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Ordered multi-material SIMP approach applied to 3D topology optimization

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Abstract

This paper presents a topology optimization framework for multi-material 3D structures to be used in mechanical load carrying applications. This framework is an extension of an ordered multi-material interpolation scheme originally proposed in 2D to the 3D minimum compliance problem implemented in MATLAB. The algorithm starts by using the Young's moduli and cost of the selected materials, then picks binary combinations with ordered densities to interpolate the value for the current iteration. Following these interpolations, the next step of the design is the solution of the mechanical compliance problem until the desired minimum compliance is met subject to volume and cost constraints. The solution scheme is based on Optimality Criteria Method and standard density filtering schemes. The main contribution of this paper is that the proposed design scheme implemented in MATLAB is an easy-to-use 3D topology optimization scheme with multi-material constituents based on a modified SIMP interpolation. Results show that the 3D code is able to deliver similar design results when compared with the existing 2D version. This effectively expands the topology optimization based design capability to many practical 3D engineering problems in a standard topology optimization setting and easy-to-use implementation in MATLAB.

Keywords: Multi-material, Topology optimization, SIMP, minimum compliance, 3D design.

1. Introduction

Topology optimization (TO) is a powerful design approach applied to different engineering applications since the seminal work in 1989 [1] ranging from static and dynamic performance of structures under mechanical and thermal loading [2] to electromagnetic designs [3] and more recently to manufacturable designs using additive manufacturing techniques [4].

TO algorithms use different material interpolation techniques such as Solid Isotropic Material with Penalization (SIMP) and Rational Approximation of Material Properties (RAMP) [5]. RAMP is proven to bypass numerical issues at zero density where SIMP is prone to numerical issues [6]. Level-set method used in TO addresses grey-scale issues more commonly faced in density based approaches [7].

Several public codes are available in literature but there is still room for improvement in leveraging these to their full potential. To the best of our knowledge, these are implemented to 2D problems or make use of a single material allowing for the design of a chosen material with void regions [8, 9]. However, their implementation in MATLAB and availability as open-source codes in addition to their easy-to-use structure have resulted in these codes to become baseline references for further studies in TO.

Attempts to extend these codes and investigate their applicability to more realistic structures also exist. The effects of applied load in terms of magnitude, direction and location on the resulting 3D structure were investigated [10]. Applications of TO algorithms to 3D is also desired as the connection with additive manufacturing has become possible and not been limited to structural TO applications only [11]. Computational optimization of the public 2D and 3D codes were pursued to increase time efficiency of the codes in another study, while a multi-material approach was introduced [12].

Similarly, the extension of single material TO algorithms to multi-material approaches in 3D has been studied in [13-15]. Another noteworthy study has been carried out on reducing the crack propagation with optimized topologies using multi-materials, based on the extended finite element method [16]. The multi-material approach improves the TO framework for structural mechanical applications by making use of relatively less compliant material in elements under higher mechanical load [17]. This material placement technique will help the design process by reducing overall material usage compared to a single material solution.

In this study, the ordered SIMP method introduced by [17] is implemented where it is adopted for binary combinations of the utilized materials. However, this

multi-material technique was implemented on the 99-line code provided in [18]. To benefit from the multi-material TO framework with multiple constraints in 3D design domains, in this paper, the existing interpolation technique is adapted to the 3D TO code provided in [9]. The resulting framework presented in this paper is based on the integration of the ordered multi-material technique to the 3D design problems based on the reference work in [9] .

2. Material and methods

2.1. Topology optimization framework for 3D multi material structures

This paper presents an enhanced TO framework for 3D multi material structures in MATLAB utilizing mainly two publicly available TO codes developed by Zuo & Saitou and Liu & Tovar [9,17]. In this section, the reference algorithms are briefly introduced and enhancements proposed by the 3D multi-material TO framework is discussed in detail. Finally, to prove the validity of the resulting 3D multi-material TO code, it is compared with the reference TO framework in 2D on the bridge design problem as in Fig. 1. Nodes at x = 0 and y = 0 coordinates are constricted at all three degrees of freedom while the nodes at the right are constricted only at the y direction. Forces are given as F, 2F, F at positions x = 1/4, x = 1/2 and x = 3/4 respectively. The boundary conditions and loads discussed are repeated throughout the z-direction for all nodes.

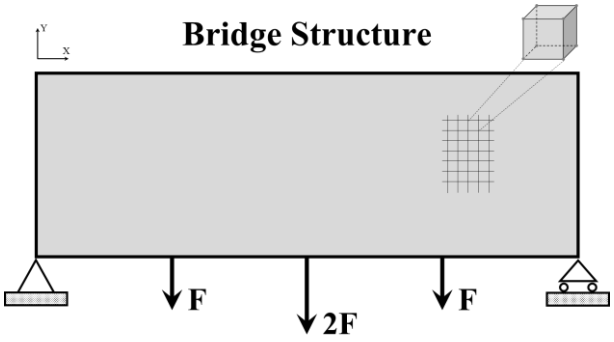


Fig 1. Bridge design problem with boundary conditions from [17].

2.1.1. Multi-material topology optimization using ordered SIMP interpolation

The multi-material 2D TO code implemented by Zuo & Saitou uses a modified version of the Solid Isotropic Material with Penalization (SIMP) material interpolation. The classical single material SIMP method on its own is not applicable to the design domains where multiple materials are used for the solution. Hence, Zuo & Saitou propose the modified SIMP strategy for multiple material usages. In this strategy, "scaling coefficient" (1) and "translation coefficient" (2) parameters for both elastic modulus (E) and cost interpolations are introduced to tailor the traditional SIMP for ordered SIMP interpolation to enable multi material solutions. In (1) and (2), E represents the elastic modulus and ρ represents the density of the materials in index *i* and *i+1,* while *p* is the penalization factor.

$$A_E = \frac{E_i - E_{i+1}}{\rho_i^p - \rho_{i+1}^p} \quad (1)$$

$$B_E = E_i - A_E \rho_i^p \quad (2)$$

These coefficients are calculated by taking binary combinations from the density ordered arrays of the materials' density, elastic modulus and cost properties which were normalized prior to the calculations as in (3). They are used for determining the effective E (4) and cost function (5) in an element for the current selection of materials. For finding the cost function's coefficients, a similar procedure is followed to (1) and (2) but E values are changed with cost values and the penalization factor is used as *1/p*.

$$\rho^i = \frac{\rho_T^i}{\rho_{max}} \ (i = 1, 2, 3, \dots n) \quad (3)$$

$$E_e(\rho_e) = A_E \rho_e^p + B_E \quad (4)$$

$$C_e(\rho_e) = A_C \rho_e^{1/p} + B_C \quad (5)$$

The performance of the aforementioned strategy is validated in a multi material problem which comprises three different materials. The material properties are provided in Table 1. By the implementation of this strategy, an E-density curve as in Fig. 2 and cost-density curve as in Fig. 3, that unify multiple materials with their specifications are drawn [17].

The developed code carries out the initialization of design domain for Finite Element Method (FEM) analysis, then proceeds with the optimality criteria method (OCM) to update the design with each iteration. The key difference compared to optimality criteria with one constraint is that the code uses two different constraints as volume fraction and cost fraction, consequently the optimization model, hence the Lagrangian function should be changed to take into account both of these constraints.

Table 1. Material properties as taken from Zuo & Saitou.

Name	Normalized density	Normalized E	Normalized cost	Color
Void	0	0	0	White
A	0.4	0.2	0.5	Blue
B	0.7	0.6	0.8	Red
C	1.0	1.0	1.0	Black

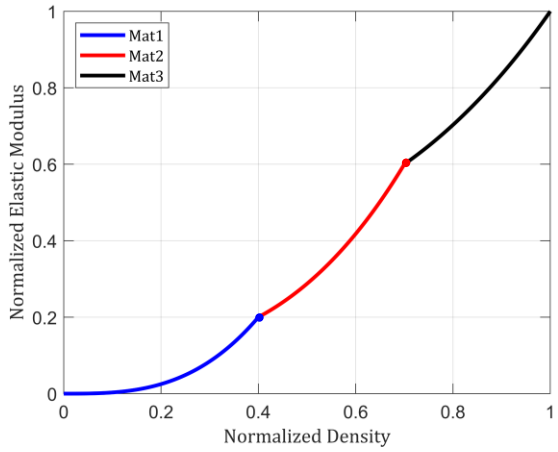


Fig 2. Ordered multi-material SIMP interpolation curve for normalized *E*.

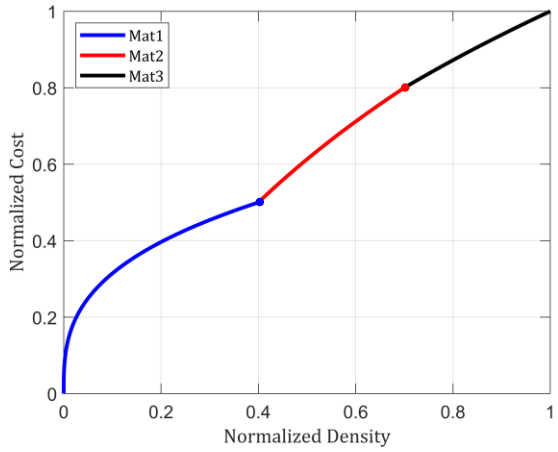


Fig 3. Ordered multi-material SIMP interpolation curve for normalized cost.

The mapping of element densities to multiple materials should be elaborated on as well. The density values are mapped to the materials considering the median value of the current combination of two materials, in such a manner that the median value is used as the boundary value for the mapping, instead of the materials' densities [17].

This ordered SIMP method was only validated for 2D problems. The ultimate goal of the present study is to adapt this method to 3D problems. For that purpose, a public 3D TO code is utilized, the structure of which code is explained in the next section.

2.1.2. 3D topology optimization code

The public 3D TO code provided in [9] takes advantage of the density-based approach which replaces homogenization method. In the code, SIMP method is used for the penalization of intermediate densities in the solution, tackling the well-known relaxation problem to overcome ill-posedness and making it suitable for standard manufacturing techniques. Unlike the original study, which focuses on three optimization problems, the main focus in this paper is on the standard minimum compliance problem. The objective function aims for the minimization of displacement under certain loads and boundary conditions subject to total volume fraction constraints [9]. In Fig. 4, the optimization structure employed is shown.

The code moves on with using the FEM to find element stiffness matrices to be used later with SIMP to assembly the general stiffness matrix. The next step uses generalized Hooke's Law to find nodal displacements with given force vectors and the assembled stiffness matrix [9].

The following step of the design process consists of updating the initial design within each iteration and comparing the objective function values in consecutive design iterations to decide on convergence. To find optimal material distribution for a given design domain, OCM is utilized in both reference codes [9, 17].

2.1.3. Implementation of ordered SIMP method to the 3D to code

In this section, changes made throughout the merging process of the reference codes will be discussed. Fig. 5 shows the modified 3D TO algorithm based on the ordered SIMP method allowing for multi-material designs. The modifications in the original 3D TO code are highlighted in the red dotted section in Fig. 5. In the following section, the changes made to the default 3D TO code will be elaborated thoroughly. MATLAB R2020b was used for the application of modifications to the original code [19].

By interchanging lines 8-10 with the lines below, the used materials' properties are given in the array format. Material properties are taken from Table 1.

```
rhoVector= [10^-8 0.4 0.7 1];
EVector= [10^-8 0.2 0.6 1];
costVector= [10^-8 0.5 0.8 1];
```

In this example, the property values are in normalized form. However, if properties aren't normalized, then these lines will simply normalize the arrays.

```
maxE = max(EVector);
maxRho = max(rhoVector);
maxCost=max(costVector);
```

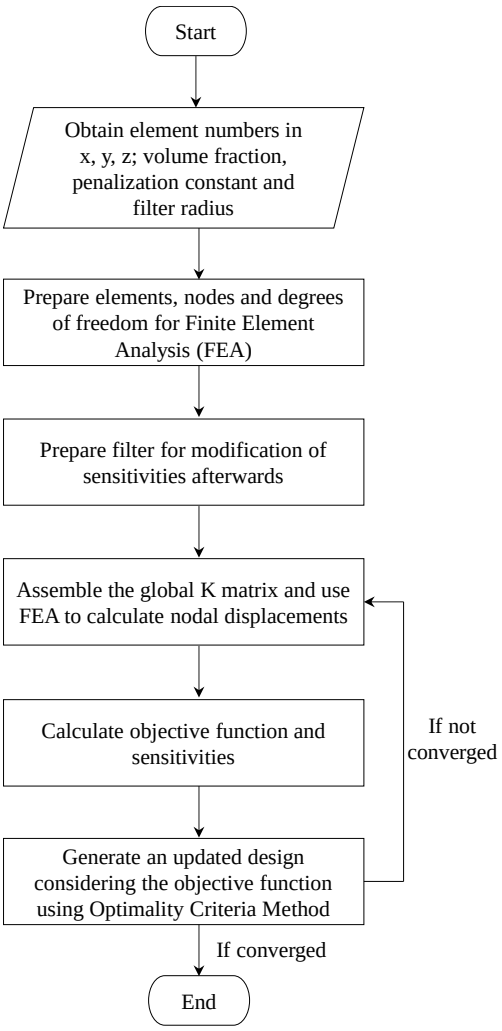


Fig 4. Step by step flowchart of the default 3D TO code from Liu and Tovar, re-interpreted by the author [9].

```
matsNumb=length(EVector);
EVector = EVector./maxE;
rhoVector = rhoVector./maxRho;
costVector = costVector./maxCost;
```

In lines 37-47, small adjustments are made to match the filter with the one in Zuo & Saitou [17]. Here, floor (...) function provided in MATLAB is used instead of ceil (...). It is also noted that both codes have the ability to work with the sensitivity or density filter. For the specific bridge design problem presented here, a sensitivity filter with radius r=3 was used., while the penalization factor was selected as 4.

Before the FEA starts in line 70, the following codes should be inserted to calculate the interpolated *E* and cost values.

```
for i = 1:nelx
 for j = 1:nely
  for k = 1:nelz
   count = 1;
   while count<matsNumb
if(rhoVector(count)<xPhys(j,i,k))&&(rhoVector(cou
nt+1)>=xPhys(j,i,k))
Ae = (EVector(count)-
EVector(count+1))/(rhoVector(count)^penal-
rhoVector(count+1)^penal);
Be = EVector(count)-
(Ae*(rhoVector(count)^penal));
      EInter(j,i,k)=Ae*(xPhys(j,i,k)^penal)+Be;
dEInter(j,i,k) = Ae*penal*(xPhys(j,i,k)^(penal-
1));
Ac=(costVector(count)-
costVector(count+1))/(rhoVector(count)^(1/penal)-
rhoVector(count+1) ^(1/penal));
```

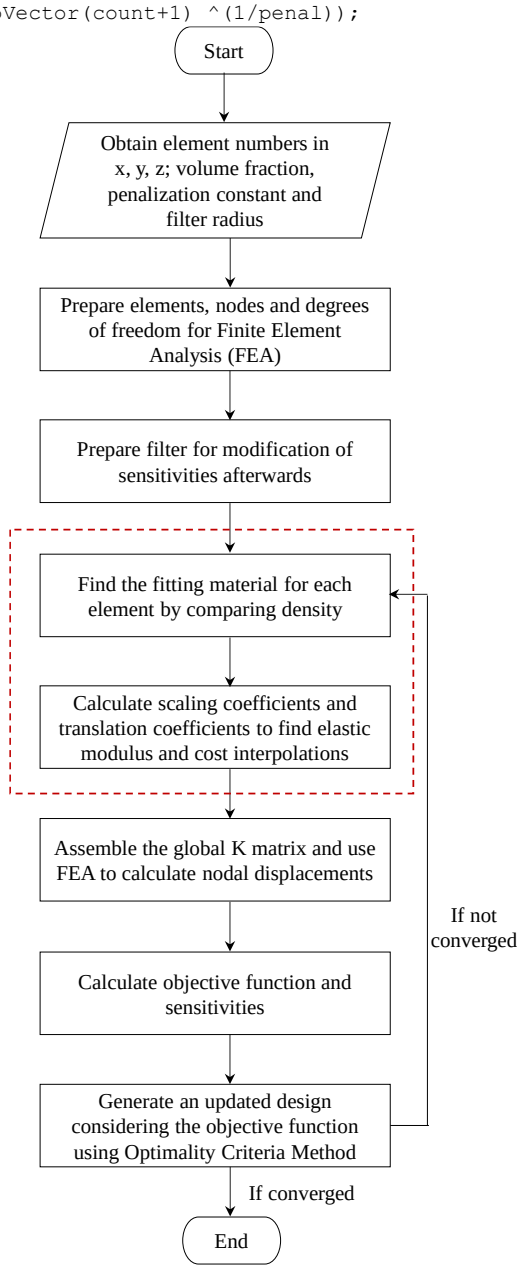


Fig 5. Step by step flowchart of the 3D TO code adapted to multi-material.

```
Bc= costVector(count)-
(Ac*(rhoVector(count)^(1/penal)));
CInter(j,i,k)=Ac*(xPhys(j,i,k)^(1/penal))+Bc;
dCInter(j,i,k) =
Ac*(1/penal)*(xPhys(j,i,k)^((1/penal)-1));
break;
end
count = count + 1;
   end
  end
 end
end
```

Line 70 is substituted with the line below to use the interpolated *E* matrix for assembling the K matrix.

```
sK = reshape(KE(:)*(EInter(:)'),24*24*nele,1);
```

Lines 75 and 76 are changed to make use of the interpolations again.

```
c = sum(sum(sum((EInter.*ce))));
dc = -dEInter.*ce;
```

Before the OCM begins, following changes are made to set equivalent parameter values with the 2D version. V2 and P2 are the introduced dynamically initialized upper limits as in the reference code.

```
moveMin = 0.001;
move0 = 0.15;
alpha = 0.96;
move = max((alpha^loop)*move0,moveMin);
dc = -1*dc;
V1=0;
V2=max(max(max(dc./dv)));
P1=0;
P2=max(max(max(dc./(CInter+x.*dCInter))));
dampingCoef = 1;
```

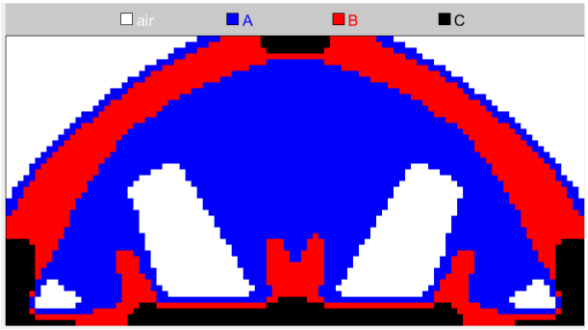
The OCM is changed to work with two constraints instead of one, therefore all iterations will be carried out with updating both bounds accordingly.

```
while (((V2-V1)/(V1+V2) > 1e-6) || ((P2-
P1)/(P2+P1)>1e-6))
 Vmid = 0.5*(V2+V1);
 Pmid = 0.5*(P2+P1);
 denominator = Vmid+Pmid.*CInter+Pmid*x.*dCInter;
 xnew = max(10^-5,max(x-
move,min(1,min(x+move,x.*sqrt(abs(dc./(denominato
r)).^dampingCoef)))));
 xPhys(:) = (H*xnew(:))./Hs;
 if sum(xPhys(:)) > volfrac*nele
  V1 = Vmid;
 else
  V2 = Vmid;
 end
 if sum(xnew(:).*CInter(:))/(nele) > costfrac
  P1= Pmid;
 else
  P2 = Pmid;
 end
end
```

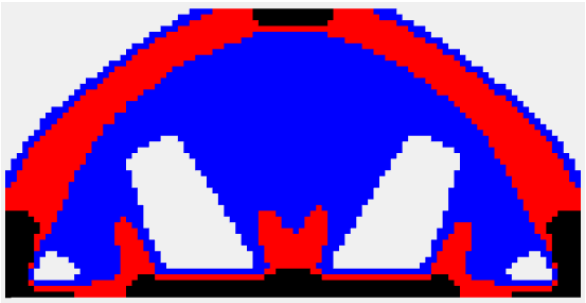
3. Results and discussion

In this section, comparative results obtained via the original 2D and 3D multi-material TO simulations are presented as shown in Fig. 6 a-b. The materials used have the same properties as in [17] where material shown with black color has a higher *E* value but also costs more, the red one has an average *E* value with average cost and material shown in blue has the lowest *E* value and costs the least. The usage of black material is prioritized for elements under high loads because of its higher *E* value, but is not favored due to its high cost. The red material is used for the transition from high density elements to low density elements where it is more cost efficient to be used instead of the black material. Blue material is used for elements where the structure connectivity is important and lower values of stiffness are required but voids cannot provide.

Optimization results with a chosen mesh of 100x50 and 100x50x1 are given in Fig. 6 a-b. The thickness in z-direction was selected as 1 element to exactly represent the 2D shell geometry of the original 2D bridge example with the developed 3D optimization code for one-to-one comparison purposes. The resulting optimal material distribution results confirm the validity of the 3D integrated multi-material code with an almost exact replication of its 2D counterpart topology and a matching convergence behavior. Convergence results are provided for normalized compliance values with respect to the total number of elements and for the resulting final volume and cost values for the optimized topologies as given in Fig. 6 c-d. Based on these results, after the same number of 123 iterative updates, the same volume fractions of 0.4 and cost fractions of 0.283 were obtained while the objective function values converged to 0.0457 and 0.0456, with the 2D and 3D code, respectively, confirming the validity of the code extension to 3D.



(a)



(b)

```
It.: 121 Obj.: 0.0457 Vol.: 0.401 Cost: 0.283 ch.:0.001
It.: 122 Obj.: 0.0456 Vol.: 0.400 Cost: 0.282 ch.:0.001
It.: 123 Obj.: 0.0457 Vol.: 0.401 Cost: 0.283 ch.:0.001
```

(c)

```
It.: 121 Obj.: 0.0455 Vol.: 0.401 Cost: 0.283 ch.:0.001
It.: 122 Obj.: 0.0454 Vol.: 0.400 Cost: 0.283 ch.:0.001
It.: 123 Obj.: 0.0456 Vol.: 0.401 Cost: 0.283 ch.:0.001
```

(d)

Fig 6. Resulting topology from (a) Zuo and Saitou's 2D and (b) the implemented 3D multi-material TO codes with their respective results given in (c) and (d).

4. Conclusions

Use of multiple materials becomes important when various constraints are taken into consideration for the TO problem [17]. Zuo and Saitou's multi-material TO code was implemented in 2D and in this study we extended it to a 3D design domain. Adaptation to 3D allows multi-material designs to address more realistic design problems. Results show that the 3D code delivers matching design results along with almost the same exact material distribution compared to the 2D code. Although this extension was only applied to the minimum compliance problem, it could be fully adapted to other 3D TO problems discussed in [9] such as force inverter and heat conduction.

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Author's statement
Conflict of interest: Authors state no conflict of interest. Informed consent: Informed consent has been obtained from all individuals included in this study. Ethical approval: The research related to human use complies with all the relevant national regulations, institutional policies and was performed in accordance with the tenets of the Helsinki Declaration, and has been approved by the authors' institutional review board or equivalent committee.

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