THE PHASE–FIELD METHOD IN OPTIMAL DESIGN

Blaise Bourdin
Department of Mathematics
Louisiana State University
Baton Rouge, LA 70803, USA
bourdin@math.lsu.edu

Antonin Chambolle
CMAP, École Polytechnique
CNRS (UMR 7641)
91128 Palaiseau Cedex, France
chambolle@cmap.polytechnique.fr

Abstract We describe the phase-field method, a new approach to optimal design originally introduced in Bourdin and Chambolle, 2000; Bourdin and Chambolle, 2003. It is based on the penalization of the variation of the properties of the designs, and its variational approximation (in the sense of Γ–convergence. It uses a smooth function, the phase-field, to represent all materials involved.

We describe our approach, and detail its application to two problems.

Keywords: Phase–field, multi-physics optimal design, perimeter penalization

Introduction

Consider the following generic optimal design problem: given a *reference domain* Ω in $\mathbf{R}^N$, some $D_0 \subset \Omega$, and two volume fractions $0 \leq \theta_1 \leq \theta_2 \leq 1$, the *admissible designs* are subsets D of Ω, such that

$$\begin{array}{l} D_0 \subseteq D \subseteq \Omega \\ \theta_1|\Omega| \leq |D| \leq \theta_2|\Omega| \end{array} \tag{1}$$

An optimal design problem is to find an admissible design D minimizing some *objective function*, F, that is :

$$\inf_{D \text{ admissible}} F(D). \tag{2}$$

In this form, optimal designs problems are very likely to be ill–posed. The geometric constraints are not enough to ensure the compactness and closedness of the set of feasible designs. Over the years, several theoretical and numerical workaround have been proposed. In the *homogenization*–based methods, one considers generalized designs, microperforated or laminated materials for example (see Kohn and Strang, 1986; Bendsøe and Kikuchi, 1988; Allaire and Kohn, 1993a; Allaire and Kohn, 1993b; Allaire and Kohn, 1994; Cherkaev and Kohn, 1997; Allaire et al., 1997; Cherkaev, 2000; Allaire, 2002, among others). Another class of numerical methods relies on heuristic "filtering" techniques (Diaz and Sigmund, 1995; Sigmund and Petersson, 1998). It was rigorously studied in Bourdin, 2001. Lastly, various penalization methods have also been suggested, where one adds an additional term to the objective function, in order to gain compactness.

Among all these choice of penalizations, "perimeter–controlled" optimization has a special place (Haber et al., 1996). It has been long understood that adding a surface term proportional to the perimeter of the designs prevents from sequences of solutions wit rapid oscilllations, and makes the problems well posed. This was indeed formalized in Ambrosio and Buttazzo, 1993, where (2) is replaced with the following free discontinuity problem:

$$\inf_{D \text{ admissible}} F(D) + \lambda \mathcal{H}^{N-1}(\partial D), \tag{3}$$

where λ is an arbitrary parameter and $\mathcal{H}^{N-1}$ represents the $N-1$–dimensional Haussdorf measure *i.e.* the length of ∂D in two dimensions, or its area in three dimensions (see Federer, 1969; Evans and Gariepy, 1992, for instance).

In the absence of an efficient numerical implementation, this method has not been widely accepted. The phase–field approach introduced in Bourdin and Chambolle, 2000; Bourdin and Chambolle, 2003 provides such a thing.

1. The phase-field method

The numerical implementation of (3) and in particular the approximation of the perimeter term are challenging. If D is a *set of finite perimeter*, then $\mathcal{H}^{N-1}(\partial D)$ is equal to the *total variation* of χ_D. If one uses *material interpolation schemes*, and replaces the characteristic function with a smooth material density ρ, with values in $[0, 1]$, then the total variation of ρ is given by

$$TV(\rho) = \int_\Omega |\nabla \rho| \, dx, \tag{4}$$

which raises two issues. Numerical minimization of an equivalent of (3) replacing the perimeter term with $TV(\rho)$ is challenging. If one tries to avoid intermediate material densities, using material penalization, for instance, then (4) becomes very stiff, and its numerical approximation non-isotropic (see Petersson et al., 1999; Chambolle, 1999).

Our approach is different. We consider a small parameter ε and introduce the functional

$$\mathcal{P}_\varepsilon(\rho) = \frac{1}{c_W} \int_\Omega \frac{\varepsilon}{2} |\nabla \rho(x)|^2 + \frac{1}{\varepsilon} W\left(\rho(x)\right)\, dx \tag{5}$$

where W is a l.s.c potential such that $W(0) = W(1) = 0$, $W(x) > 0$ if $x \notin \{0, 1\}$, $W(x) \geq c_1|x|^2 - c_2$ for some $c_1 > 0$ and c_2, and $c_W = \int_0^1 \sqrt{2W(t)}\, dt$. We also extend the objective function F by a $\mathcal{F}$, defined for any density field $\rho(x) \in L^1(\Omega)$, and such that

$$\mathcal{F}(\chi_D) = F(D), \tag{6}$$

for any set D of finite perimeter, and such that $\mathcal{F}(\rho)$ depends continuously on ρ. Then, we consider the following regularization of the optimal design problem:

$$\inf_{\rho \in \mathcal{D}_A} \mathcal{F}(\rho) + \lambda \mathcal{P}_\varepsilon(\rho), \tag{7}$$

where the set of admissible designs is

$$\mathcal{D}_A = \left\{ \rho \in H^1(\Omega), \rho(x) = 1 \text{ a. e.in } D_0, \text{ and } \theta_1|\Omega| \leq \int_\Omega |\rho(x)|\, dx \leq \theta_2|\Omega| \right\}.$$

It is well-known (see Alberti, 2000; Modica and Mortola, 1977a; Modica and Mortola, 1977b; Dal Maso, 1993; Braides, 2002 for instance) that if for any small ε there exists a subsequence ρ_{ε_j} of the sequence ρ_ε of minimizers of (7) and a subset $D \in \Omega$, such that $\rho_{\varepsilon_j} \to \chi_D$ almost everywhere in Ω, then D is a solution of (3). Practically, this means that solving the regularized problem (7) for a "small enough" ε will lead to a good approximation of the solution of (3).

This approach has several advantages over the classical ones. It is independent of the choice of $\mathcal{F}$, provided that condition (6) is satisfied. In the case of structural optimization, for instance, this means that the debate over the mechanical soundness of various material interpolation law is unrelevant in our case (although it might be used in the numerical implementation as in Bourdin and Chambolle, 2003). From the expression of $\mathcal{P}_\varepsilon$, it is clear that for a given ε, the minimizing sequences of designs are bounded in $H^1(\Omega)$. Classical numerical methods, finite elements or finite differences can be applied without fear of mesh-dependency, checkerboards, or anisotropy for instance.

One of the drawback of the method, which is indeed true of all perimeter controlled optimal design method, is that the solution of (3) may not be an open set and regular set. Optimal sets for the penalized problems are sets of finite perimeter, a very wide class of sets that contains very "pathological" sets. If one wishes to carry out a very rigorous analysis of the method applied to a specific objective function, one has to study the regularity of the solutions. This is done in Ambrosio and Buttazzo, 1993 for the thermal conductivity problem

and in Chambolle and Larsen, 2003 in the case of compliance optimization, for instance.

Lastly, the penalization term in (7) takes into accounts only the part of the perimeter of D *inside* the computational domain. In other words, it does not account for the part of the boundary of D that lies along $\partial\Omega$. This can easily addressed (see Bourdin and Chambolle, 2003 or Bourdin et al, 2000 for a similar problem in fracture mechanics). For the sake or simplicity, we do not discuss this issue in this paper.

In the following section, we describe the application of the phase field in the classical context of compliance optimization, then extend it to a multi-phase problem with design-dependent loads. Note that it has already been used in more complicated problems (Burger and Stainko, 2003) and that extension to more general problems involving multiple materials and multiple physics are in progress.

2. A classical example: compliance optimization

We consider here the classical problem of the design of structure with maximal stiffness under given loads. Let Γ_0 and $\Gamma_f \in \partial\Omega$ be disjoint subsets of the boundary of Ω standing at strictly positive distance from each other. Let f, be a given force on Γ_f, and $\mathbf{A}$ be the linear Hooke's law of an elastic material occupying a subset $D \subset \Omega$. The compliance of D under the load f is defined by

$$F(D) = -\inf_{u=0 \text{ on } \Gamma_0} \int_D \mathbf{A}e(u) : e(u)\, dx - 2\int_{\Gamma_f} f \cdot u\, dx, \tag{8}$$

where and $e(u)$ is the symmetrized gradient of u. It is easy to show that the perimeter-controlled optimal design associated with this objective function is well-posed, in the class of sets of finite perimeter. A little more care has to be taken while applying the phase–field regularization, however. Indeed, the straightforward extension of F to characteristic functions χ_D is not continuous. Following a now classical approach, we introduce an arbitrarily weak fictitious material with Hooke's law $\delta\mathrm{A}$ ($\delta > 0$), and extend the compliance as

$$F_\delta(D) = -\inf_{u=0 \text{ on } \Gamma_0} \int_\Omega \left((1-\delta)\chi_D + \delta\right) \mathbf{A}e(u) : e(u)\, dx - 2\int_{\Gamma_f} f \cdot u\, dx. \tag{9}$$

Note that this step is not strictly related to the phase-field method, but simply about gaining continuity of the objective function with respect to design changes. In Bourdin and Chambolle, 2003, it is shown using Γ–convergence, that when $\delta \to 0$, the minmizers of $F_\delta(D) + \lambda\mathcal{P}(D)$ converges to that of $F(D) + \lambda\mathcal{P}(D)$.

A trivial way to extend F_δ to arbitrary density functions $\rho(x)$ is to consider *any* function continuous monotonous function S such that $S(0) = 0$ and $S(1) = 1$, and

$$\mathcal{F}_\delta(\rho) = - \inf_{u=0 \text{ on } \Gamma_0} \int_\Omega ((1-\delta)S(\rho) + \delta)\, \mathbf{A}e(u) : e(u)\, dx - 2 \int_{\Gamma_f} f \cdot u\, dx. \tag{10}$$

Once again, it is shown in Bourdin and Chambolle, 2003 that when $\varepsilon \to 0$, the minimizer $\rho_{\delta_\varepsilon}$ of $\mathcal{F}_\delta(\rho) + \lambda \mathcal{P}_\varepsilon(\rho)$ converge to a χ_{E_δ}, where E_δ minimizes $F_\delta(D) + \lambda \mathcal{P}(D)$ among all admissible designs D. Sending then δ to 0, one obtains convergence of $v_{\delta,\varepsilon}$ to the minimizers of $F(D) + \lambda \mathcal{P}(D)$.

Figure 1 presents a numerical example obtained by Arnaud Anantharaman and Alain Griveau under Antonin Chambolle's supervision, at École Polytechnique. It corresponds to a beam clamped on its lower-left and lower-right corners, and loaded in its center. The density of gray corresponds to the value of the phase field ρ. The function W used here is

$$W(t) = \begin{cases} t(t-1)/2 & \text{if } 0 \le t \le 1 \\ +\infty & \text{otherwise,} \end{cases}$$

and the material interpolation law is $S(t) = t^2$.

Note that the density function ρ, has very little intermediate values. Indeed, the second term in (5) penalizes them. The transition of ρ from 0 to 1 along the edges of the designs is still smooth, meaning that piecewise linear finite element, for instance, will provide a good interpolation. It is known indeed that the with of the transition layer around the edges of the designs is of the order of $\varepsilon\pi$, for any $\varepsilon > 0$. This gives an estimate on how small shall one set the regularization parameter, in relation with the mesh size, for example.

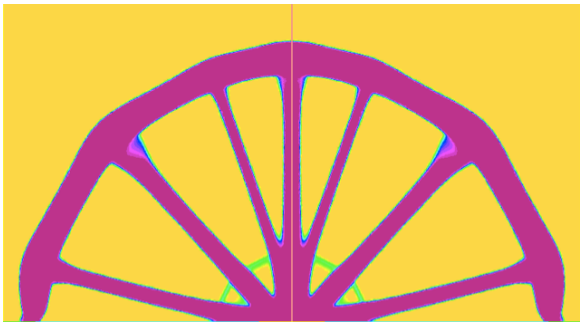

Figure 1. Optimal design of a beam using the phase field method.

3. Extension to design-dependent loads

Another strength of our approach is that the phase field also provides a simple way to represent the edges of the designs, and is easy to extend to the case of more than two phases.

In Bourdin and Chambolle, 2003, we consider the problem of the minimization of the compliance of structures submitted to fixed pressure loads on parts of their boundary. We consider a domain Ω partitioned in three subsets S (the structure), L (some liquid under a give pressure p), and V the void. The compliance of this system is given by

$$F(S,L,V) = \inf_u \int_S \mathrm{A}e(u) : e(u)\,dx - 2\int_{\partial L} pu(x)\cdot\nu_L(x)\,d\mathcal{H}^{N-1}(x), \quad (11)$$

where ν_L is the outer normal to the set L, and u varies among kinematically admissible displacement fields which we do not explicit here. A generalization of the perimeter energy to this three phase case would is

$$\Lambda(S,L,V) = \mathcal{H}^{N-1}(\partial S\cap\partial L)+\mathcal{H}^{N-1}(\partial S\cap\partial V)+\mathcal{H}^{N-1}(\partial L\cap\partial V). \quad (12)$$

Intuitively, however, it is clear that if the interface in between the liquid and the void sets has length > 0, then the compliance (11) is infinite. Indeed, we show (in 2D only) that if $F(S,L,V) < \infty$ then $\mathcal{H}^{N-1}(\partial L \cap \partial V) = 0$, in which case we have

$$\Lambda(S,L,V) = \mathcal{H}^{N-1}(\partial L) + \mathcal{H}^{N-1}(\partial V). \quad (13)$$

Another consequence of that is that it allows the use of a *scalar* phase field: following the analysis of the previous section, we introduce a fictitious material of Hooke's law $\delta\mathrm{A}$, a phase field ρ, and three material interpolation functions S, L, V such that

$$\left\{\begin{array}{l} V(-1)=1, V(0)=V(1)=0 \\ S(-1)=0, S(0)=1, S(1)=0 \\ L(-1)=L(0)=0, L(1)=1 \end{array}\right. \quad (14)$$

In this case, one can approximate $F(S,L,V)$ by a function $F_\varepsilon(\rho)$ similar to (5) where W is now a three-well function such that $W(-1)=W(0)=W(1)=0$ and $W(x)>0$ if $x\notin\{-1,0,1\}$. Lastly, the compliance $F(S,L,V)$ becomes

$$\mathcal{F}_{\delta,\epsilon}(S,L,V) = \inf_u \int_\Omega \left((1-\delta)S(\rho)+\delta\right)\mathrm{A}e(u) : e(u)\,dx - 2\int_\Omega pu(x)\cdot\nabla L(\rho)\,dx. \quad (15)$$

Note in particular how the surface intergral over ∂L was approximated in terms of $\nabla L(\rho)$. Again using Γ–convergence with respect to δ first and then ε, one can show that the minimizers of $\mathcal{F}_{\delta,\varepsilon} + \lambda\mathcal{P}_\varepsilon$ converge to that of $F(S,L,V) + \lambda\Lambda(S,L,V)$.

Figure 2 represents the design of a piston subject to pressure forces in its lower side, and clamped along the black rectangle on the top left corner. The black colored region correspond to $\rho = 1$, *i.e.* the liquid, the gray area to $\rho = 0$ (the structure), and the white are to the void ($\rho = -1$). The white line correspond to the level line $1/3$ of ρ and the black one to $\rho = -1/3$. The three design correspond to decreasing parameters λ. As expected, the complexity of the topology of the designs increases when λ decreases.

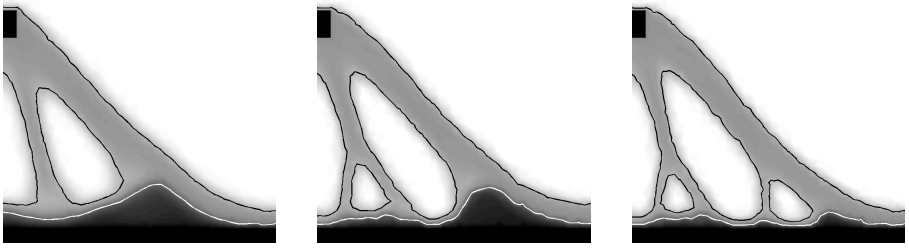

Figure 2. Optimal design of a piston.

References

Alberti, G. (2000). Variational models for phase transitions, an approach via Γ–convergence. In *et al.*, G. B., editor, *Calculus of Variations and Partial Differential Equations*, pages 95–114. Springer–Verlag. (Also available at `http://cvgmt.sns.it/papers/`).

Allaire, G. (2002). *Shape optimization by the homogenization method*. Springer-Verlag, New York.

Allaire, G., Bonnetier, É., Francfort, G., and Jouve, F. (1997). Shape optimization by the homogenization method. *Numer. Math.*, 76(1):27–68.

Allaire, G. and Kohn, R. (1993a). Explicit optimal bounds on the elastic energy of a two-phase composite in two space dimensions. *Quart. Appl. Math.*, 51(4):675–699.

Allaire, G. and Kohn, R. (1993b). Optimal bounds on the effective behavior of a mixture of two well-ordered elastic materials. *Quart. Appl. Math.*, 51(4):643–674.

Allaire, G. and Kohn, R. (1994). Optimal lower bounds on the elastic energy of a composite made from two non-well-ordered isotropic materials. *Quart. Appl. Math.*, 52(2):311–333.

Ambrosio, L. and Buttazzo, G. (1993). An optimal design problem with perimeter penalization. *Calc. Var. Partial Differential Equations*, 1(1):55–69.

Bendsøe, M. and Sigmund, O. (2002). *Topology Optimization.* Springer, Berlin

Bendsøe, M. and Kikuchi, N. (1988). Generating optimal topologies in structural design using a homogenization method. *Comput. Methods Appl. Mech. Engrg.*, 71(2):197–224.

Bourdin, B. (2001). Filters in topology optimization. *Int. J. Numer. Meth. Engrg*, 50:2143–2158.

Bourdin, B. and Chambolle, A. (2000). *Optimisation topologique de structures soumises à des forces de pression*. Actes du 32ème Congrès National d'Analyse Numérique. SMAI, editor (2000)

Bourdin, B. and Chambolle, A. (2003). Design-dependent loads in topology optimization. *ESAIM: Control, Optimisation and Calculus of Variations*, 9:19–48.

Bourdin, B., Francfort, G.A. and Marigo, J.-J. (2000). *Numerical experiments in revisited brittle fracture* J. Mech. Phys. Solids 48(4):797–826.

Braides, A. (2002). Γ–*convergence for beginners.* Oxford Lecture Series in Mathematics and its Applications, vol.Ê22. Oxford University Press, Oxford.

Burger, M. and Stainko, R. (2003). *Phase-field relaxation of topology optimization with local stress constraints* to appear.

Chambolle, A. (1999). Finite differences discretizations of the Mumford-Shah functional. *M2AN Math. Model. Numer. Anal.*, 33(2):261–288.

Chambolle, A. and Larsen, C. (2003). C^∞ regularity of the free boundary problem for a two-dimensional optimal compliance problem *Calc. Var. Partial Differential Equations*, 18(1):77–94

Cherkaev, A. (2000). *Variational methods for structural optimization*. Springer-Verlag, New York.

Cherkaev, A. and Kohn, R., editors (1997). *Topics in the mathematical modelling of composite materials*. Birkhäuser Boston Inc., Boston, MA.

Dal Maso, G., (1993). *An introduction to* Γ*-convergence.* Birkhäuser.

Diaz, A. and Sigmund, O. (1995). Cherckerboard patterns in layout optimization. *Struct. Optim.*, 10:40–45.

Evans, L. and Gariepy, R. (1992). *Measure theory and fine properties of functions*. CRC Press, Boca Raton, FL.

Federer, H. (1969). *Geometric measure theory*. Springer-Verlag, New York.

Haber, R.B., Jog C.S. and Bendsøe, M.P. (1996). A new approach to variable-topology shape design using a constraint on the perimeter. Struct. Optim. 11 (1996), 1–12.

Kohn, R. and Strang, G. (1986). Optimal design and relaxation of variational problems. I-III. *Comm. Pure Appl. Math.*, 39(3):113–137, 139–182, 353–377.

Modica, L. and Mortola, S. (1977a). Il limite nella Γ–convergenza di una famiglia di funzionali ellittici. *Boll. Un. Mat. Ital. A (5)*, 14(3):526–529.

Modica, L. and Mortola, S. (1977b). Un esempio di Γ^-–convergenza. *Boll. Un. Mat. Ital. B (5)*, 14(1):285–299.

Petersson, J. Beckers M., and Duysinx, P. (1999). Almost isotropic perimeters in topology optimization : theoretical and numerical aspects *Proceedings of the Third World Congress on Structural and Multidisciplinary Optimization (Amherst, NY)*

Sigmund, O. and Petersson, J. (1998). Numerical instabilities in topology optimization: A survey on procedures dealing with checkerboards, mesh-dependencies and local minima. *Struct. Opt.*, 16(1):68–75.

Wang, M.Y. and Zhou, S.W. (2004). Phase transition: a variational method for structural topology optimization. *CMES: Computer Modeling in Engineering & Sciences*, 6(6):547–566.