Checkerboard instabilities
in topological shape optimization algorithms

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Abstract

Checkerboards instabilities for an algorithm of topological design are studied on a simple example. The algorithm uses orthogonal rank-2 laminates as design variables, which need to be regularized as the associated Hooke's laws are degenerate. When the displacements are approximated by $Q1$ or $Q1$-bubble elements, the discrete operator is linearized, and its eigenvalues are computed in terms of the regularization parameter.

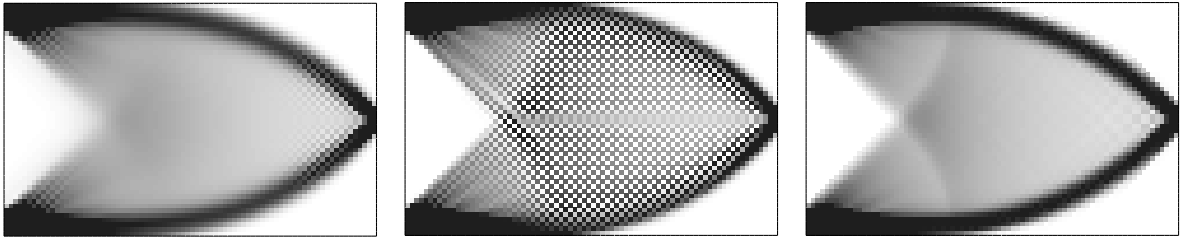Keywords: Checkerboard instabilities, topological optimization.

Figure 1: *2d cantilever: beginning of instabilities (iteration 80, left), after convergence (iteration 400, middle), after convergence with a proper filtering process (iteration 400 right).*

1 Introduction

Algorithms for shape optimization by the homogenization method have become very popular in structural design. Several versions have been developed [2], [1] and commercial software companies are now offering packages, based on this methodology, that perform shape optimization.

The basic problem consists in distributing some elastic material in a given volume, in order to design the shape that is most performant under given solicitations with respect to some design criterion. Typically, the problem is formulated as the minimization of a cost functional associated with the stress field, over a set of characteristic functions that represents the possible distributions of a given elastic material, with Hooke's law A_0. In the most studied case, the objective function is the compliance, *i.e.*, the work of prescribed external loads, applied on the boundary of the volume where the shape is to be designed.

Homogenization pitches in, because this basic formulation does not translate into a sound optimization problem, from the point of view of the calculus of variations. It turns out that the kind of cost functional considered does not have the proper convexity properties, and a relaxation of the formulation is necessary. From a numerical point of view, the natural formulation of the

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optimization problem yields numerical algorithms that are unstable under mesh refinements. The relaxation is performed via homogenization theory, and amounts to reset the problem as one of finding the most performant distribution of a specific family of porous materials, so as to minimize the extended objective function. The appropriate porous materials are viewed as composites made of mixtures of the original material A_0 and voids. The original formulation can then be replaced by that of minimizing the extended compliance with respect to two fields: the admissible stresses or strains, and the parameters that describe a sufficiently large class of admissible composites (the design variables).

M. Bendsoe and his collaborators use a saddle-point formulation using the strains and the design variables [6]. We favor using the stresses and the design variables that describe a particular family of composites, the so-called rank N laminates. Our choice is motivated by the fact that one can explicitly determine the laminate, the compliance of which is optimal under a given stress field. Thus, a natural numerical algorithm consists in iteratively solving an elasticity problem to compute the stress field (for some fixed design variables) then in updating the design variables (for a fixed stress field) using explicit optimality conditions [1]. In the computations reported there, the elastic displacement is discretized with $Q1$ finite elements, while the design parameters are chosen piecewise constant.

If a lot of progress has been made concerning the mathematical study of the continuous problem, not much is known concerning the numerical analysis of the different algorithms that have been proposed. Most of them, however, show checkerboard type instabilities on the density of the material A_0 in the composite, the variable that serves to visualize the results. Such instabilities are typical features of saddle-point problems, and the traditional remedies applied to computations for Stokes problem provide a satisfactory cure. Computations using higher order elements for the displacement have been reported to be checkerboard-free (see for example [6]), filtering the checkerboard modes of the density on macro-elements also gives good results [1], [3]. Another approach [7], consists in seeking a bound on the total perimeter of the shape.

Several authors invoke the Babuška-Brezzi inf-sup condition [4], to explain the appearance of checkerboard. In [5], Diaz and Sigmund consider a patch of four elements, and show that the discrete compliance computed with linear finite elements (respectively with quadratic elements) is lower (respectively higher) than that of the solution to the continuous problem obtained by homogenization.

In this note, we study a simple example where the algorithm of [1] produces these instabilities and we try to relate them with the choice of rank-N laminates as design variables. As explained above, the algorithm is based on an alternate directions method, where the stress field and the design parameters are updated iteratively. At each iteration, the new design parameters, are those of the optimal rank-N laminate ($N = 2$ in 2d, $N = 3$ in 3d). In 2d, the laminate which is optimal under a stress field σ is a rank-2 laminate with layers in orthogonal directions (the principal directions of σ), and proportions within the layers that depend on the principal stresses. Only three parameters are necessary to describe those materials: the overall density of A_0, θ, a direction $n = (\cos(\alpha), \sin(\alpha))$ and a proportion m. The 4×4 elasticity tensor of the laminate $(\theta, n, m) = (\theta, (1, 0), m)$ has non-zero coefficients of the following form, in terms of the Lamé coefficients κ and μ of A_o :

$$A_{1111} = \frac{4\kappa\mu(\kappa + \mu)\theta(1 - \theta(1 - m))(1 - m)}{4\kappa\mu\,(\kappa + \mu)^2(1 - \theta) - m(1 - m)\theta^2} \,, \quad A_{2222} = \frac{4\kappa\mu(\kappa + \mu)\theta(1 - \theta m)m}{4\kappa\mu\,(\kappa + \mu)^2(1 - \theta) - m(1 - m)\theta^2}$$

$$A_{1122} = A_{2211} = \frac{4\kappa\mu(\kappa - \mu)\theta^2 m(1 - m)}{4\kappa\mu\,(\kappa + \mu)^2(1 - \theta) - m(1 - m)\theta^2}$$

In particular, it is degenerate (since $A_{1212} = 0$), and cannot withstand shear stresses. The tensor corresponding to $\alpha \neq 0$, is deduced from the one above by a rotation of α, and thus bears the same feature. This difficulty originates in the fact that we are dealing with mixtures of A_0 and of a degenerate Hooke's law, namely void. In [1], the formulation is justified by considering mixtures of A_0 with a weaker material, and by letting the strength of the latter tend to 0. However sound mathematically, the degenerate Hooke's law has to be taken into account numerically, since it might lead to ill-posed problems in the alternate direction algorithm. Therefore, the numerical computations are performed by regularizing the Hooke's law of the laminate. A small positive parameter η is added to the diagonal terms corresponding to shear, when the matrix is expressed in the principal directions of lamination. We want to study on a simple example, the influence of this coefficient on the checkerboard patterns.
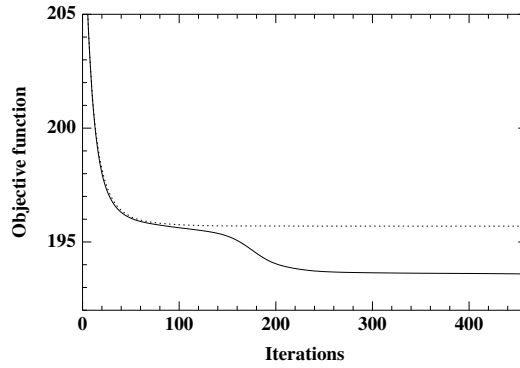

Figure 2: *A typical convergence plot. The objective function suddenly decreases after appearance of checkerboards (solid line), while the convergence is smooth if the checkerboard filtering is used (dashed line).*

2 A 2d test-case

Checkerboard instabilities usually appear in "gray" zones of intermediate densities of composite material, when the algorithm has almost converged. They typically occur in very fine meshes, when the stress field is almost constant over neighbouring elements. In order to understand what triggers their appearance, we study the smallest test-case we could find, that shows these instabilities. It consists in a patch of 4 elements (2×2) on $[-1, 1]^2$. A symmetry condition is imposed on the planes $x = 0$ and $y = 0$. An external pressure p_1 (respectively p_2) is applied on the sides $x = \pm 1$ (resp. $y = \pm 1$), cf. Figure 3. We choose the constraint on the weight (cf. [1]) so that the optimal solution is a uniform laminate with $\theta = 1/2$, $, n = (1, 0)$, $m = \frac{|p_2|}{|p_1| + |p_2|}$. We choose as initial design this configuration slightly perturbed on each element, and apply the algorithm of [1]. Checkerboards are obtained if the displacement is discretized with $Q1$ elements. When $Q2$ elements are used, the initial errors disappear after a few iterations and the algorithm converges to the uniform solution.

We propose to analyse this phenomenon by an explicit computation, and linearize the operator that is iterated during the algorithm. This operator transforms a configuration $(\theta_k, n_k, m_k), 1 \leq k \leq 4$ of design parameters, constant on each element, (and the associated Hooke's laws A^k) into an updated configuration in the following way. We consider regularized Hooke's laws $A^k(\eta)$, obtained by adding $\eta > 0$ on the shear components A^k_{1212}, A^k_{2121} of A^k, when the tensors are expressed in the coordinates defined by $(n_k, n_k^{\perp})$. The solution to the discrete elasticity problem
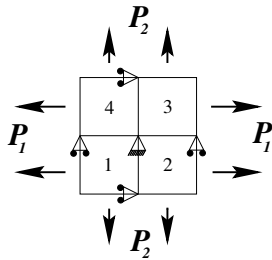
Figure 3: *the 2×2 patch.*

with Hooke's laws $A_k(\eta)$ is then computed and we obtain the associated stress fields (mean stress on each element). Then we use the optimality conditions (cf. [1]) to compute the new design parameters.

We linearize this operator about the configuration $(\theta_k, n_k, m_k) = (1/2, (1,0), \frac{|p_2|}{|p_1|+|p_2|})$, for different choices of discretizations of the displacement, namely for $Q1$ and so-called $Q1$-bubble elements. The latter are the $Q1$ 4-nodes elements with an additional node at the center, associated to the biquadratic shape function $16xy(1-x)(1-y)$ in the reference element $[0,1]^2$. For the Stokes problem, $Q1$ elements are known to produce checkerboard patterns on the pressure, whereas the $Q1$-bubble seem to produce stable results. In the first case, our test case has 12 degrees of freedom for the displacement, and 20 in the second.

To linearize the operator, we consider configurations of the form $(1/2 + \theta_k, (1, \alpha_k), \frac{|p_2|}{|p_1|+|p_2|} + m_k)$, compute exactly the displacement and make a Taylor expansion of the resulting design variables. The computations have been made using the Maple symbolic calculator. They are made easier with the following result :

Proposition 2.1 *Checkerboard errors are stable for the linearized operator, i.e., if $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4$, $\theta_1 = -\theta_2 = \theta_3 = -\theta_4$, $m_1 = -m_2 = m_3 = -m_4$, then the new error has the same symmetries.*

This property helps us to reduce the amount of computations, restricting the number of degrees of freedom to the half of the whole set, using pointwise symmetries with respect to $(0,0)$. Note that a uniform error on the direction only (*i.e.*, $(\theta_k, n_k, m_k) = (0, (0, \alpha), 0)$, $1 \le k \le 4$) produces checkerboards.

Due to this proposition, an error, which has a checkerboard symmetry is described by only 3 variables, and its damping or magnifying reduces then to the computation of the eigenvalues of a 3×3 matrix.

Proposition 2.2 *For the $Q1$ and the $Q1$-bubble elements in 2d, if $\eta > 0$ is small enough and if $|p_1|/|p_2|$ is close to 1, the error matrix has an eigenvalue greater than 1. Moreover, its largest eigenvalue tends to 1 when the regularizing parameter η tends to 0^+.*

This last proposition indicates that small values of η should minimize the appearance of instabilities. From a numerical point of vue, however, small values of η lead to ill-conditioned systems and larger roundoff errors.

The $Q1$-bubble element seems to slightly enhance the stability, as the larger eigenvalue is lower than that of the $Q1$ case. Numerical tests on the global algorithm are underway to determine if these elements lead however to stable solutions without filtering.
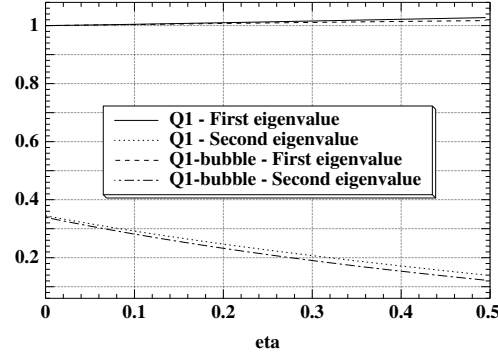
Figure 4: *Plot of the 2 first eigenvalues of the error matrix when $p_2 = 2p_1$ (the third one is 0), for Q1 and Q1-bubble element, as functions of η.*

The condition $|p_1|/|p_2|$ close to 1, for the eigenvalue to be greater than one, confirms the numerical intuition that checkerboards are initiated in zones where the resulting stresses are close to a uniform hydrostatic pressure.

In the context of damage simulation, similar relaxed formulations and algorithms are used, involving the lamination of two non-degenerate materials. In this case, no checkerboard instabilities have been reported.

In 3d, the formula for the optimal laminates are quite more complicated (see [1]). They involve two regimes of orthogonal rank-3 and orthogonal rank-2 laminates. In contrast with the rank-2, the Hooke's laws in the orthogonal rank-3 regimes are non-degenerate. Numerical tests suggest that checkerboard appearance is rare in 3d, and occur when a rank-2 laminate regime is reached. These last remarks support the claim that checkerboards are a consequence of the degeneracy of the rank-2 laminates.

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