,L) - u_d(L)|^2 + 2\int_0^L (u(x,L) - u_d(x))u_L(x,L)dx.$$

Here u_L stands for the derivative of the solution with respect to the "shape paparemter" L.

The key point is then computing $v = u_L$.

Taking into account that, in the interior of the interval (0, L) the equation -u'' = f is independent of L, the derivative $v = u_L$ necessarily satisfies the equation

$$-v''=0.$$

On the other hand, since the boundary condition at x = 0 is independent of L we also have

$$v(0) = 0.$$

The most delicate point is computing the boundary condition at x = L. There we use the boundary condition

$$u(L,L)=0.$$

After derivation this gives:

$$u_L(L,L) + u_x(L,L) = 0.$$

In other words,

$$v(L) = -u_x(L,L).$$

Thus, v., the derivative of the state with respect to the "sahpe parameter" L satisfies a non-homogeneous boundary condition in which the right hand side coincides with the normal derivative of the reference solution.

This is a systematic fact in optimal design problems, whose derivative is always a boundary control problem, the normal derivative of the state being the control.



To choose the optimal domain Ω within the class of domains, embedded in the pavé D and containing the subdomain ω , subject to some optimality criterium.

Numerical approximation in 2-d elliptic optimal shape design

Work in collaboration with D. Chenais, C. R. Acad. Sci. Paris, Ser. I (2004)

OPTIMAL DESIGN

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OPTIMIZATION PROCESS INVOLVING GEOMETRIES AND SHAPES.

Elliptic optimal design. Control= Shape of the domain. State equation = Dirichlet Laplacian.

Dimension n = 2, Šveràk: There exists an optimal domain in the class of all open subsets of a given bounded open set, whose complements have a uniformly bounded number of connected components.

Key point: compactness of this class of domais with respect to the complementary-Hausdorff topology and the continuous dependence of the solutions of the Dirichlet laplacian in H^1 with respect to it.



It is well known that, when the number of holes is unlimited, homogenization phenomena arise and the minimum is not achieved. Cioranescu-Murat: $-\Delta \rightarrow -\Delta + \mu$.

COMMON COMPUTATIONAL/NUMERICAL PRACTICE:

* Continuous optimal design \rightarrow discrete finite-element version.

* Compute the discrete optimal shape (discrete optimization or shape and topological derivatives, level set methos,...)

The choice of one method or another depends very much on the expertise and computational capacities.

THE PROBLEM:

Do these methods converge? YES!

This is a proof of the efficiency that most methods employed to solve optimal design problem computationally exhibit.

One may use different tools at the discret level:

- Shape derivatives;
- Topological derivatives;
- Discrete Optimization.

But numerical experiments are often of a surprisingly good accuracy (R. Feijoo, R. Tarocco, C. Padra,...)

We consider a finite-element discrete version of this problem and prove that the discrete optimal domains converge in that topology towards the continuous one.

Key point : finite-element approximations of the solution of the Dirichlet laplacian converge in H^1 whenever the polygonal domains converge in the sense of H^c -topology.

This provides a rigorous justification to the most common engineering to optimal design.

OPTIMAL SHAPE DESIGN+NUMERICS

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NUMERICS+OPTIMAL SHAPE DESIGN



The triangulation of the pavé and the fixed subdomain (constraint) from which all admissible discrete domains have to be built.



The class of admissible domains for the discrete problem. This time the admissible domains need to be unions of triangles from the discrete mesh. Let D be a bounded open lipschitz connected subset of \mathbb{R}^2 .

Denote by $\sharp_c \Omega$ the number of connected components of $\overline{D} \setminus \Omega$.

For a fixed $N \in \mathbf{N}$, we consider the family of admissible domains

$$\mathcal{O}^N = \{ \Omega \subset D; \ \Omega \text{ open}, \ \sharp_c \Omega \leq N \},\$$

and the H^c -topology defined by the metric

$$d_{H^c}(\Omega, \ \Omega') = \max\{\max_{x \in \overline{D} \setminus \Omega} \ d(x, \ \Omega'), \ \max_{x' \in \overline{D} \setminus \Omega'} \ d(x', \ \Omega)\}.$$

 \mathcal{O}^N is H^c -compact.

For $f \in H^{-1}(D)$ and $\Omega \in \mathcal{O}^N$, let y_{Ω} be the solution of the Dirichlet problem in Ω :

$$-\Delta y = f$$
 in Ω ; $y = 0$ on $\partial \Omega$;

or, in variational form,

$$y_{\Omega} \in H_0^1(\Omega); \quad \int_{\Omega} \nabla y_{\Omega} \cdot \nabla z = \langle f, z \rangle_{H^{-1}(\Omega), H_0^1(\Omega)}, \quad \forall z \in H_0^1(\Omega).$$

Optimal design problem:

 $\min_{\Omega \in \mathcal{O}^N} j(\Omega), \quad \text{with} \quad j(\Omega) = \langle f, y_{\Omega} \rangle_{H^{-1}(\Omega), H^1_0(\Omega)} = \int_{\Omega} |\nabla y|^2 dx.$

Šveràk proved that a minimizer Ω^* does exist in \mathcal{O}^N .

For each h > 0 we introduce a regular triangular mesh $(\mathcal{T}_h)_h$ of the domain D of size h and the family \mathcal{O}_h^N of polygonal open subsets of D union of triangles in $(\mathcal{T}_h)_h$ belonging to the class \mathcal{O}^N .

The finite-element space $V_h(\Omega_h) \subset H_0^1(\Omega_h)$ constituted by continuous and piecewise P_1 polynomial (over triangles).

The Galerkin finite-element approximation:

$$y_h \in V_h(\Omega_h); \quad \int_{\Omega_h} \nabla y_h \cdot \nabla z_h = \langle f, z_h \rangle_{H^{-1}, H^1_0(\Omega_h)}, \quad \forall z_h \in V_h(\Omega_h).$$

The discrete optimal design problem:

$$\min_{\Omega \in \mathcal{O}_h^N} j(\Omega), \quad \text{with} \quad j_h(\Omega) = \int_{\Omega_h} |\nabla y_h|^2 dx.$$

The ingredients of the proof: **Г**-convergence

FACT 1: Any $\Omega \in \mathcal{O}^N$, can be approximated by $\Omega_h \in \mathcal{O}_h^N$ as follows:

$$F = \overline{D} \setminus \Omega, \quad F_h = \bigcup_{T \in \mathcal{T}_h, T \cap F \neq \emptyset} T, \quad \Omega_h = \overline{D} \setminus F_h.$$

It is easy to prove that $d_{H^c}(\Omega_h, \Omega) \xrightarrow{h \to 0} 0$, and $\sharp_c \Omega_h \leq N$ for any h. We then prove that

$$\widetilde{y_h} \stackrel{h \to 0}{\longrightarrow} \widetilde{y_\Omega} \quad \text{strong} - H^1(D)$$

 $j_h(\Omega_h) := \langle f, y_h \rangle_{H^{-1}(\Omega), H^1_0(\Omega_h)} \stackrel{h \to 0}{\longrightarrow} j(\Omega).$

This result guarantees the convergence of the Galerkin finite-element approximations with respect to the H^c - convergence of domains.

FACT 2: The same occurs if Ω_h is an arbitrary sequence of admissible domains H^c -converging to Ω .

FACT 3: The existence of a minimizer Ω_h^{\star} for j_h in the class \mathcal{O}_h^N for each h > 0 is obvious since \mathcal{O}_h^N has a finite number of elements.

FACT 4: The results above and a standard Γ -convergence argument allow showing that any H^c -accumulation point Ω^* of discrete optimal domains Ω_h^* is an optimal domain for the continuous problem.

CONCLUSION:

We have given a rigorous mathematical answer to the issue of whether control and numerics commute depends in a very sensitive way on:

* The control requirement one imposes: Stronger control requirement produce instabilities more easily.

* The model under consideration, and in this sense, the wave equation is the most unstable one;

* The numerical scheme: correct dispersivity and dissipativity properties are needed to capture correctly high frequency components.

OPEN PROBLEMS:

* Analyze the same issue in thye context of the Neumann problem. The problem is more difficult even for the continuous Laplacian;

* Analyze the problem of finding the discrete optimal shape. Compare different strategies: discrete optimization, descent methods,...

* When applying descent methods for obtaining the discrete optimal shapes analyze the possible use of the continuous gradient for computing descent directions (continuous versus discrete gradients).

* Obtain convergence rates.

* Address more complex models: Elasticity and Stokes equations, Navier-Stokes,

Work carried out within the EU Networks

"Homogenization and Multiple Scales" (A. Damlamian)

and

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"Smart Systems" (B. Miara).
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With the support of the Spanish MCYT (Ministerio de Ciencia y Tecnologia).