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New approximations for sequential optimization with discrete material interpolations

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1. Abstract

The Discrete Material Optimization (DMO) [1] is a technique employed in structural optimization problems, dealing with the choice of discrete candidate materials over a certain structural domain. It is based on the use of material interpolations, functions of design variables, which can be seen as weighted sums of these candidates. Its goal is to select the weights' values by means of optimization techniques, in a way that the material being represented by the interpolation can assume the constitutive characteristics of one and only one of the proposed candidates.

At the literature, the DMO was successfully employed in optimization problems of laminated composites, where the desire was to find orientation stacking sequence and material distribution in laminae of plates and shells. Such problems involve in their formulation compliance [1], natural frequencies [2], buckling loads [2, 3], etc. The solutions of these problems were all obtained by the Method of Moving Asymptotes (MMA) [4], which is grounded in Sequential Approximate Optimization (SAO) concepts also known as Approximation Concepts in optimization [5]. However, in many cases, such results do not provide final designs showing full convergence to well (uniquely) selected materials.

This work presents a new solution strategy to DMO problems based on the proposal of a new class of second generation approximations [6] based on using DMO weights to define proper intermediate variables, which is shown to bring improvements in the utilization of SAO techniques. The results obtained show that such approximations provide superior convergence to DMO compliance minimization (maximization of stiffness) problems in terms of uniquely selected materials and final optimized designs.

2. Keywords: second generation approximations, discrete material optimization, sequential approximate optimization

3. Discrete Material Optimization

The Discrete Material Optimization (DMO) [1] technique permits to choose by optimization candidate materials in domains/subdomains of structures by using interpolations of such candidates in the form of the Eq.(1). This interpolation represents the variable material $\mathbf{C}(\mathbf{x})$ which can be seen as a weighted sum of the discrete candidates $\mathbf{C}_i$, where the weights w_i are functions of the variables $\mathbf{x}$, assumed as design variables.

$$\mathbf{C}(\mathbf{x}) = w_1(\mathbf{x})\mathbf{C}_1 + w_2(\mathbf{x})\mathbf{C}_2 + ... + w_i(\mathbf{x})\mathbf{C}_i + ... + w_n(\mathbf{x})\mathbf{C}_n = \sum_{i=1}^{n} w_i(\mathbf{x})\mathbf{C}_i \tag{1}$$

The desire is always to set one of the weights equal to 1 and the others to zero in the end of an optimization process, therefore selecting in $\mathbf{C}(\mathbf{x})$ one of the n candidate materials in the end of the optimization. Common interpolation functions, or weights $w_i(\mathbf{x})$, used in Eq.(1) are the DMO4, the DMO5 and the SFP (Shape Function with Penalization)[7]:

$$\text{DMO4:} \qquad w_i = (x_i)^p \prod_{j=1;j\neq i}^{n} [1-(x_j)^p] \tag{2}$$

$$\text{DMO5:} \qquad w_i = \frac{\hat{w}_i}{\sum_{i=1}^{n}\hat{w}_i} \qquad \text{and} \qquad \hat{w}_i = (x_i)^p \prod_{j=1;j\neq i}^{n} [1-(x_j)^p] \tag{3}$$

$$\text{SFP:} \qquad \begin{array}{ll} w_1 = \left[\dfrac{1}{4}(1-x_1)(1-x_2)\right]^p & w_2 = \left[\dfrac{1}{4}(1+x_1)(1-x_2)\right]^p \\ w_3 = \left[\dfrac{1}{4}(1+x_1)(1+x_2)\right]^p & w_4 = \left[\dfrac{1}{4}(1-x_1)(1+x_2)\right]^p \end{array} \tag{4}$$

The DMO4 deals with any number of candidate materials, the DMO5 is a normalized version of the prior to ensure $\sum_{i=1}^{n} w_i = 1$ in order to better represent material characteristics during optimization and the SFP, in the present form, is able to interpolate only $n = 4$ candidate materials, but in this case reduces in a half the number of necessary design variables x_i in comparison to the DMO4/5. The variables x_i are $0 \leq x_i \leq 1$ in DMO4/5 and $-1 \leq x_i \leq 1$ in SFP. The p is a penalty factor to avoid mix of materials (weights w_i not or 0 or 1) in the final optimized designs. Using common finite element notation, a DMO compliance c minimization problem has the form:

$$\begin{aligned} \text{minimize:} \quad & c = \mathbf{f}^{\mathrm{T}}\mathbf{u} \\ \text{subjected to:} \quad & \mathbf{K}(w_i(\mathbf{x}))\mathbf{u} = \mathbf{f} \\ & g(\mathbf{x})_M = M(w_i(\mathbf{x})) \leq M_{max} \\ & x_{min} \leq x_i \leq x_{max} \end{aligned} \tag{5}$$

The dependence of the design variables $\mathbf{x}$ is inserted in the problem by using the interpolations $\mathbf{C}(\mathbf{x})$ to compose the structure stiffness matrix $\mathbf{K}$. The problem counts with a mass constraint $g(\mathbf{x})_M$ which is important when distributing materials with distinct densities over subdomains of a structure.

4. Improved SAO Approximations for DMO

The solutions of DMO problems like in Eq.(5) are usually based in the efficient Method of Moving Asymptotes (MMA) [4]. In some cases, however, it is reported in the literature a difficulty of convergence in terms of obtaining well selected materials [8]. In order to achieve improvements in this sense, new approximations for use with Sequential Approximate Optimization (SAO) techniques are here proposed. They are based on using the weights $w_i(\mathbf{x})$ to define intermediate variables to compose second generation [6] approximations, in this specific case to the compliance c in Eq.(5). A good indicative that such procedure will result in improved approximations is the fact that the interpolated material $\mathbf{C}(\mathbf{x})$ in Eq.(1) varies linearly with the $w_i(\mathbf{x})$ and these weights have an explicit dependency on the design variables $\mathbf{x}$. Having as base a compliance first order Taylor series expansion, it is possible to write a direct approximation [5] in the $w_i(\mathbf{x})$ as:

$$\tilde{c}_{D-w}(\mathbf{x}) = c(\mathbf{w}_0) + \sum_{i=1}^{n} (w_i(\mathbf{x}) - w_{0i}) \left(\frac{\partial c}{\partial w_i}\right)_{\mathbf{w}_0} \tag{6}$$

A conservative approximation [5] in the $w_i(\mathbf{x})$ can be written as:

$$\tilde{c}_{C-w}(\mathbf{x}) = c(\mathbf{w}_0) + \sum_{i=1}^{n} (w_i(\mathbf{x}) - w_{0i}) \frac{w_{0i}}{w_i(\mathbf{x})} \left(\frac{\partial c}{\partial w_i}\right)_{\mathbf{w}_0} \tag{7}$$

A MMA approximation [4] in the $w_i(\mathbf{x})$ can be written as:

$$\tilde{c}_{MMA-w}(\mathbf{x}) = c(\mathbf{w}_0) + \sum_{i=1}^{n} \left[(w_{0i} - L_i) - \frac{(w_{0i} - L_i)^2}{w_i(\mathbf{x}) - L_i}\right] \left(\frac{\partial c}{\partial w_i}\right)_{\mathbf{w}_0} \tag{8}$$

The intermediate variables used in Eq.(6) to (8) are respectively $w_i(\mathbf{x})$, $1/w_i(\mathbf{x})$ and $1/(w_i(\mathbf{x}) - L_i)$. It is important to highlight that the approximations in the Eq.(7) and (8) already consider the fact that the derivative of the compliance c with respect to a material weight w_i is given by:

$$\frac{\partial c}{\partial w_i} = -\mathbf{u}^T \frac{\partial \mathbf{K}}{\partial w_i} \mathbf{u} \tag{9}$$

This derivative is always negative since the stiffness matrix derivative appearing in Eq.(9) is positive definite. They will be assessed in solving the compliance minimization problem given by Eq.(5), using SAO in the space of the design variables x_i, since the approximations in Eq.(6) to (8) are ultimately explicit functions of the design variables x_i. For comparison with the new proposed approximations, two common and well used classical approximations in structural optimization will also be included in this evaluation: the conservative and MMA approximations [5, 4] based on first order expansions in terms of simpler intermediate variables, respectively x_i,$1/x_i$ and $1/(x_i - L_i)$, $1/(U_i - x_i)$. Due to this, they are referred in the results session ahead as *approximations in* x_i.

It should be mentioned that other types of approximations available in the literature [5, 9] can be created over the concept of intermediate variables in terms of the $w_i(\mathbf{x})$. Here, only the most common types are tested, which are the direct, conservative and MMA.

5. Results

Results for two cases will be presented in order to illustrate the proposed approximations assessment. SAO is performed for the problem in Eq.(5) using the Conjugate Gradient (CG) method as preferred solver, since the approximations in the $w_i(\mathbf{x})$ are no longer separable in the x_i and due to this a dual solution (like in the CONLIN and MMA methods) can not be directly developed. Relying over second level convex approximations could perhaps be a good choice. However, at this stage it was decided to use a more straightforward solver. Additional details, like the moving limits strategy employed for the x_i variables and the followed rules for MMA asymptotes updates are fully described in [10].

The first case is a problem from [7], whose aim is to distribute the same unidirectional fiber reinforced composite material at the orientations 0, ±45 and 90 degrees in sixteen equal subdomains of a membrane subjected to load and boundary conditions as shown in Fig.1. The DMO4, DMO5 and SFP interpolations are used, together with several values of p. The number of design variables x_i defined is $16 \times 4 = 64$ with DMO4/5 and $16 \times 2 = 32$ with SFP. The material interpolations used in each one of the sixteen subdomains are of the form:

$$\bar{\mathbf{Q}}(\mathbf{x}) = w_1(\mathbf{x})\bar{\mathbf{Q}}_{-45} + w_2(\mathbf{x})\bar{\mathbf{Q}}_0 + w_3(\mathbf{x})\bar{\mathbf{Q}}_{45} + w_4(\mathbf{x})\bar{\mathbf{Q}}_{90} \tag{10}$$

The results obtained are shown in Tab.1, where it can be seen that the approximations which provided the best designs in terms of lowest compliance values, well selected materials and number of iterations spent are the direct approximation in the $w_i(\mathbf{x})$, which converged well with DMO4/5 and SFP, followed by the MMA approximation in the $w_i(\mathbf{x})$, which converged well with DMO4 and SFP but not with the DMO5. It can be noticed that the well converged results are equal or better than the ones from [7], reproduced in Tab.1 for comparison. The best designs encountered are depicted in Fig.1, in terms of compliance c.

The second case presented is also a membrane problem based in a very similar one in [8] whose loads, boundary conditions and mesh are shown in Fig.2. It consists of a four point bending case treated by symmetry boundary conditions. The aim now is to choose materials among an unidirectional fiber reinforced composite at the orientations 0, ±45 and 90 degrees and a soft foam, in each one of the 768 finite elements of the mesh. The DMO4 and DMO5 interpolations are used. The SFP is not suitable anymore, since five candidate materials are considered. The number of design variables x_i defined is $768 \times 5 = 3840$, a much bigger problem. Now, the penalty parameter p is considered variable throughout the optimization, starting from $p = 1$ at the 10 first iterations, after that going to $p = 2$ for more 10 iterations and finally to $p = 2.5$ up to the end of the solution. The material interpolations used are of the form:

$$\bar{\mathbf{Q}}(\mathbf{x}) = w_1(\mathbf{x})\bar{\mathbf{Q}}_{-45} + w_2(\mathbf{x})\bar{\mathbf{Q}}_0 + w_3(\mathbf{x})\bar{\mathbf{Q}}_{45} + w_4(\mathbf{x})\bar{\mathbf{Q}}_{90} + w_5(\mathbf{x})\mathbf{Q}_f \tag{11}$$

In this second problem, materials with different densities are distributed in the domain of the structure being optimized. Therefore, the mass constraint $g_M(\mathbf{x})$ in Eq.(5) is important and set in such a way that 75% of the membrane is to be filled by foam. This constraint is included in the compliance minimization using an Augmented Lagrangian Method (ALM). The results found with DMO4 presented convergence and are depicted in Fig.2. (The results obtained with DMO5 did not converge.) From this figure, it can be noticed that the direct approximation in the $w_i(\mathbf{x})$ and the MMA approximation in the $w_i(\mathbf{x})$ were the ones wich provided the best designs to be found in terms of well selected materials, final material topologies and lowest compliance values. Furthermore, the case with the MMA approximation in $w_i(\mathbf{x})$ was the one which provided the best of all compliance values found and in a small number of iterations, only 66. This is indeed a very good result for this problem considering its size in number of variables. The superior convergence qualities of the MMA approximation in the $w_i(\mathbf{x})$ in comparison to the same approximation in the x_i can be illustrated by the graph in Fig.3. In this graph it can be seen that, when the intermediate variable $w_i(\mathbf{x})$ is used, a smoother convergence is guaranteed for both the compliance $\tilde{c}(\mathbf{x})$ and for the mass constraint $g_M(\mathbf{x})$ over the iterations run.

6. Conclusions

It is concluded that approximations using intermediate variables based on the weights $w_i(\mathbf{x})$ are of superior quality for DMO problems of compliance minimization solved by SAO techniques. The best

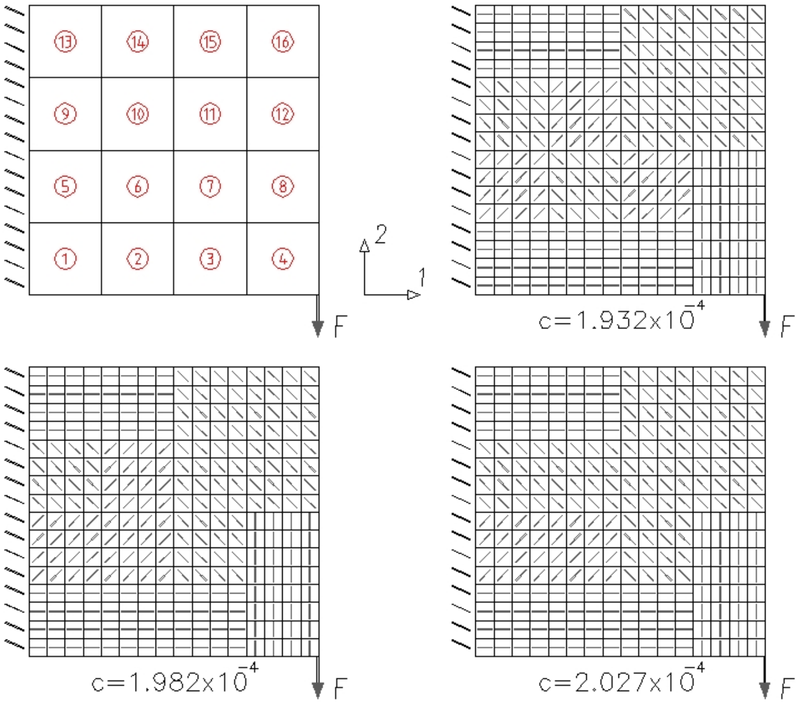

Figure 1: Membrane test case from [7]: material orientations are chosen in 16 sub-domains. Some of the best results in terms of compliance c and orientations found are included.

Table 1: Membrane test case from [7]: convergence results for compliance c minimization, using several compliance approximations.

Interpolation Scheme	DMO4 p=2	DMO4 p=3	DMO4 p=5	DMO5 p=2	DMO5 p=3	DMO5 p=5	SFP p=2	SFP p=3	SFP p=5
Solution from [7], based on the MMA method.									
Result[a]	n/r	n/r	mixed mat.	n/r	n/r	selected mat.	selected mat.	selected mat.	selected mat.
Objective c^b $\times 10^{-4}$			-			4.176	2.027	2.027	2.027
Iterations	-	-	18	-	-	5	4	4	4
Using compliance conservative approximation in the x_i and CG.									
Result	not converged	not converged	not converged	not converged	not converged	not converged	not converged	mixed mat.	mixed mat.
Objective c $\times 10^{-4}$	-	-	-	-	-	-	-	9.588	1.715
Iterations	-	-	-	-	-	-	-	5	5
Using compliance MMA approximation in the x_i and CG.									
Result	not converged	selected mat.	not converged	not converged	not converged	not converged	not converged	selected mat.	selected mat.
Objective c $\times 10^{-4}$	-	2.323	-	-	-	-	-	2.027	2.027
Iterations	-	100	-	-	-	-	-	3	3
Using compliance direct approximation in the $w_i(\mathbf{x})$ Eq.(6) and CG.									
Result	selected mat.	selected mat.	selected mat.	not converged	selected mat.	selected mat.	not converged	selected mat.	selected mat.
Objective c $\times 10^{-4}$	1.932	2.033	2.056	-	2.027	2.027	-	2.027	2.027
Iterations	7	3	5	-	2	2	-	3	3
Using compliance conservative approximation in the $w_i(\mathbf{x})$ Eq.(7) and CG.									
Result	mixed mat.	mixed mat.	mixed mat.	mixed mat.	mixed mat.	mixed mat.	mixed mat.	mixed mat.	mixed mat.
Objective c $\times 10^{-4}$	2.038	2.043	2.046	1.394	1.394	1.395	2.044	2.017	2.032
Iterations	41	38	34	22	23	23	44	25	22
Using compliance MMA approximation in the $w_i(\mathbf{x})$ Eq.(8) and CG.									
Result	selected mat.	selected mat.	selected mat.	mixed mat.	mixed mat.	mixed mat.	mixed mat.	selected mat.	selected mat.
Objective c $\times 10^{-4}$	1.932	1.982	2.061	1.394	1.394	1.396	2.041	2.027	2.027
Iterations	8	5	5	12	16	13	7	3	3

[a]n/r - not reported
[b]Calculated based on material selection results shown in [7]

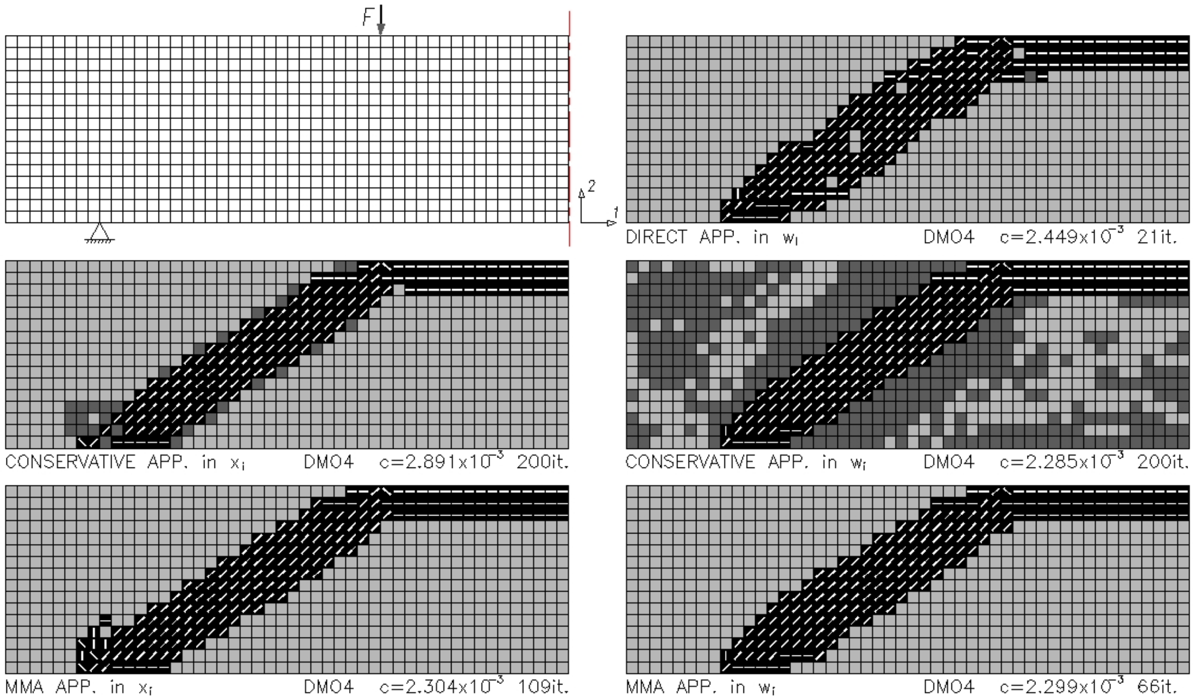

Figure 2: Membrane test case based in [8]: load/boundary conditions and DMO4 results. Black is fiber composite and the white lines indicate material orientation, light gray is foam and dark gray means mixture of candidates.

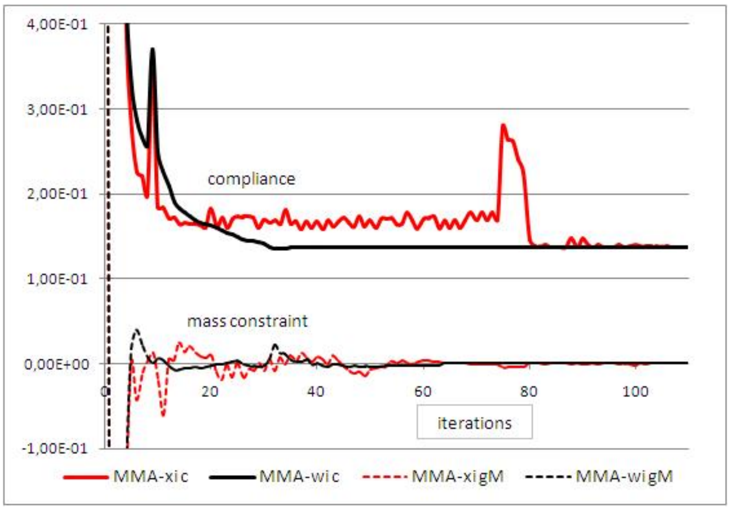

Figure 3: Membrane test case based in [8]: normalized values of compliance c and mass constraint g_M plotted in terms of iterations for DMO4 cases with MMA approximations in x_i and $w_i(\mathbf{x})$ from Fig.(2).

approximations in this sense were the direct and MMA approximation based on the weights $w_i(\mathbf{x})$. They had a better performance in comparison to classical approximations. However, they were not able to consistently improve the optimization performance when using DMO5. This will be the focus of a next work.

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