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Treatment of numerical instabilities in topology optmization using the LSM/IGABEM coupling

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Abstract. The volume reduction characteristic of topology optimization techniques is attractive to both academia and industry. This interest stems from financial reasons and environmental aspects. This study addresses a topology optimization formulation for structural elements based on the coupling between the Level Set Method (LSM) and the Isogeometric Boundary Element Method (IGABEM). The former method describes the boundary evolution whereas the latter determines the mechanical fields. As in IGABEM, isogeometric descriptions have been used in LSM, which provide accuracy, robustness, solution generality, and direct communication between both methods. The coupling between the methods has been written by defining the normal velocity to the reference level set curve through the shape sensitivity of the augmented Lagrangian function. A heuristic topology modification addresses the deficiency of LSM in generating holes. This study clarifies the possibility of encountering numerical instability problems when using the studied coupling formulation or similar ones involving penalty methods. An effective treatment is proposed, also reducing the dependence on the parameters of the heuristic criterion for the process success. The results verify its robustness by comparing them with those from other coupling formulations between LSM and BEM where results from the Solid Isotropic Material with Penalization (SIMP) are the reference.

Keywords: LSM, IGABEM, topology optimization, penalty coefficient.

1 Introduction

The scarcity of natural resources, the need for commitment to controlling pollutant emissions, the interest in reducing production costs, and the constant pursuit of profit maximization are environmental and market factors that have driven interest in structural optimization studies. Among the various formulations proposed in the field, delivering a structure with optimal volume is a common goal under different circumstances. Because this characteristic addresses or mitigates the aforementioned issues, the field has received considerable attention from both academia and industry in recent decades. Topology optimization, the focus of the present study, is a branch of structural optimization. It allows for complete alteration of the structure's topology [1]. As such, it is regarded as the most complete and versatile variant.

Among the various approaches for implementing the topology optimization process, this study focuses on the Level Set Method (LSM). Originally, the method was developed to describe interface motion using the Hamilton-Jacobi differential equation [2, 3]. Its formulation defines the boundary as a level curve of a potential function known as the level set function. Sethian and Wiegmann [4] originally applied the LSM for topology optimization problems. Their method employs the finite difference procedure developed by Wiegmann and Bube [5] to solve the linear elasticity subproblems. Also, the stress field on the current configuration leads to the velocity field required to evolve the boundary along time.

The dissemination of LSM in the field of topology optimization was driven by its coupling with the Finite Element Method (FEM), which replaced the previously mentioned solver for accessing the mechanical quantities of the domain [6]. The coupling with FEM attracted the attention of engineering researchers due to its widespread use in the field. As a result, LSM was also coupled with other numerical methods, such as the Boundary Element Method (BEM).

The first formulation of topology optimization coupling the BEM and the LSM was applied to the classical

problem of compliance minimization under a volume equality constraint [7]. The methods demonstrated excellent compatibility, as BEM inherently relies on boundary discretization. Leveraging this feature, a formulation was later proposed in which BEM was embedded into the Eulerian mesh of the level set, aligning the nodes of the mechanical model with those of the level curve [8].

A limitation of LSM arises from the fact that its topological modifications occur only through the merging of holes within the domain. The method, by its nature, is unable to generate new holes. To overcome these shortcomings, earlier studies, such as those previously cited, initiated the optimization process with a domain already containing multiple pre-defined holes. Although this strategy partially addresses the issue, it may introduce a dependency of the final result on the initial configuration of the domain. To explore alternative approaches, a process for topology modification by hole insertion was developed based on the topological derivative of the objective function at internal points [9]. In a coupling formulation with BEM, there is a correlation between the results obtained using topological derivative-based hole insertion and another one using von Mises stress evaluation at internal points [10]. Additional results for other examples employing hole insertion driven by von Mises stress can be found in the literature, further demonstrating its robustness [11, 12].

Another innovation introduced in the last three cited works is the use of Non-Uniform Rational B-Splines (NURBS) for discretizing the level curve of the level set function. Over this isogeometric mesh, boundary elements with Lagrangian polynomial interpolation bases discretize the mechanical problem domain. This methodology was also adopted in the implementation of shape sensitivity within the optimization algorithm [13]. In this approach, a strategy based on Lagrange multipliers was employed, with the adjoint solution obtained using the bisection method [14]. Furthermore, the optimization process within this coupling framework was investigated using the augmented Lagrangian method combined with the von Mises stress criterion for hole insertion [15, 16].

Building on the pioneering isogeometric formulations in numerical methods led by Hughes, Cottrell, and Bazilevs [17] in FEM, the technology has been progressively adapted to BEM (IGABEM) in parallel with the development of recent optimization studies [18, 19]. Exploiting computational aspects of IGABEM, this approach improves significantly the accuracy for elastoastatic problem in comparison to conventional Lagrangian interpolation. [20]. These advantages, combined with the avoidance of the cost associated with remeshing using Lagrangian interpolation elements, led to the implementation of IGABEM in the most recent optimization framework employing the augmented Lagrangian method [21]. However, some convergence issues have been identified in applications and developments based on this latest formulation [22].

The present study discusses aspects of the latest formulation, such as the influence of the initial choice and the progression of the penalty parameter throughout the analysis. The convergence verification process of the approach is examined, and a methodology for this purpose is proposed. In particular, numerical instability issues inherent to the process are clarified, and successful strategies for their mitigation are addressed. The avoidance of these instabilities leads to robust results, consistent with expectations reported in the literature. Furthermore, this improvement reduces the dependence of optimization success on the selection of heuristic topology modification parameters.

2 Formulations

This section addresses the formulations used in the developed topology optimization process through the coupling between LSM and IGABEM. The methodologies for evaluating the evolution of the level set function over time and the adopted IGABEM formulation are presented herein. Subsequently, the construction of the optimization process based on the augmented Lagrangian method is described, detailing the coupling between the methods.

2.1 Level Set Method

The LSM consists of defining a domain Ω, of arbitrary dimension and representing the analysis body, through its boundary Γ, one dimension smaller. That description is on a design domain D, having the same dimension as Ω. The mapping is performed by a potential function ϕ called the level set function, such that

$$\begin{cases} \mathbf{x} \in \Omega \mid \phi(\mathbf{x}) > c \\ \mathbf{x} \in \Gamma \mid \phi(\mathbf{x}) = c \\ \mathbf{x} \in D \backslash \Omega \mid \phi(\mathbf{x}) < c \end{cases}, \tag{1}$$

where c is an arbitrary constant, typically assigned a zero value. The Hamilton-Jacobi differential equation describes the evolution of ϕ over time t. This mathematical model preserves the characteristics of an Initial Value Problem (IVP) that lacks an analytical solution. Therefore, discrete solution methods in time and space are required. In the context of topology optimization, first-order approximation methods obtains robust results. So, the present formulation adopts the discrete approach presented by Sethian [23]. Thus, considering a two-dimensional analysis, the discrete evolution equation is represented by

$$\phi_{ij}^{n+1} = \phi_{ij}^{n} - \Delta t \left[\max\left(\overline{v}_{ij}, 0\right) \nabla^{+} + \min\left(\overline{v}_{ij}, 0\right) \nabla^{-} \right], \tag{2}$$

where the index n indicates a point along the time axis, and the indices i and j correspond to the horizontal and vertical positions, respectively, of each point in the grid required for spatial discretization. Sethian [23] provides the formulae for calculating the ∇ terms.

For the numerical stability of the IVP discrete solution process, the prescribed time step must satisfy the Courant-Friedrichs-Lewy (CFL) condition [24]. In the initialization and reinitialization processes of the level set function, it was assumed that the value at a given point corresponds to its shortest distance to the boundary. Finally, for topology modification, this study adopts a von Mises stress criterion similar to that used in previously cited works [10, 11, 15, 16, 21]. Holes are created if $\sigma_{ij}^{v}\left(t^{n}\right) < \rho \max\left[\sigma_{ij}^{v}\left(t^{0}\right)\right]$, where ρ is a prescribed removal rate.

2.2 Isogeometric Boundary Element Method

Similar to the classical BEM formulation, which uses elements with basis functions described by Lagrangian polynomials, IGABEM also starts from the discretization of the Somigliana Identity, or boundary integral equation. This study uses a IGABEM formulation on that NURBS curves lead to geometric and functional boundary representation. Thus, for any source point on the boundary, the integral equation may be represented in its discrete form as

$$\frac{1}{2} c_{kj}\left(\hat{\xi}\right) u_j = \sum_{p=1}^{np} \left[\int_{-1}^{1} p_j \, c_{ij}\left(\xi\right) \, u_{ki}^{*}\left(\xi\right) \, \tilde{J}\left(\overline{\xi}\right) \, \hat{J}\left(\xi\right) \, d\xi \right] - \sum_{p=1}^{np} \left[\int_{-1}^{1} u_j \, c_{lj}\left(\xi\right) \, p_{kl}^{*}\left(\xi\right) \, \tilde{J}\left(\overline{\xi}\right) \, \hat{J}\left(\xi\right) \, d\xi \right]. \tag{3}$$

In the above equation, the indexes i and k indicate the directions of analysis, while the index j represents each component of displacement u or traction p at the control points of a NURBS curve. The terms $\mathbf{u}^{*}$ and $\mathbf{p}^{*}$ derive from the Kelvin fundamental solution [25–27]. The sum is taken over the number of patches, which are isogeometric discretization blocks. In two-dimensional analysis, a patch corresponds to a single NURBS curve. The tensor $\mathbf{c}$ on the right-hand side of the equation contains the scattering of the basis functions for each integrated NURBS curve. On the left-hand side, the scattering corresponds to the basis functions of the NURBS curve to which the source point belongs. The symbol ξ denotes the integration space, where the Gaussian space has been adopted for the application of Gauss-Legendre quadrature. When this symbol is overlined, it represents the support space of the NURBS basis functions, referred to as the parametric space. The symbol J represents the Jacobian of the space transformation. A hat accent indicates the mapping from the integration space to the parametric space, while a tilde denotes the mapping from the parametric to the physical space. It is worth noting that the integrals in eq. (3) may be weakly singular if the integrated patch contains the source point. To address these integrals, the current implementation adapts the singularity subtraction process to IGABEM [28, 29].

For each source positioned on the boundary, there is a discretized integral equation following the form of eq. (3). This leads to a linear system of equations relating displacements and tractions at control points. Thus, the configurations of a Boundary Value Problem (BVP) are established. One can solve the system after applying the essential and natural boundary conditions through column exchanges.

The adopted heuristic topology modification criterion requires the evaluation of the Cauchy stress at points within the domain. In BEM formulations, it is possible to modify the boundary integral equation by applying the displacement-to-stress transformation process. In IGABEM, the discretization of this modified equation can be written as

$$\sigma_{km} = \sum_{e=1}^{np} \left[\int_{-1}^{1} p_j \, c_{ij}\left(\xi\right) \, d_{kim}^{*}\left(\xi\right) \, \tilde{J}\left(\overline{\xi}\right) \, \hat{J}\left(\xi\right) \, d\xi \right] - \sum_{e=1}^{np} \left[\int_{-1}^{1} u_j \, c_{lj}\left(\xi\right) \, s_{klm}^{*}\left(\xi\right) \, \tilde{J}\left(\overline{\xi}\right) \, \hat{J}\left(\xi\right) \, d\xi \right], \tag{4}$$

where the tensors $\mathbf{d}^*$ and $\mathbf{s}^*$ result from the transformation applied to $\mathbf{u}^*$ and $\mathbf{p}^*$. The BEM literature provides their expressions [25–27]. It is important to note that these kernels tend to be hypersingular, requiring a considerable number of integration points for sufficiently accurate evaluation of the integrals, especially near the boundary. To mitigate this issue, the implementation utilizes the cubic transformation of quadrature. It increases the process accuracy while keeping the same number of integration points [30, 31]. If the internal point lies within the grid cell containing the boundary, is Cauchy stress tensor is approximated by that of the closest boundary point. An adaptation to the 2D IGABEM of an indirect process that requires no integrals evaluates this tensor at boundary points [32].

2.3 Optimization

The optimization problem of this study consists of $min\left[C\left(\Omega\right)\right]$ subject to $V\left(\Omega\right) - \overline{V} = 0$. It is a nonlinear constrained problem. The symbol C denotes the compliance function of the domain, V represents the volume function, and $\overline{V}$ is a prescribed volume. The augmented Lagrangian method can rewrites this problem on a function

$$\mathcal{A}\left(\Omega, \lambda^k, \gamma^k\right) = C\left(\Omega\right) + \lambda^k \left(V\left(\Omega\right) - \overline{V}\right) + \frac{\gamma^k}{2}\left(V\left(\Omega\right) - \overline{V}\right)^2, \tag{5}$$

where λ is the Lagrange multiplier, γ is a penalty coefficient, and k denotes the iteration index of the algorithm. The multiplier is pseudo-analytically updated as $\lambda^{k+1} = \lambda^k + \gamma^k \left(V\left(\Omega\right) - \overline{V}\right)$, while γ is incremented at each step by $\gamma^{k+1} = \delta\,\gamma^k$. Larger values of δ tend to accelerate the process; however, they also increase the likelihood of ill-conditioning [33, 34]. Previous studies have shown that, for the coupling employed, δ values closer to unity tend to yield better results. This factor, combined with the numerical stability condition of the LSM, results in a slower evolution of the process. Thus, the convergence state in the current approach is identified when the compliance exhibits little oscillation over some tens of iterations.

The coupling strategy defines the normal velocity of the boundary as

$$\overline{v}\left(\Gamma\right) = -\frac{\partial \mathcal{A}}{\partial \Omega} = -\left[\mathcal{E}\left(\Omega\right) + \lambda^k + \gamma^k\left(V\left(\Omega\right) - \overline{V}\right)\right]. \tag{6}$$

Consequently, the evolution of the level set function proceeds in the direction of minimizing the augmented Lagrangian according to the shape. The function $\mathcal{E}$ denotes the internal work density. It is evaluated using IGABEM. The formulation of eq. (6) also enables a numerical compatibility procedure for defining the initial value of γ based on the geometry, stiffness, and loading parameters of the domain. By setting $\gamma^0 = \left(O\,P^2\right) / \left(E\,h^0\left(\Omega\right)\right)$, the influence of the penalty term is scaled consistently for different values of the quantities involved in the expression. Furthermore, eq. (6) is valid only on the boundary. Therefore, one requires a regularization process to extend the normal velocity throughout the domain D [35].

3 Results

A short cantilever plate bending structure, where a load is applied at the corner of its lower right end, exemplifies the described optimization procedure. Figure 1 illustrates its configuration along with its stiffness and loading parameters. This example is commonly addressed in the topology optimization literature. A single NURBS representation discretizing each segment with different boundary conditions initializes the mechanical model. A total of 50 integration points per isogeometric element integrate the fundamental kernels. A $168 \times 112\,\mathrm{mm}^2$ grid with a point spacing of $2.8\,\mathrm{mm}^2$ performs the spatial discretization of the level set function. The target volume is 30% of the original volume. For the heuristic hole insertion criterion, $\rho = 2\%$ is considered with an increment of 1% at each evolution step of the LSM. A value of $O = 10^{-1}$ is adopted for computing γ^0.

Figure 2 presents the achieved results by the proposed formulation. Around iteration 350, one can observe the occurrence of instabilities. Geometrically, the domain begins to expand and contract abruptly in cycles. That eventually leads to code failure. Despite the low slope, the compliance curve is still trending downwards before the instabilities. It indicates that the domain illustrated in the figure still has potential for further evolution. Upon consulting the literature, one can identify several possible modifications to the standard update scheme of the augmented Lagrangian method. In particular, alternatives limiting the γ value growth successfully corrected these

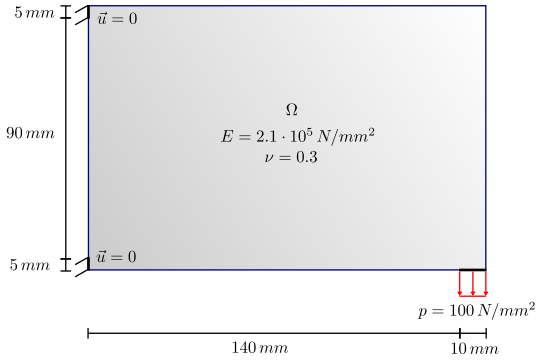
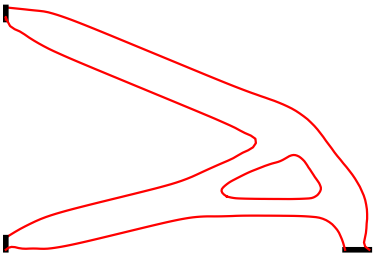
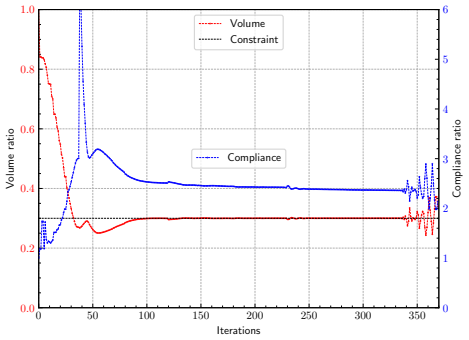


Figure 1. Short plate bended by a loading applied to the corner of its lower face

instability issues. The implemented modifications consisted of adopting a maximum value for γ and refraining from updating it if current configuration satisfies the constraint within a specified tolerance [36, 37]. Based on analyses of the behavior of γ throughout the process, the authors establish a maximum value of $O^{max} = 5.0 \cdot 10^0$. Together with a tolerance of 10^{-3} for the constraint, as detailed on Alg. 1, one can obtain the results shown in Fig. 3. Clearly, the achieved compliance value is lower than that obtained in the previous process. Moreover, the domain configuration is more consistent with established results in the literature obtained using the Solid Isotropic Material with Penalization (SIMP) [21]. This configuration, in fact, shows greater agreement with SIMP when compared to other ones produced by different methodologies involving the LSM/BEM coupling [15, 16, 21].



(a)



(b)

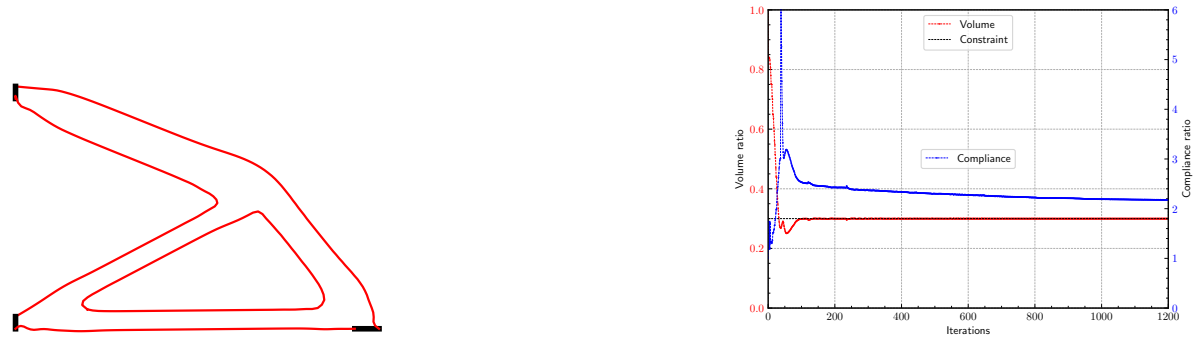
Figure 2. Inital results: (a) domain; (b) convergence

Algorithm 1. Penalty coefficient stabilized update

```
while not(convergence) do
    if |V − V̄| > 10^−3 then
        γ ← min(δ.γ, γ^max)
    end if
end while
```

4 Conclusions

The achieved results highlight the occurrence of instabilities in the described process, as previously reported in the literature. Modifications to the update scheme of γ demonstrate clear success in addressing these instabilities. As a result, for the discussed example, these modifications lead to significantly improved outcomes compared to the untreated process. These results also show present greater consistency with the established SIMP solutions when compared to those obtained by other authors employing similar LSM/BEM coupling approaches. The convergence plots further illustrate the anticipated slowness of the process and underscore the need to verify convergence by analyzing the recent history of iterations.



(a) (b)

Figure 3. Improved results: (a) domain; (b) convergence

Further discussions on the optimization process and the parameters λ and γ, as well as applications to additional examples, may be found in the main author's master's dissertation [38].

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