XLI CILAMCE
XLI Ibero-Latin American Congress on Computational Methods in Engineering
16-19 November, 2020 FOZ DO IGUAÇU PARANÁ - BRAZIL

Assessment of penalty parameters in density-based topology optimization

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Abstract. The present paper discusses two penalty parameters — the penalty parameter of intermediate densities (PPID) and the penalty parameter of the density field gradient (PPDFG) — in the context of density-based topology optimization problems considering a Solid Isotropic Microstructure with Penalization (SIMP). Both parameters aim to control the influence of functional terms added to the cost functional to regularize the optimization problem. PPID aims to the reduction of intermediate densities regions and, consequently, finding out a better definition of the material contour. PPDFG, in its turn, has as its purpose to mitigate the checkerboard phenomenon. Displacements, strains, and stresses are obtained via the Finite Element Method, with relative densities defined at element nodes. The mathematical solution of the optimization problem is carried out taking into account the Augmented Lagrangean Method. The numerical experiment planning consisted of performing a series of combinations between the penalty parameters and different finite element meshes, to check their influence on the checkerboard phenomenon, mesh dependence, intermediate densities regions extension, structural topology, and values of the cost functional. In particular, the optimization problem aims to minimize the compliance of the structure with a constraint on the material volume. From the results obtained in this work, it is possible to verify that PPGDF can mitigate or inhibit the mesh dependence, avoid coarse contours, and the occurrence of the checkerboard phenomenon — conversely, for high values, extensive intermediate densities regions appear, causing a sharp increase in the structure compliance. In addition, PPGDF has a greater influence than PPID, which, for the optimization problem presented, exerted little variation in the compliance of the structure.

Keywords: Density-based topology optimization, Finite Element Method, SIMP, Augmented Lagrangian Method.

1 Introduction

In the last decades, there have been several works on the application and development of techniques for topology optimization of continuum structures aiming to assist in the design of a structure that satisfies a certain set of constraints and minimizes one or more performance functions. In general, the topology optimization process seeks to determine the optimal topology by specifying the existence of the material or its absence. Among the optimization methods frequently used there are density-based methods (Bendsøe [1]; Bendsøe and Sigmund [2, 3]), topological derivative (Amstutz and Novotny [4]; Amstutz et al. [5]), level set (Wang et al. [6]; van Djik et al. [7]) and evolutionary methods (Huang and Xie [8]).

To solve an optimization problem using density-based methods, the design variables are relative material densities, ρ, where $\rho = 0$ and $\rho = 1$ indicate, respectively, the absence and the existence of the material. In particular, due to its simplicity and robustness, the density-based method, considering a Solid Isotropic Microstructure with Penalization (SIMP) (Bendsøe [1]; Bendsøe and Sigmund [2]), has been widely used in the most diverse problems. Intrinsic to the application of density-based methods to optimization problems involving the evaluation of functions or variables via methods of approximation and discretization, numerical instabilities may arise, e.g mesh dependency, checkerboard phenomenon, and local minimums (Bendsøe and Sigmund [3]; Sigmund and Petersson [9]). Besides, another point to be considered is obtaining a topology with a well-defined material boundary — i.e. a material-void transition zone tending to zero and without jagged boundaries.

In order to overcome such adversities, different approaches have been proposed. In particular, Allaire and Kohn [10] propose the insertion of a term for energy functional so that any value of intermediate density is penalized, thus regions with a porous microstructure are reduced. Haber et al. [11] introduce the Perimeter Method in which a constraint on the perimeter of the topology is considered that leads to convergent solutions concerning mesh refinement. Petersson and Sigmund [12] add, to the classic compliance minimization problem with a constraint on the material volume, local constraints on the components of the density field gradient. Such constraints are controlled by a weighting parameter, allowing to change the complexity of the final topology —

and reduces or mitigates the appearance of a checkerboard and provides a mesh-independent solution. Sigmund [13] proposes a filter, to generate mesh independence, that modifies the sensitivity of an element considering its sensitivities in a small fixed neighborhood by a weighted average operation. Pereira [14], Fancello and Pereira [15] and Pereira et al. [16] propose a modification of the optimization problem by adding two functionals, each of them with its penalty parameter — the penalty parameter of intermediate densities (PPID) and the penalty parameter of the density field gradient (PPDFG) — with the main focus on a mass minimization problem with local stress constraints solved numerically via Augmented Lagrangian Method. In this case, the term for penalizing density gradients is intended to avoid or mitigate the checkerboard phenomenon. Such an approach is also used in the work of Silva et al. [17] in the solution of a compliance minimization problem with a constraint on the volume with an analysis aimed mainly at controlling discretization errors via h-adaptivity. Additionally, the works of Sigmund and Petersson [9], Diaz and Sigmund [18], Borrvall and Petersson [19], Borrvall [20], Hägg and Wadbro [21], among others, can be cited.

In this context, the current work aims to systematically analyze the influence of PPID and PPDFG in the characterization of a structural optimization problem to minimize compliance with a volume constraint, considering the SIMP model. Numerical experiments are planned in such a manner to possibly assess energy functional, mesh dependency, checkerboard phenomenon, the extension of the material transition zones, and the complexity of the optimal topology.

2 Formulation of the density-based topology optimization problem

The topological optimization problem addressed in this work is the minimization of the compliance of a continuum structure with an equality constraint on the material volume considering a density-based method with a SIMP microstructure (Bendsøe [1]; Bendsøe and Sigmund [2]). The SIMP model allows a continuous relative densities field variation, ρ, between 0 (void) and 1 (solid material). For this formulation, the energy functional or cost functional, $c(\rho)$, is given by

$$c(\rho) = \int_{\Omega} \frac{1}{2} \left(\nabla^s \boldsymbol{u}\right)^T \boldsymbol{D}_\rho(\rho) \left(\nabla^s \boldsymbol{u}\right) d\Omega \text{ , with } \boldsymbol{D}_\rho(\rho) = \rho^q \boldsymbol{D}_0 , \tag{1}$$

where $\boldsymbol{u}$ is the vector field of displacements and Ω is the domain of the problem. In particular, the material constitutive tensor, $\boldsymbol{D}_\rho$, acts as a penalty for intermediate densities. Still in eq. (1), $\boldsymbol{D}_0$ is the constitutive stiffness tensor of the solid material (here considered isotropic and elastic) and q is the exponent, whose literature suggests — based on topological sensitivity assessments — the cubic dependence for plane linear elasticity problems (Amstutz [22]). The equality constraint for the volume of the structure, h_V, is shown in eq. (2) and imposes that the volume functional, V, is equal to a fraction, λ, of the initial volume, V_0,

$$h_V(\rho) = V(\rho) - \lambda V_0 = 0 . \tag{2}$$

At this point, it is worth mentioning that the current work seeks to evaluate the numerical solution of the optimization problem with a similar approach as presented in Silva et al. [17], as well as in the works of Pereira [14], Fancello and Pereira [15] and Pereira et al. [16] in the context of mass minimization problems with local stress constraints. Initially, two functionals, F_m and F_ρ, dependent on the relative density field, are added into the cost functional to regularize the problem. Subsequently, considering the Augmented Lagrangean Method (Bertsekas [23]), the volume constraint, h_V, is incorporated into the cost functional, eq. (1) , by the insertion of a quadratic external penalty, r_K, and a Lagrange multiplier, η_K. In this way, the K^{th} minimization sub-problem is presented in eq. (3) with only a lateral constraint on the design variables (i.e. the relative densities):

$$\begin{aligned} &\min_{\rho \in L^\infty(\Omega)} \left[\overline{L}_K(\rho, r_K, \eta_K) = c(\rho) + r_m F_m(\rho) + r_\rho F_\rho(\rho) + \eta_K h_V(\rho) + r_K h_V(\rho)^2 \right] \\ &\textit{Subject to :} \ \{0 < \rho_{min} \le \rho(\boldsymbol{x}) \le 1, \quad \forall \boldsymbol{x} \in \Omega. \end{aligned} \tag{3}$$

For the proposed problem, the F_ρ functional aims to inhibit the appearance of numerical instabilities such as the checkerboard (Pereira [14]; Fancello and Pereira [15]; Pereira et al. [16]; Borrvall [20]); and the F_m functional, in its turn, seeks to mitigate the occurrence of extensive intermediate densities regions (Allaire and Kohn [10]; Allaire and Frankfurt [24]; Pereira [14]; Fancello and Pereira [15]; Pereira et al. [16]). These functionals are expressed mathematically as:

$$F_m(\rho) = \int_{\Omega} \rho(1-\rho)\, d\Omega \quad \text{and} \quad F_\rho(\rho) = \int_{\Omega} (\nabla\rho)^T (\nabla\rho)\, d\Omega . \tag{4}$$

Furthermore, r_m and r_ρ are called, respectively, as the penalty parameter of intermediate densities (PPID) and the penalty parameter of the density field gradient (PPDFG); and a minimum value for density $\rho_{min} = 0.01$ was adopted to avoid numerical singularities (Pereira et al. [16]; Fin et al. [25]). According to Bertsekas [23], eq. (3) represents the K^{th} optimization problem from a sequence of finite problems that must be solved. After the convergence of each subproblem, the r_K and η_K parameters are updated taking into account the standard updating rule given by (Bertsekas [23]; Silva et al. [17])

$$\eta_{K+1} = \eta_K + 2 r_K h_V(\rho), \tag{5}$$

$$r_{K+1} = min\{z r_K ; r_K^{max}\}, \text{ with } z > 1 \ e \ r_K > 0, \forall K \in \mathbb{N}, \tag{6}$$

where z is a constant scalar that defines the increase rate of r_K, $r_K^{máx}$ is a higher limit for r_K, and $\mathbb{N}$ is the set of natural numbers. To solve each problem, the Conjugated Gradient Method was used for search direction determination; and the Golden Section Method for calculating the step size along this direction. Both methods can be found in Arora [26]. Besides, the Adjoint Method is used to obtain the sensitivity analysis of the Augmented Lagrangean functional.

3 FEM model and numerical planning

The mechanical model evaluated in this paper is shown in Fig. 1 and consists of a simply supported beam with a central load *P*. Except for the definition of material and geometric parameters, this model has been studied in numerous works in the scope of minimizing compliance with a volume constraint (Costa Jr. and Alves [27]; Tovar and Khandelwal [28]). Both essential and natural boundary conditions are applied along a length, *L*, of the edge to avoid stress concentration. A two-dimensional linear elasticity problem was created considering a plane stress state with mechanical properties, geometry, and optimization parameters summarized in Tab. 1. To reduce the computational cost, the model was implemented considering the symmetry about the vertical axis. The domain discretization was carried out with a criss-cross pattern, with Constant Strain Triangle elements, to obtain two distinct meshes (one coarse and one fine) to assess the mesh dependence on the studied optimization problem. For both meshes, factorial planning of the penalties parameters r_m and r_ρ was carried out over a wide range to enable an assessment of their influence on the optimal structure obtained. This procedure was performed in Matlab®. The initial density field was defined as a homogeneous field that satisfies the equality constraint on the material volume. Besides, the quadratic external penalty for the first subproblem, r_{ini}, was set as four times the energy functional for the initial density field; and its maximum value defined as $r_K^{max} = 100 r_{ini}$. The Lagrange multiplier for the first subproblem is equal to zero. Adding up, it was considered that the K^{th} problem converged when the following criteria are met: (i) $\|\boldsymbol{\rho}_{K+1} - \boldsymbol{\rho}_K\| < 10^{-3}\sqrt{ndv}$, (ii) $\left|\bar{L}_{K+1} - \bar{L}_K\right| < 10^{-4}\bar{L}_{ini}$, and (iii) $r_K = r_K^{max}$. In this case, *ndv* indicates the number of design variables under analysis.

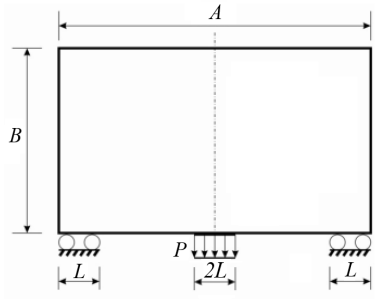

Figure 1. Mechanical model scheme.

Table 1. Numerical planning.

	Category	Parameter	Value
FEM model	Mechanical properties	Young's Modulus [Pa]	1
		Poisson's Ratio [-]	0.3
	Geometry	*A* [m]	20
		B [m]	12
		Thickness [m]	1
		L [m]	1
	Neumann boundary	*P* [N]	1
	Domain discretization	Coarse mesh	Criss-cross [20;24] (1920 elements)
		Fine mesh	Criss-cross [40;48] (7680 elements)
Optimization parameters		r_m [N.m]	0 0.25 0.50
		r_ρ [N.m]	0 0.005 0.05 0.5
		λ	0.3
		z	1.5

4 Numerical results and discussion

The optimal topologies for the different sets of penalty parameters, according to the numerical planning described in Tab. 1, are presented for the coarse and fine meshes, respectively, in Fig. 2 and Fig. 3. For both meshes, considering fixed r_m values, one should note its influence on the optimal topologies found. Corroborating results exposed by Pereira [14] and Pereira et al. [16], as r_ρ increases, there is a reduction in the number of ramifications of the optimal structure (i.e., their complexity decreases). Such behavior is justified since this parameter is associated with the penalty of the density field gradient. To put it another way, its increase tends to lead to topologies with a reduced variation of this field, evidenced here by the reduction of the complexity of the structure. On the other hand, if r_ρ is excessively high, there is a tendency to eliminate both holes in the domain and high regions with intermediate densities, which should be avoided. Furthermore, the higher r_ρ value, the greater the tendency to obtain topologies with smoother boundaries, avoiding jagged boundaries and facilitating the posterior design aiming the structure manufacture.

Regarding the checkerboard phenomenon occurrence — being this the main reason for the insertion of the penalty of density gradients term to the cost functional (Pereira et al. [16]) — this numerical instability did not markedly feature for both meshes evaluated. Nevertheless, the optimal topology in Fig. 3, considering both penalty parameters null, exhibited this phenomenon in some regions of its domain.

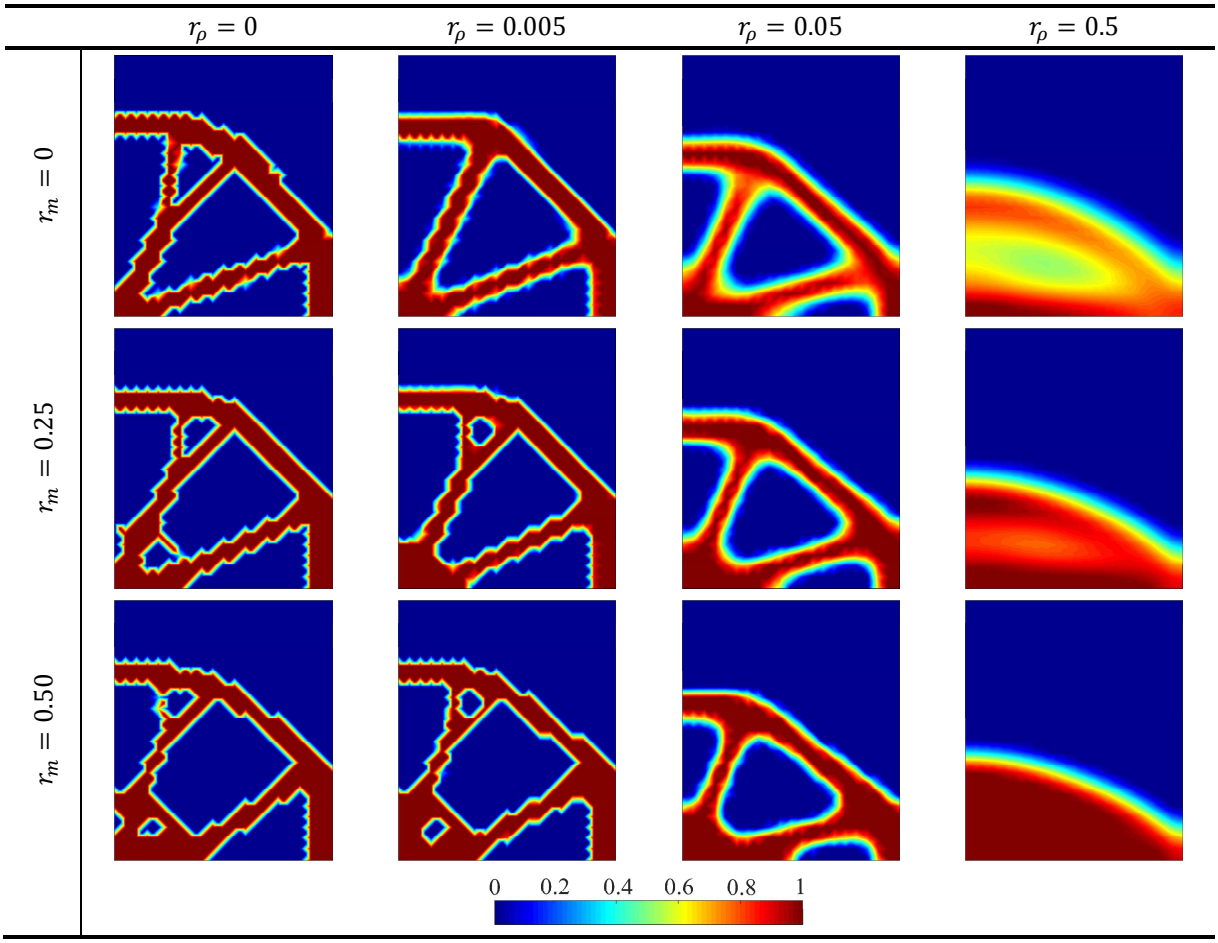

Figure 2. Optimal topologies, for the coarse mesh, as a function of r_m and r_ρ parameters.

Another relevant aspect in optimization problems solved via density-based methods is the mesh dependence (Bendsøe and Sigmund [3]; Sigmund and Petersson [9]). A comparison between Fig. 2 and Fig. 3 shows that the increase of r_ρ tends to generate optimal solutions with no mesh dependence. That is, similar topologies are found for meshes with distinct refinements. Indeed, numerical experiments suggest that $r_\rho = 0.05$ is the most adequate. Such behavior is also pointed out in the numerical experiments conducted by Silva et al. [17] in the scope of minimum compliance with a volume constraint using the same approach analyzed here.

Likewise, an analysis of the effect of r_m variation, for fixed r_ρ values, can be performed. In general, considering low r_ρ values (between 0 and 0.005), Fig. 2 and Fig. 3 show that an r_m increase leads to a tendency of enhancement of the structure complexity. Conversely, for higher values of r_ρ (between 0.05 and 0.5), no significant changes in the connectivity of the structure are identified and the reduction of intermediate densities is remarkable.

Therefore, given the mechanical model evaluated and the numerical experiments carried out here, a joint analysis of Fig. 2 and Fig. 3 points out that the appropriate values are $r_m = 0.5$ and $r_\rho = 0.05$. Not to mention that the fine mesh topology should be preferred due to its fewer discretization errors. Moreover, Silva et al. [17] emphasize this aspect, evaluating the same problem addressed here, and propose an h-adaptivity technique to control discretization errors, which guarantee solutions with global errors, evaluated according to the energy norm, below a prescribed allowable error value.

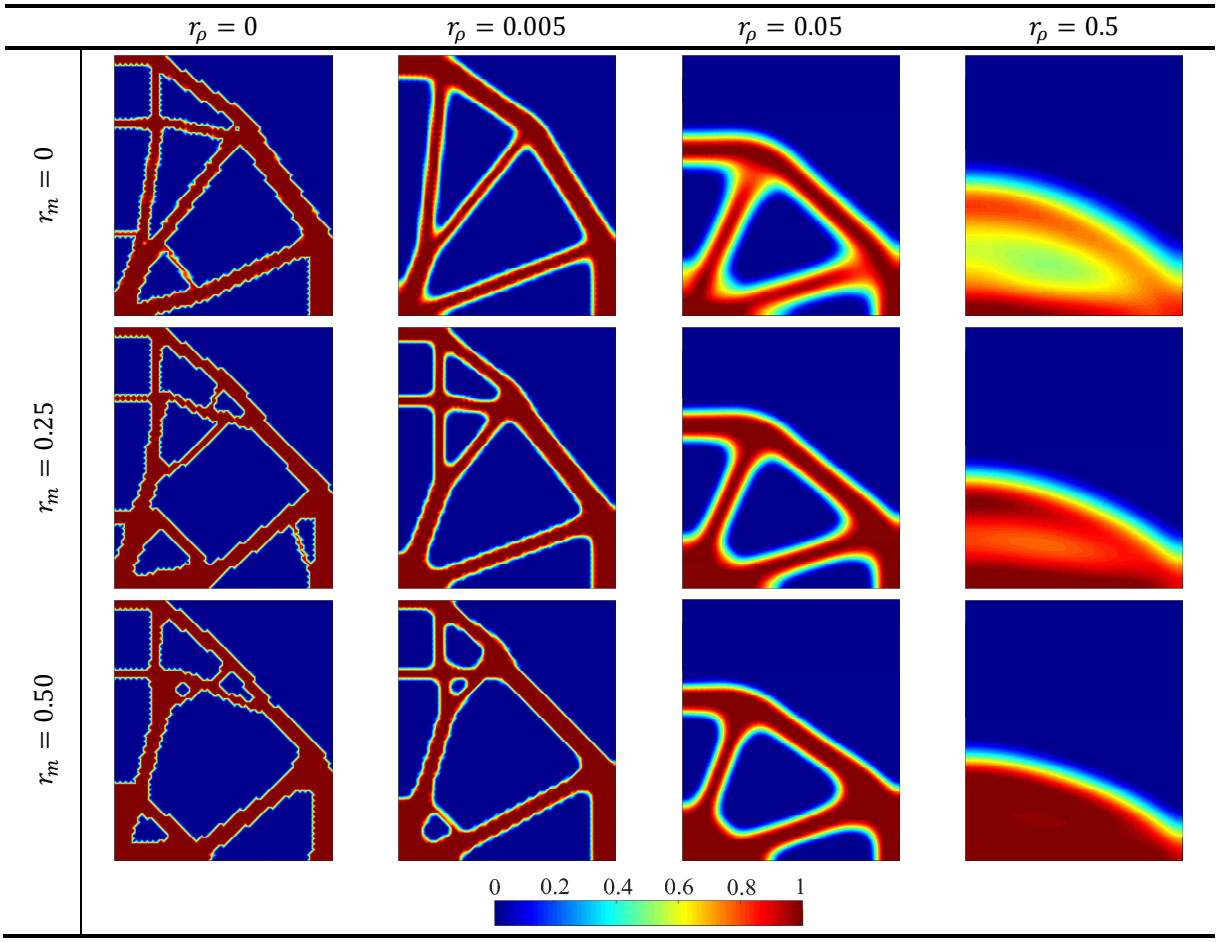

Figure 3. Optimal topologies, for the fine mesh, as a function of r_m and r_ρ parameters.

Additionally, similar behavior is observed in Fig. 4 between the coarse and fine meshes regarding the quantitative evaluation of the energy functionals, intermediate densities penalty, and densities gradient penalty. The increase in r_ρ generates a reduction in F_ρ functional; as already discussed and verified qualitatively by Fig. 2 and Fig. 3. Such reduction is provided by the smoothing of the density field, represented by regions with intermediate densities with a consequent increase in F_m. Thus, accompanied by topological solutions with an increase in intermediate densities (i.e. more porous material regions), there is an increase in the energy functional. On the other hand, r_m has little influence on the structure's energy, mainly for higher r_ρ values.

Besides, as observed in Figs. 2 and Fig. 3 — and already pointed out by several studies (Maute and Ramm [29]; Costa Jr. and Alves [27]; Silva et al. [17]) in structural optimization problems solved via density-based methods and with design variables linked to finite element discretization — finer meshes generate topologies with a better definition of the material-void interface. In this context, concerning the methodology applied, F_m and F_ρ might be interpreted as a quantitative measure of the material boundary resolution, where higher F_ρ and lower F_m

for a solution with no mesh dependence indicate a better-defined topology (Silva et al. [17]). For instance, considering the topology with $r_m = 0.5$ and $r_\rho = 0.05$, the coarse mesh has $F_m = 5.8$ and $F_\rho = 52.7$ while the fine mesh has $F_m = 5.2$ and $F_\rho = 58.3$.

In the light of the above, the modification in the optimization problem presented suggests that both penalty parameters evaluated must be carefully defined, since higher or lower values of them might cause or even accentuate mesh dependence, widen material-void transition, non-smooth boundaries, and checkerboard occurrence.

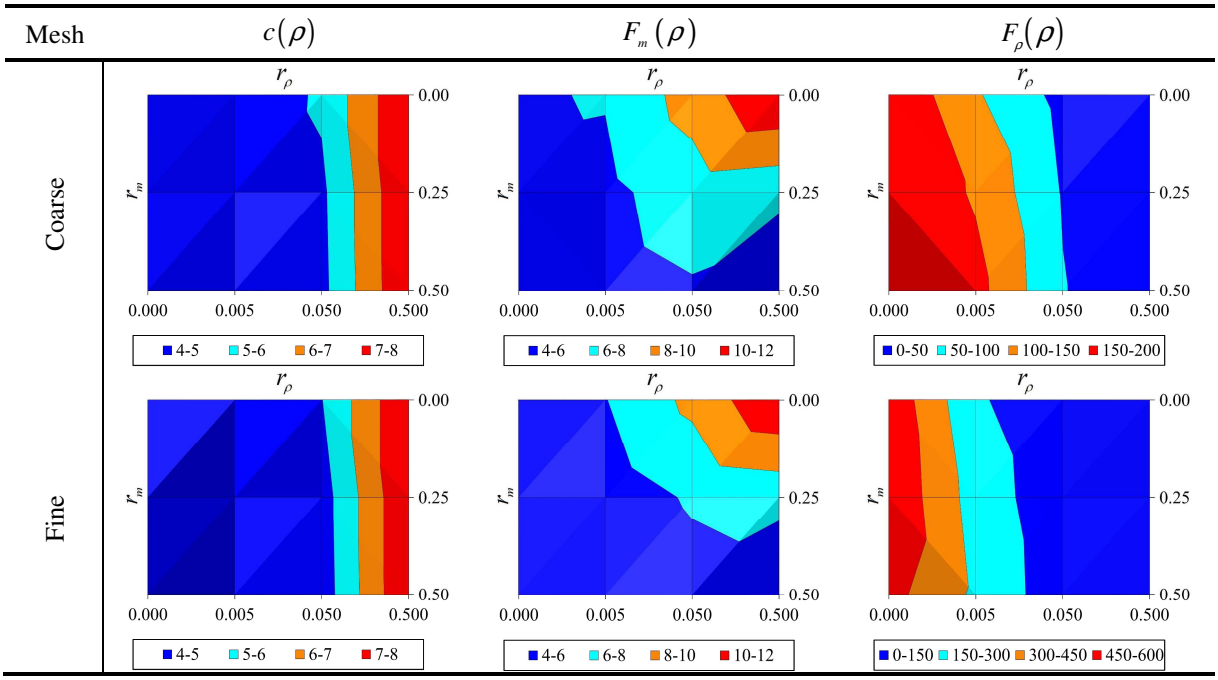

Figure 4. Maps of functional values as a function of r_m and r_ρ parameters.

5 Conclusions

From the present work — which applies a density-based topology optimization to minimize compliance with a constraint on the material volume and whose objective is to discuss the influence of two penalty parameters, r_m and r_ρ, in the optimal structures obtained — it can be concluded that:

(i) The penalty parameter r_ρ has a more pronounced influence than r_m on the problem's energy functional, which increases proportionally with r_ρ. Low r_m values might generate regions of intermediate densities in the topology and this occurrence must be minimized or avoided. In contrast, lower r_ρ values enhance the appearance of complex final topology, mesh dependence, more coarse boundaries, and checkerboard. However, when r_ρ is higher, large regions of material-void transition can appear in the topology, causing increased compliance.

(ii) To have an optimum structure that can be manufactured, both parameters studied must be carefully defined to avoid the instabilities and problems described. Adding up, although the parameter r_ρ provides a trend of mesh independence; finer meshes generate topologies with a better definition of the structure boundaries and with smaller discretization errors.

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References

[1] M. P. Bendsøe, "Optimal shape design as a material distribution problem". *Structural Optimization*, vol. 1, n. 4, pp. 193–202, 1989.
[2] M. P. Bendsøe and O. Sigmund, "Material interpolation schemes in topology optimization". *Archive of Applied Mechanics (Ingenieur Archiv)*, vol. 69, n. 9–10, pp. 635–654, 1999.
[3] M. P. Bendsøe and O. Sigmund, *Topology Optimization: Theory, Method and Application*. Springer, 2003.
[4] S. Amstutz and A. A. Novotny, "Topological optimization of structures subject to von Mises stress constraints". *Structural and Multidisciplinary Optimization*, vol. 41, n. 3, pp. 407–420, 2010.
[5] S. Amstutz, A. A. Novotny and E. A. Souza Neto, "Topological derivative-based topology optimization of structures subject to Drucker-Prager stress constraints". *Computer Methods in Applied Mechanics and Engineering*, vol. 233–236, pp. 123–136, 2012.
[6] M. Y. Wang, X. Wang and D. Guo, "A level set method for structural topology optimization". *Computer Methods in Applied Mechanics and Engineering*, vol. 192, n. 1–2, pp. 227–246, 2003.
[7] N. P. van Dijk, K. Maute, M. Langelaar and F. van Keulen, "Level-set methods for structural topology optimization: a review". *Structural and Multidisciplinary Optimization*, vol. 48, n. 3, pp. 437–472, 2013.
[8] X. Huang and Y. M. Xie, *Evolutionary Topology Optimization of Continuum Structures: Methods and Applications*. John Wiley and Sons, 2010.
[9] O. Sigmund and J. Petersson, "Numerical instabilities in topology optimization: A survey on procedures dealing with checkerboards, mesh-dependencies and local minima". *Structural Optimization*, vol. 16, pp. 68–75, 1998.
[10] G. Allaire and R. V. Kohn, "Topology optimization and optimal shape design using homogenization". In: M. P. Bendsøe and C. A. Soares Mota (ed.), *Topology Design of Structures.* Kluwer, Boston, pp. 207–218, 1993.
[11] R. B. Haber, C. S. Jog and M. P. Bendsøe, "A new approach to variable-topology shape design using a constraint on perimeter". *Structural Optimization*, vol. 11, n. 1–2, pp. 1–12, 1996.
[12] J. Petersson and O. Sigmund, "Slope constrained topology optimization". *International Journal for Numerical Methods in Engineering*, vol. 41, n. 8, pp. 1417–1434, 1998.
[13] O. Sigmund, "On the design of compliant mechanisms using topology optimization". *Mechanics of Structures and Machines*, vol. 25, n. 4, pp. 493–524, 1997.
[14] J. T. Pereira, Otimização Topológica de Componentes Mecânicos com Restrições sobre o Critério de Falha Material. PhD thesis, Federal University of Santa Catarina, 2001.
[15] E. A. Fancello and J. T. Pereira, "Structural topology optimization considering material failure constraints and multiple load conditions". *Latin American Journal of Solids and Structures*, vol. 1, n. 1, pp. 3–24, 2003.
[16] J. T. Pereira, E. A. Fancello and C. S. Barcellos, "Topology optimization of continuum structures with material failure constraints". *Structural and Multidisciplinary Optimization*, vol. 26, n. 1–2, pp. 50–66, 2004.
[17] J. Silva, J. T. Pereira and D. A. F. Torres, "h-adaptive topology optimization considering variations of material properties and energy error density recovery". *Engineering Computations*, vol. ahead-of-print, n. ahead-of-print, pp. ahead-of-print, 2020.
[18] A. R. Diaz, O. Sigmund, "Checkerboard patterns in layout optimization". *Structural Optimization*, vol. 10, n. 1, pp. 40–45, 1995.
[19] T. Borrvall, J. Petersson, "Topology optimization using regularized intermediate density control". *Computer Methods in Applied Mechanics and Engineering*, vol. 190, pp. 4911–4928, 2001.
[20] T. Borrvall, "Topology optimization of elastic continua using restriction". *Archives of Computational Methods in Engineering*, vol. 8, n. 4, pp. 351–385, 2001.
[21] L. Hägg and E. Wadbro, "Nonlinear filters in topology optimization: existence of solutions and efficient implementation for minimum compliance problems". *Structural and Multidisciplinary Optimization*, vol. 55, pp. 1017–1028, 2017.
[22] S. Amstutz, "Connections between topological sensitivity analysis and material interpolation schemes in topology optimization". *Structural and Multidisciplinary Optimization*, vol. 43, n. 6, pp. 755–765, 2011.
[23] D. P. Bertsekas, *Constrained Optimization and Lagrange Multiplier Methods*. Athena Scientific, 1996.
[24] G. Allaire and G. A. Francfort, "A numerical algorithm for topology and shape optimization". In: M. P. Bendsøe and C. A. Soares Mota (ed.), *Topology Design of Structures.* Kluwer, Boston, pp. 239–248, 1993.
[25] J. Fin, L. A. Borges and E. A. Fancello, "Structural topology optimization under limit analysis". *Structural and Multidisciplinary Optimization*, vol. 59, n. 5, pp. 1355–1370, 2019.
[26] J. S. Arora, *Introduction to Optimum Design*. Elsevier Academic Press, 2017.
[27] J. C. A. Costa Jr. and M. K. Alves, "Layout optimization with h-adaptivity of structures". *International Journal for Numerical Methods in Engineering*, vol. 58, n. 1, pp. 83–102, 2003.
[28] A. Tovar and K. Khandelwal, "Topology optimization for minimum compliance using control strategy". *Engineering Structures*, vol. 48, pp. 674–682, 2013.
[29] K. Maute and E. Ramm, "Adaptive topology optimization". *Structural Optimization*, vol. 10, pp. 100–112, 1995.