The 9th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2024
3–7 June 2024, Lisboa, Portugal

A PLUGIN FRAMEWORK FOR LARGE-SCALE MULTI-FORMULATION TOPOLOGY OPTIMIZATION

Neiva M.B.[1], Nale A.[2], Menezes I.F.M.[1] and Chiozzi A.[3]

[1] Department of Mechanical Engineering
Pontifical Catholic University of Rio de Janeiro
Rua Marquês de São Vicente, 225, Rio de Janeiro 22453, Brazil

[2] Department of Architecture
University of Ferrara
Via della Ghiara, 36, Ferrara 44121, Italy

[3] Department of Environmental and Prevention Sciences
University of Ferrara
C.so Ercole I d'Este, 32, Ferrara 44121, Italy

Key words: Topology Optimization, Large-Scale Simulation, Plugin Framework

Summary. Topology optimization is a design computational method that aims to find the best distribution of material to maximize some performance measures within a given domain under prescribed constraints. The technique has found a wide range of applications due to its flexibility in addressing different problems. In particular, the pioneering work of Sigmund [1] and Bendsøe and Kikuchi [2] on single and multiple materials has paved the way for developing new formulations and educational codes. These codes demonstrate the potentiality of topology optimization in structural mechanics to generate optimized layouts. Advances and extensions have been proposed, including periodic and non-periodic microstructures. Motivated by these previous works, we propose a plugin-based framework that allows the treatment of a multi-material formulation for large-scale structural problems. Standard compliance minimization is used, and the proposed implementation enables handling multiple materials with different stiffness properties, i.e., isotropic and anisotropic materials, as well as various constraints. The plugins are implemented to allow the user to customize the specific problem to address. Moreover, the software allows new features to be added to the pre-existing code to extend or change the formulation already implemented. Numerical examples are presented to demonstrate the capabilities and validate the main features of the proposed framework. The authors are investigating potential extensions of this work to consider more complex formulations, such as stress constraints and multiphysics problems.

1 INTRODUCTION

Topology optimization is a computational method that allows designing the optimal layout of a given domain subjected to user-defined constraints and proper loading and support conditions. This technique leverages its potential to embed numerical optimization methods with finite element analysis (FEA). As a consequence, topology optimization deals with the main limitations related to the finite element method (FEM). In particular, topology optimization has emerged sensitive to numerical instabilities, such as checkerboard patterns. Efforts to face and overcome these limitations have been proposed using restriction methods for Solid Isotropic Method Penalization (SIMP) problems, such as perimeter control [3, 4], sensitivity filter [5], density filter [6], and projection filter [7]. In addition, filtering techniques allow, with adequate discretization, to provide the smoothness of the design field. Despite some limitations, topology optimization is a pervasive methodology that handles different physics and problems, e.g., structural optimization and thermal and fluid management. So, in this context, a modular code can provide adequate flexibility and versatility to change the formulation and the analysis method, the solver, and the update scheme. Initially, many available routines were focused on specific topology optimization problems, such as the 99-line [1] and 88-line [8], combining the topology formulation and the numerical analysis methods to preserve the compactness of the code. Then, educational codes were presented to increase the readability and efficiency of the technique, such as PolyTop [9], which offers a general FE framework based on isoparametric polygonal finite elements integrated with a modular code structure for topology optimization. Indeed, taking advantage of this code organization, it was extended for multi-materials problems with PolyMat [10] and for dynamics with PolyDyna [11]. In addition, some examples [12, 13] leverage on pre-computation of element and global stiffness matrix by considering a discretion of all equal elements and same material in order to speed-up the problem resolution. Despite being computationally efficient for the problem addressed, these codes present memory allocation issues in Matlab for large-scale problems. The filtering sparse matrix also requires storing a large amount of memory. Another issue presented in these Matlab codes is associated with the solution of large linear systems of equations that arise from finite element analyses. Therefore, strategies to efficiently deal with large-scale problems have received increasing interest in the literature in the past few years. Indeed, a parallel framework for topology optimization PETSc [14] was proposed to solve fluids and solid mechanics problems integrated with the method of moving asymptotes (MMA). Amir et al. [15] proposed a multigrid preconditioned conjugate gradient (MGCG) solver to improve the computational performance for solving 3D structural topology optimization problems. To overcome the mentioned memory and performance limitations, we propose a framework based on plugins to handle large-scale structural topology optimization for multi-material problems. The proposed topology optimization approach is integrated into TopSim [16], a C++ software developed at Tecgraf/PUC-Rio for high-performance finite element analysis. Using plugins provides versatility in implementing different topology optimization features and allows for easy-to-extend existing codes. Here, we exploit the implementation of a multi-material formulation with a homogenization approach to optimize an assigned layout, selecting the optimal microstructures concurrently with the optimal macrostructural topology during the optimization process. The paper is organized as follows: Section 2 details the main features of topology optimization and its integration in a plugin-based framework, Section 3 outlines the main results and novelty aspect of the proposed implementation and finally Section

4 provides conclusions and future perspectives.

2 MATERIALS AND METHODS

The multi-material formulation for static linear elasticity topology optimization problem in a continuum setting is stated as follows:

$$\begin{aligned} \min_{\mathbf{z}} \quad & C(\mathbf{z}) = \mathbf{U}^T \mathbf{K}(\mathbf{z})\, \mathbf{U} \\ \text{s.t.} \quad & g_j - \overline{V}_j \leq 0,\ j = 1, ..., N^c \\ & 0 \leq z_e^m \leq 1,\ e = 1, ..., N^e,\ m = 1, ..., N^m \\ \text{with:} \quad & \mathbf{K}(\mathbf{z})\, \mathbf{U}(\mathbf{z}) = \mathbf{F} \\ & \overline{\mathbf{z}} = \mathcal{P}\mathbf{z} \end{aligned} \tag{1}$$

where the volume constraints $g_j = \sum_{m \in \mathcal{G}_j} \sum_{\ell \in \mathcal{E}_j} V_\ell m_v(y_{\ell m}) / \sum_{\ell \in \mathcal{E}_j} V_\ell$ are defined through the element densities, z_e^m, evaluated in the element centroids. The constraints, $j = 1, ..., N_c$, where N_c is the total number of constraints, are controlled by the element, $\mathcal{E}$, and the material $\mathcal{G}$ index, which allows to define global and local constraints subdividing regions of the design space to provide flexibility to the designer. The optimization is density-based [17], where the discretized design domain is associated with the optimized design variable. This method is combined with the classical theory of homogenization [18], which allows a multi-material formulation to handle both isotropic and anisotropic materials, as depicted in Figure 1.

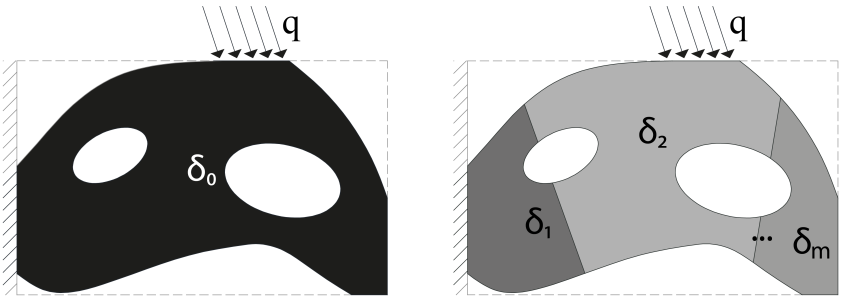

Figure 1 Conceptual illustration of material distribution shaping the optimal layout with single (a) and multi-material (b) formulation. The optimal layout is depicted with the extended design domain and boundary conditions.

The material properties are provided to the iterative process by defining the homogenized material density matrix C_m^H. The iterations are performed using a gradient-based method alternating design variable update and finite element analysis (FEA). It consists of an Eulerian approach, allowing the non-re-mesh at each iteration to take account of new boundaries between materials and voids. An issue with the topology optimization problem is that the solution is not unique, i.e., by increasing the mesh refinement, the objective function decreases, meaning that the problem is not well-posed and is mesh-dependent. However, this problem can be overcome by introducing a density filter. The filter represents a convolution factor over the design variable z, which allows the control of the minimum length scale of the optimal topology by defining a weighting function:

$$\mathbf{P}_{i,j} = \frac{p(i,j)A_j}{\sum_{k=1}^{N} p(i,k)A_k} \qquad (2)$$
$$p(i,j) = max\{0, [r_{min} - dist(i,j]^q\}$$

where the distance $p(i,j)$ is computed over the neighborhood centroids of elements (i,j) in a user-defined radius r_{min} by the operator $dist(i,j)$. The order of the filter is computed according to the user-defined parameter q, where for two-dimensional problems a cone convolution is preferred by setting a linear filter $q = 1$, but quadratic ($q = 2$) and cubic ($q = 3$) can be used. The filtered design variable y is calculated by applying the filter $\mathbf{P}_{ij}$ to the design variables z. In this work, the filter is calculated efficiently using recursion, a technique for making a function call itself. Figure 2 illustrates the implemented filtering technique.

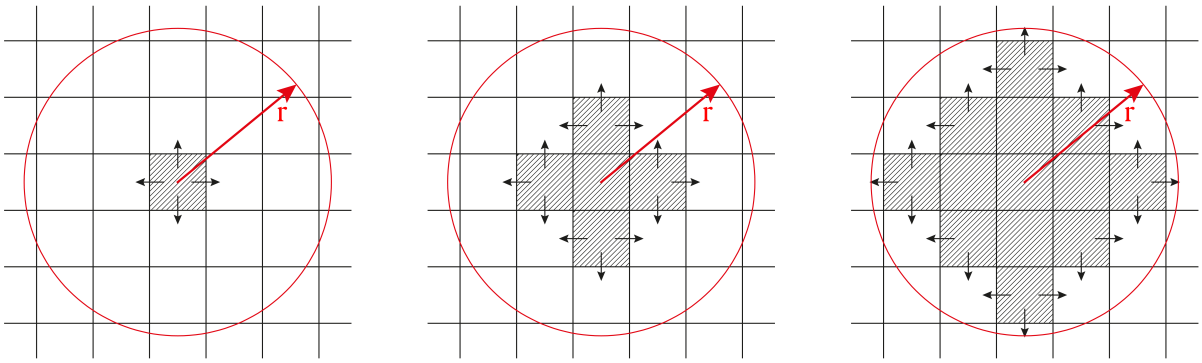

Figure 2 Filtering technique of design variables.

In particular, this work proposes a different strategy to compute the filter, which is particularly expensive to implement, as suggested by the educational code PolyTop [9]. Indeed, a loop for every element [9] to compute the distance to the other elements in the mesh is performed in order of $O(n)$ and, once the vector holding all distances is obtained, a sort is performed in order of $O(n\log(n))$. Therefore, the entire algorithm has order of $O(n^2\log(n))$. The proposed implementation allows for reducing the order, where the built-in sort algorithm is performed only once by Tops [22], with an order of $O(n\log(n))$, and, using the recursion, the total algorithm order remains $O(n)$. It is a density filter and represents a restriction method for SIMP problem, which is a common technique used to reduce mesh-dependency and the topology optimization problem to be well-posed. In addition, filtering technique allows to address well-known problem in topology optimization, such as checkerboard patterns. In addition, it works as convolution operator over design variables, providing density continuity in the design space and a minimum-length control in the optimal layout, which is particularly useful for additive manufacturing applications. In particular, the design variables are penalized by a modified SIMP (Solid Isotropic Material Penalization) method, which enforces the solution to a 0/1 pattern, while the voids are modeled as an Ersatz material. The multi-material framework is tailored by a multi-material interpolation scheme [10], which is derived from interpolation scheme of discrete systems (DMO) [19, 20]:

$$\mathbf{K} = \sum_{m=1}^{N^m} w_{em} \prod_{\substack{p=1 \\ p \neq m}}^{N^m} (1 - \gamma w_{ep}) \mathbf{K}_m^H, \; e = 1, ..., N^e \tag{3}$$

where the parameter γ handles the mixing of materials in the continuation scheme, starting from a convex formulation (i.e., p=1 and γ=0) without mixing for $\gamma = 0$ to a non-convex optimization by increasing the penalization and mixing parameters. Then, the design variables $w_i^e = 1$ and $w_{j \neq i}^e = 0 \; \forall e$ are updated with the Optimality Criteria (OC) [1] for two-phase topology optimization problems, while to accommodate multiple materials and constraints the Zhang-Paulino-Ramos (ZPR) update scheme [21] is adopted, which is a sequential linear programming (SLP) technique. The presented multi-material topology optimization framework has been implemented and integrated into TopSim. The plugin framework for multi-material optimization is shown in Figure 3.

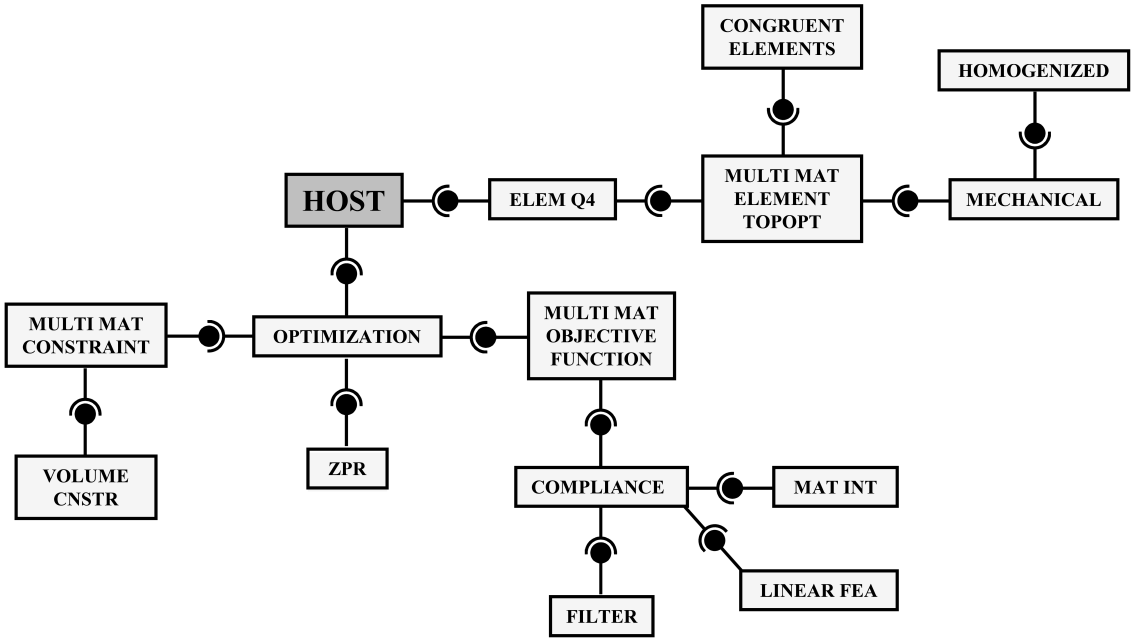

Figure 3 Plugin-based framework for multi-material topology optimization with 4-noded quadrilateral elements and ZPR update scheme.

The approach allows the optimization of structures, including multiple materials with different stiffness properties. These features are included in the optimization process through the stiffness material matrix D_m^H calculated by the classical theory of homogenization [18]. This information is computed in the `"Homogenized"` plugin. The multi-material interpolation function, which is built inside the `"MultiMat Element TopOpt"` plugin, provides the local interpolated stiffness matrix [19] starting from the single-material stiffness material computed in `"Mechanical"`, which are calculated separately with the information located in `"Homogenized"`. The plugin `"Congruent elements"` provides information about identical elements. Then, in the `"Optimization"` plugin, the Topology Optimization is performed by computing the objective

function `"Compliance"` and the constraint function `"Volume Cnstr"` of the current problem. Finally, the design variables are updated by an update scheme, e.g., `"ZPR"`, which can be substituted with OC, GCMMA, MMA, and SDM under appropriate amendments.

3 RESULTS AND DISCUSSION

The numerical simulations are performed in static linear elasticity with Quad-4 (Q4) elements. The discretized space adopted for the FEA matches the design variable space. The example presented here is the Messerschmitt-Bölkow-Blohm (MBB) Beam, a well-known benchmark for topology optimization. Figure 4 depicts the geometry, loading, and boundary conditions. The problem is set dimensionless and solved on half of the domain by taking advantage of symmetry conditions. A distributed vertical load $q = 0.5$ is applied on a beam, with length $L = 3$ and height $H = 1$, for a length of $x = L/16$.

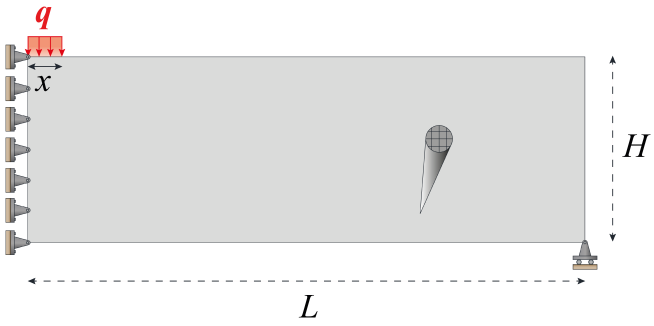

Figure 4 MBB Beam 2D Symmetric Domain with assigned boundary and load conditions.

The single and multi-material formulations have been tested as single isotropic material and homogenized multiple lattice microstructures. Figure 5 shows the microstructural shape and elastic surface.

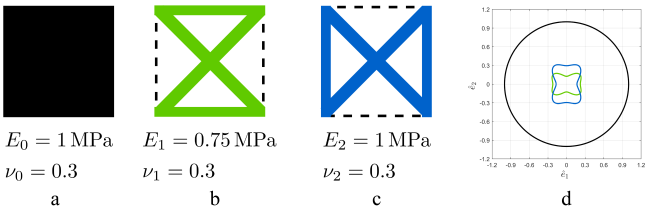

Figure 5 Microstructural material used in topology optimization: a) isotropic, b) and c) lattice microstructures, and d) homogenized elastic surfaces of assigned microstructures.

Two types of discretization have been adopted. We ran the first group of simulations with 30000 elements to investigate the local minimum achieved with different solvers and filter radii to the length scale of the optimal layout. Then, a fine mesh of 360000 elements is used to test the computational efficiency of the topology optimization algorithm. As update schemes, we adopted the OC and ZPR Update Scheme to address a single-material, see Figure 6, and a multi-material topology optimization problem, see Figure 7.

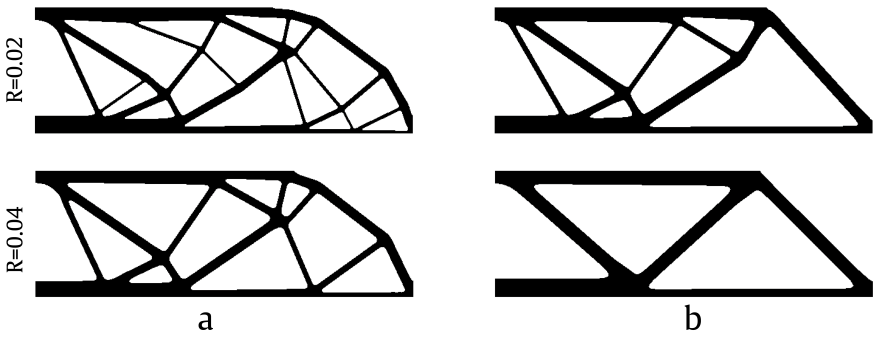

Figure 6 Numerical solution with single isotropic material: a) OC update scheme, b) ZPR update scheme.

The result for single-material is achieved using an isotropic material, as depicted in Figure 5b. Here, different update schemes and filter radii have been used to show the influence on the local minimum. Then, motivated by investigating the multi-material formulation, we considered two lattice microstructures with different stiffness properties oriented orthogonally.

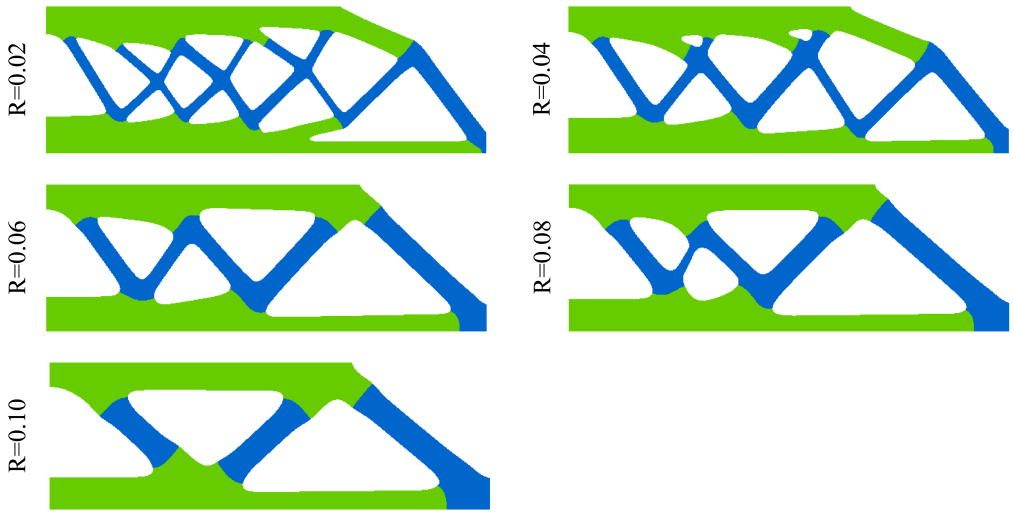

Figure 7 Numerical solution with multi-material applying different filter radii.

The solutions clearly show the density filter's influence on controlling the length scale and, consequently, the local minimum achieved. This first group of numerical simulations with 30000 elements has been solved with a direct FE solver. Then, we adopted a larger discretization of 360000 elements. In this case, we considered a single-material isotropic, and the solver adopted is the Preconditioned Conjugate Gradient (PCG), which allows the FEA to speed up. The numerical solutions are performed using a modified SIMP approach, and the optimization parameters are detailed in Table 1.
In the last numerical result presented here, the domain is discretized using 360000 elements, as illustrated in Figure 8.

Table 1 Numerical parameters for single-material (SM) and multi-material (MM) optimization with discretization of 30000 elements (30k) and 360000 elements (360k).

Parameter	Description	SM 30k	MM 30k	SM 360k
p	SIMP penalization factor	[1:0.5:4]	[1 1.5 2 3 4]	[1:0.5:4]
γ	MM weight penalization factor	[ ]	[0 0.2 0.5 0.8 1]	[ ]
q	Filter exponent	1	1	1
R	Filter radius	[0.02 0.04]	[0.02:0.02:0.10]	0.04
$move_{\text{OC}}$	OC move	0.2	[ ]	[ ]
η_{OC}	OC exponent	1/2	[ ]	[ ]
$move_{\text{ZPR}}$	ZPR move	0.2	0.2	0.2
η_{ZPR}	ZPR exponent	1/2	1/2	1/2
$\overline{v}$	Volume Fraction	0.3	0.3	0.3
max_{iter}	Maximum iterations	150	150	150
tol	Convergence tolerance	0.02	0.02	0.02

Figure 8 Numerical solution with single-material isotropic topology optimization.

Figure 9 shows the convergence of the objective function along the optimization iterations for each penalization factor.

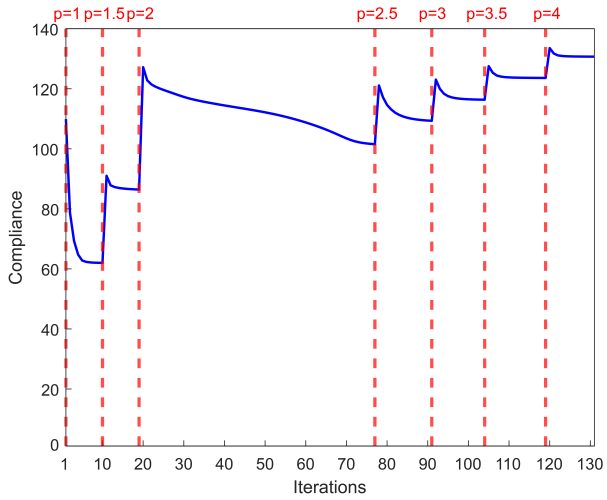

Figure 9 Convergence plot for single-material isotropic example using 360000 elements in the mesh.

4 CONCLUSIONS

In this work, we presented a general framework for topology optimization based on plugins, where a robust and efficient topology optimization formulation is embedded with high-performance finite element analysis (FEA) software. In addition, we showcased the algorithm's efficiency using a 2D benchmark numerical example with singular and multiple materials. We performed a simulation with a fine mesh to demonstrate the capabilities of the implemented plugins to face a high-resolution solution. Future works will focus on implementing a stress constraint formulation to handle structural problems, including materials failure limit and yield functions. Additionally, attention will be paid to the design freedom of the material design space, such as porosity and orientation.

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