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# Diverse Topology Optimization using Modulated Neural Fields

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## Abstract

Topology optimization (TO) is a family of computational methods that derive near-optimal geometries from formal problem descriptions. Despite their success, established TO methods are limited to generating single solutions, restricting the exploration of alternative designs. To address this limitation, we introduce *Topology Optimization using Modulated Neural Fields* (TOM) – a data-free method that trains a neural network to generate structurally compliant shapes and explores diverse solutions through an explicit diversity constraint. The network is trained with a solver-in-the-loop, optimizing the material distribution in each iteration. The trained model produces diverse shapes that closely adhere to the design requirements. We validate TOM on established 2D and 3D TO benchmark problems. Our results show that TOM generates more diverse solutions than any previous method, all while maintaining near-optimality and without relying on a dataset. These findings open new avenues for engineering and design, offering enhanced flexibility and innovation in structural optimization.<sup>1</sup>

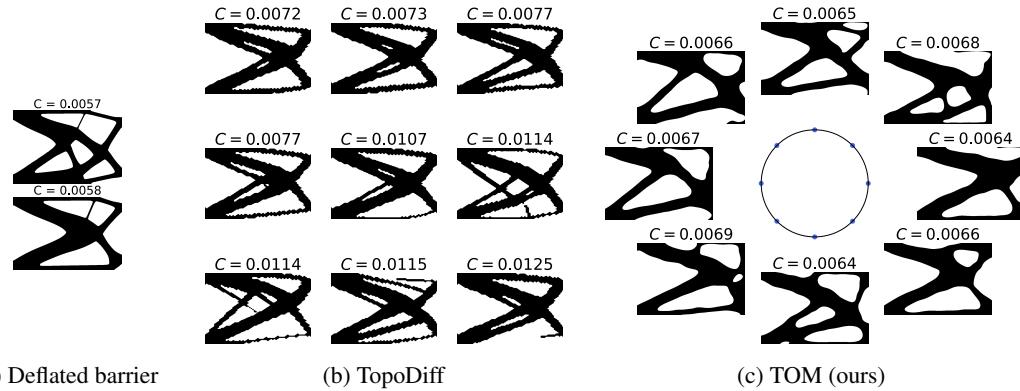


Figure 1: Solutions to the cantilever problem generated by three TO methods. (a) *Deflated barrier* – a classical TO method generating high-quality but few solutions. (b) *TopoDiff* – a data-driven diffusion model generating many, but low-quality solutions. (c) *TOM* – our modulated neural field trained with a solver-in-the-loop and a diversity constraint generating diverse near-optimal structures. Here, we use a circular modulation space to capture a smooth manifold of solutions. All methods minimize the structural compliance  $C$ , which measures the total displacement of the loaded shape.

<sup>1</sup>The code will be made public upon acceptance.

15 **1 Introduction**

16 Topology optimization (TO) is a computational design technique to determine the optimal material  
17 distribution within a given design space under prescribed boundary conditions. A common objective  
18 in TO is the minimization of structural compliance, which measures the displacement under load. Due  
19 to the non-convex nature of TO problems, these methods generally provide near-optimal solutions,  
20 with no guarantees of converging to global optima [1].

21 Traditional TO methods are limited to producing a single design. However, generating multiple diverse  
22 solutions is important to balance performance with other considerations, such as manufacturability,  
23 cost, and aesthetics. Therefore, we propose **Topology Optimization using Modulated Neural Fields**  
24 (TOM), an approach to generate diverse, near-optimal designs: A neural network parametrizes the  
25 shape representations and is trained to generate near-optimal solutions. The model is optimized using  
26 a solver-in-the-loop approach [43], where the neural network iteratively adjusts the design based on  
27 feedback from a physics-based solver.

28 To enhance the diversity of solutions, we introduce an explicit diversity constraint during training.  
29 TOM not only enables the generation of multiple, diverse designs but also leverages machine learning  
30 to explore the design space more efficiently than traditional TO methods [36].

31 Empirically, we validate our method on TO for linear elasticity problems in 2D and 3D. Our results  
32 demonstrate that TOM obtains more diverse solutions than prior work while being substantially faster  
33 and remaining near-optimal. This addresses a current limitation in TO and opens new avenues for  
34 automated engineering design.

35 Our main contributions are summarized as follows:

- 36 1. We introduce TOM, the first method for data-free, solver-in-the-loop neural network training,  
37 which generates diverse solutions adhering to structural requirements.
- 38 2. We introduce a novel diversity constraint variant for neural density fields based on the  
39 Chamfer discrepancy that ensures the generation of distinct and meaningful shapes and  
40 enhances the exploration of the designs.
- 41 3. Empirically, we demonstrate the efficacy and scalability of TOM on 2D and 3D prob-  
42 lems, showcasing its ability to generate a variety of near-optimal designs. Our approach  
43 significantly outperforms existing methods in terms of solution diversity.

44 **2 Background**

45 **2.1 Topology optimization**

46 TO is a computational method developed in the late 1980s to determine optimal structural geometries  
47 from mathematical formulations [6]. TO iteratively updates a material distribution within a design  
48 domain under specified loading and boundary conditions. Due to the non-convex nature of most  
49 TO problems, convergence to a global minimum is not guaranteed. Instead, the goal is to achieve a  
50 near-optimal solution, where the objective closely approximates the global optimum. There are four  
51 prominent method families widely recognized in TO. In this work, we focus on *SIMP* and refer the  
52 reader to Yago et al. [47] for a more detailed introduction.

53 **Solid isotropic material with penalization (SIMP)** is a prominent TO method we adapt for TOM.  
54 SIMP operates on a mesh with mesh points  $\mathbf{x}_i \in \mathcal{X}, i \in \{1, \dots, N\}$  in the design region. The aim  
55 is to find a binary density function at each mesh point  $\rho(\mathbf{x}_i) \in \{0, 1\}$ , where  $\rho(\mathbf{x}_i) = 0$  represents  
56 void and  $\rho(\mathbf{x}_i) = 1$  represents solid material. To make this formulation differentiable, the material  
57 density  $\rho$  is relaxed to continuous values in  $[0, 1]$ . A common objective of SIMP is to minimize the  
58 compliance  $C$ , a measure of deformation under load. The SIMP objective is then formulated as a  
59 constrained optimization problem:

$$\begin{aligned} \min : \quad & C(\rho) = \mathbf{u}^T \mathbf{K}_\rho \mathbf{u} \\ \text{s.t. :} \quad & V = \sum_{i=1}^N \rho_i v_i \leq V^* \\ & 0 \leq \rho_i \leq 1 \quad \forall i \in N \end{aligned} \tag{1}$$

60 where  $\mathbf{u}$  is the displacement vector,  $\mathbf{K}_\rho$  is the global stiffness matrix,  $V$  is the shape volume, and  
61  $V^*$  is the target volume. The density field is optimized iteratively. In each iteration, a finite element  
62 (FEM) solver computes the compliance and provides gradients to update the density field  $\rho$ . To  
63 encourage binary densities, intermediate values are penalized by raising  $\rho$  to the power  $p > 1$ . Hence,  
64 the stiffness matrix is defined as  $\mathbf{K}_\rho = \sum_{i=1}^N \rho_i^p \mathbf{K}_i$ , where  $\mathbf{K}_i$  describes the stiffness of solid cells  
65 and depends on material properties.

66 **TO for multiple solutions.** Generating multiple design alternatives for TO problems is crucial for  
67 many real-world engineering cases where single optima often don't exist. However, classical TO  
68 algorithms typically yield a single solution and do not ensure convergence to a global minimum.  
69 Papadopoulos et al. [32] introduce the deflated barrier (DB) method, an extension of the classical  
70 SIMP approach that can find multiple solutions. By employing a search strategy akin to depth-first  
71 search, DB identifies multiple solutions without relying on initial guess variations, thereby enhancing  
72 design diversity.

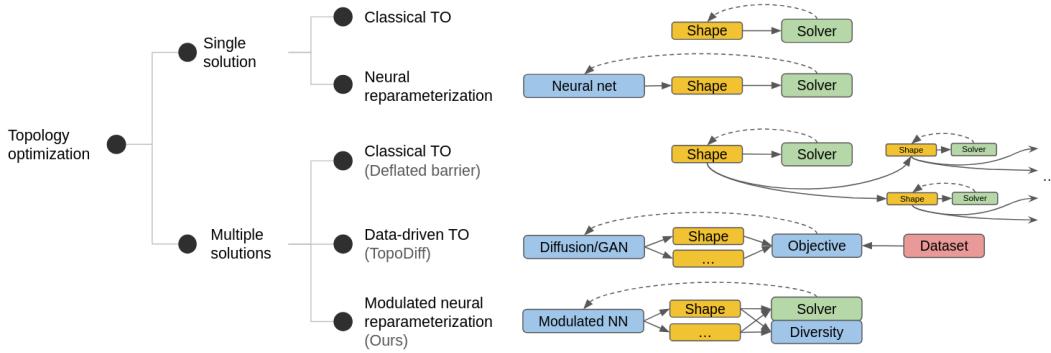


Figure 2: Taxonomy of classical and neural topology optimization methods. The dashed lines indicate iterative updates, such as gradient descent. TOM is the first data-free method to produce multiple shapes with a neural network.

## 73 2.2 Shape generation with neural networks

74 **Neural fields** offer a powerful framework for geometry processing, utilizing neural networks  
75 to model shapes implicitly. This approach enables high-quality and topologically flexible shape  
76 parameterizations [12]. The two prevalent methods for representing implicit shapes are signed  
77 distance functions (SDF) [33, 2] and density (or occupancy) [29] fields. We opt for the density  
78 representation due to its straightforward compatibility with SIMP optimization.

79 Given a  $d_x \in \{2, 3\}$  dimensional domain  $\mathcal{X} \subset \mathbb{R}^{d_x}$ , a neural density field employs a neural network  
80  $f_\theta : \mathcal{X} \rightarrow (0, 1)$  with parameters  $\theta$  to define the shape  $\Omega := \{x \in \mathcal{X} | f_\theta(x) \geq \tau\}$  as the  $\tau \in [0, 1]$   
81 super-level-set of  $f_\theta$ .

82 **Conditional neural fields.** While a neural density field represents a single shape, a *conditional*  
83 neural field represents a set of shapes with a single neural network [26]. Generally, one can condition  
84 on text, point clouds, or other modalities of interest [49]. In this work, we use a modulation code  
85  $\mathbf{z} \in \mathbb{R}^{d_z}$  as an additional input to the network. The resulting network  $f_\theta(\mathbf{x}, \mathbf{z})$  parametrizes a set of  
86 shapes. There are different ways to incorporate the modulation vector into the network, such as input  
87 concatenation [33], hypernetworks [17], or attention [35]. In this work, we use input concatenation,  
88 as it is simple and fast to train.

89 **Diversity constraint** can be used to modify the TO problem formulation (1) to facilitate the discovery  
90 of multiple solutions. The diversity constraint introduced in geometry-informed neural networks  
91 (GINNs) [8] defines a diversity measure  $\delta$  on the set of shapes  $\{\Omega_i\}$  as

$$\delta(\{\Omega_i\}) = \left( \sum_j \left[ \min_{k \neq j} d(\Omega_j, \Omega_k) \right]^{1/2} \right)^2. \quad (2)$$

92 This measure builds upon a chosen dissimilarity function  $d(\Omega_i, \Omega_j)$ . Essentially,  $\delta$  encourages  
93 diversity by maximizing the distance between each shape and its nearest neighbor.

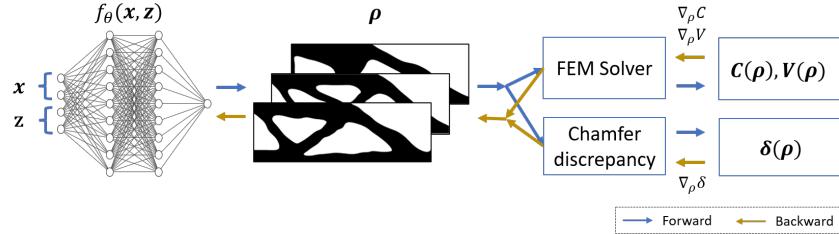


Figure 3: A single iteration of TOM trained with  $M = 3$  shapes in parallel. In each iteration, the input to the network consists of the mesh vertices  $\{\mathbf{x}_i\}_{i=1,\dots,N}$  and modulation vectors  $\{\mathbf{z}_j\}_{j=1,\dots,M}$ . The network outputs densities  $\rho_j$  at the vertices  $\mathbf{x}_i$  for each shape. The densities are passed to the FEM solver, which computes the compliances  $C_j$  and volumes  $V_j$ , as well as their gradients  $\nabla_\rho C_j$  and  $\nabla_\rho V_j$ . The diversity loss  $\delta(\rho)$  and its gradient  $\nabla_\rho \delta$  are based on the Chamfer discrepancy between the surface points of the shapes.

94 GINNs utilize a dissimilarity function on the shape boundary, but their approach is limited to signed  
 95 distances (SDFs). In Section 3.2, we show how to adapt the Chamfer discrepancy as a  
 96 dissimilarity function on density fields.

### 97 2.3 Topology optimization with neural networks

98 Figure 2 presents an overview of various TO methods that search for either single or multiple solutions,  
 99 further categorized by their use of neural networks.

100 **Neural reparameterization** uses a neural network to represent the material distribution in a  
 101 discretization-free manner. Existing work explores training a single shape by parametrizing the  
 102 material *density* [40, 9, 10, 18] or *boundary* [13], which is optimized with a solver-in-the-loop. NITO  
 103 [31] uses modulation of a neural field to introduce constraints on the boundary of a *single* shape.  
 104 NTopo [48] uses a conditional neural field to generate individual solutions for different topology  
 105 optimization problems, adapting to factors like target volume or force vector position. TOM, however,  
 106 finds multiple solutions, not just one per setting.

107 **Data-driven neural TO** uses a dataset of generated solutions to train neural networks that can  
 108 then generate diverse solutions. Most prior works use generative adversarial networks (GANs)  
 109 [16, 15, 44, 30]. Recent work showed the superiority of diffusion models for data-driven TO [25].  
 110 Data-driven methods require a large amount of compute to generate a dataset and train a large  
 111 generative model and aim to *amortize* these costs by fast inference on new, unseen problem settings.

## 112 3 Method

### 113 3.1 TO using modulated neural fields

114 **Definitions.** Let  $\mathcal{X} \subset \mathbb{R}^{d_x}$  be the domain of interest in which there is a shape  $\Omega \subset \mathcal{X}$ . Let  $\mathcal{Z} \subset \mathbb{R}^{d_z}$   
 115 be a discrete or continuous modulation space, where each  $\mathbf{z} \in \mathcal{Z}$  parametrizes a shape  $\Omega_{\mathbf{z}}$ . The  
 116 possibly infinite set of all shapes is denoted by  $\Omega_{\mathcal{Z}} = \{\Omega_{\mathbf{z}} | \mathbf{z} \in \mathcal{Z}\}$ . The modulation vectors  $\{\mathbf{z}_i\}$  are  
 117 sampled according to a probability distribution  $p(\mathcal{Z})$ .

118 For density representations a shape  $\Omega_{\mathbf{z}}$  is defined as the set of points with a density greater than  
 119 the level  $\tau \in [0, 1]$ , formally  $\Omega_{\mathbf{z}} = \{\mathbf{x} \in \mathcal{X} \mid \rho_{\mathbf{z}}(\mathbf{x}) > \tau\}$ . While some prior work on occupancy  
 120 networks [28] treats  $\tau$  as a tunable hyperparameter, we follow Jia et al. [19] and fix the level at  
 121  $\tau = 0.5$ . We model the density  $\rho_{\mathbf{z}}(\mathbf{x}) = f_{\theta}(\mathbf{x}, \mathbf{z})$ , corresponding to the modulation vector  $\mathbf{z}$  at a  
 122 point  $\mathbf{x}$  using a neural network  $f_{\theta}$ , with  $\theta$  being the learnable parameters.

123 **TO using modulated neural fields.** Our approach, akin to standard SIMP, formulates a constrained  
 124 optimization problem aiming to minimize an objective function for multiple shapes simultaneously,  
 125 while adhering to a volume constraint for each shape. Central to our method is the introduction  
 126 of a diversity constraint, denoted as  $\delta(\Omega_{\mathcal{Z}})$ , which is defined over multiple shapes to reduce their  
 127 similarity. This leads to the following constrained optimization problem:

$$\begin{aligned}
\text{min : } & \mathbb{E}_{\mathbf{z} \sim p(\mathcal{Z})} [C(\rho_{\mathbf{z}})] \\
\text{s.t. : } & V_{\mathbf{z}} = \int_{\mathcal{X}} \rho_{\mathbf{z}}(\mathbf{x}) d\mathbf{x} \leq V^* \\
& 0 \leq \rho_{\mathbf{z}}(\mathbf{x}) \leq 1 \quad \delta^* \leq \delta(\Omega_{\mathcal{Z}})
\end{aligned} \tag{3}$$

128 where  $V^*$  and  $\delta^*$  are target volumes and diversities, respectively. TOM updates the density fields of  
129 multiple shapes iteratively. In each iteration, the density distribution of each shape is computed and  
130 the resulting densities are passed to the FEM solver. The FEM solver calculates the compliance loss  
131  $C$  and gradients  $\nabla C$ . To accelerate the computation, parallelization of the FEM solver is employed  
132 across multiple CPU cores, with a separate process dedicated to each shape.  
133 The diversity loss and its gradient are computed on the GPU using PyTorch [34], along with any  
134 optional geometric losses similar to GINNs.  
135 We use the adaptive augmented Lagrangian method (ALM) [4] to automatically balance multiple loss  
136 terms. Additionally, we gradually increase the sharpness parameter  $\beta$  of the Heaviside filter (Equation  
137 14), which acts as annealing. The complete TOM method is concisely presented in Algorithm 1.

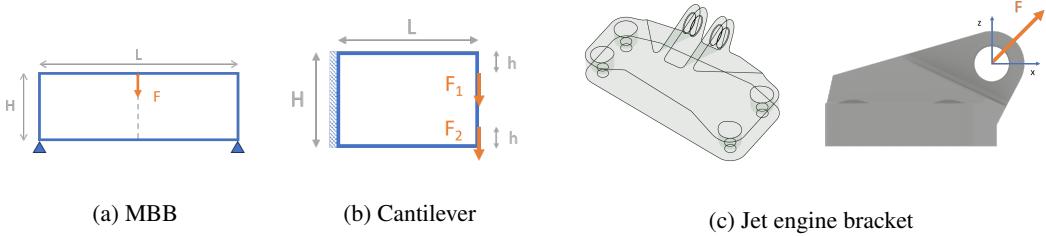


Figure 4: Three benchmark problem definitions. (a) *MBB*: The boundary is fixed at the attachment points at the bottom left and right corners. The dotted line indicates the symmetry axis at  $\frac{L}{2}$  where the force  $F$  is applied. (b) *Cantilever*: Forces  $F_1, F_2$  are applied at distance  $h$  from the upper and lower boundaries. The left boundary is fixed. (c) *Jet engine bracket*. Left: Available design region with six cylindrical interfaces where the shape must attach. Right: A diagonal force is applied at the two central interfaces. The bracket is fixed at the four side interfaces.

### 138 3.2 Diversity

139 The diversity loss, defined in Equation 2, requires the definition of a pairwise dissimilarity measure  
140 between shapes. GINNs [8] use boundary dissimilarity, which is easily optimized for SDFs since  
141 the value at a point is the distance to the zero level set. However, this dissimilarity measure does not  
142 apply to our density field shape representation. Hence, we propose a boundary dissimilarity based on  
143 the chamfer discrepancy.

144 **Diversity via differentiable chamfer discrepancy.** To define the dissimilarity on the boundaries of  
145 a pair of shapes  $(\partial\Omega_1, \partial\Omega_2)$ , we use the one-sided chamfer discrepancy (CD):

$$CD(\partial\Omega_1, \partial\Omega_2) = \frac{1}{|\partial\Omega_1|} \sum_{x \in \partial\Omega_1} \min_{\tilde{x} \in \partial\Omega_2} \|x - \tilde{x}\|_2 \tag{4}$$

146 To use the CD as a loss, it must be differentiable w.r.t. the network parameters  $\theta$ . However, the  
147 chamfer discrepancy  $CD(\partial\Omega_1, \partial\Omega_2)$  depends only on the boundary points  $x_i \in \partial\Omega$  which only  
148 depend on  $f_\theta(x_i)$  implicitly. Akin to prior work [11, 7, 27], we apply the chain rule and use the  
149 level-set equation to derive

$$\frac{\partial CD}{\partial \theta} = \frac{\partial CD}{\partial x} \frac{\partial x}{\partial y} \frac{\partial y}{\partial \theta} = \frac{\partial CD}{\partial x} \frac{\nabla_x f_\theta}{|\nabla_x f_\theta|^2} \frac{\partial y}{\partial \theta} \tag{5}$$

150 where  $y = \rho$  is the density field in our case. We detail this derivation in Appendix C.3. Finding  
151 surface points on density fields is substantially harder than for SDFs, as there is no reliable gradient  
152 information to exploit for root finding. Therefore, we employ a robust algorithm detailed in Algorithm  
153 2.

154 **Geometric constraints** We utilize geometric constraints similar to GINNs, leveraging the continuous  
 155 field representation to learn finer details, particularly at interfaces. Further details are provided in  
 156 Table 5 and Appendix B.

157 **4 Experiments**

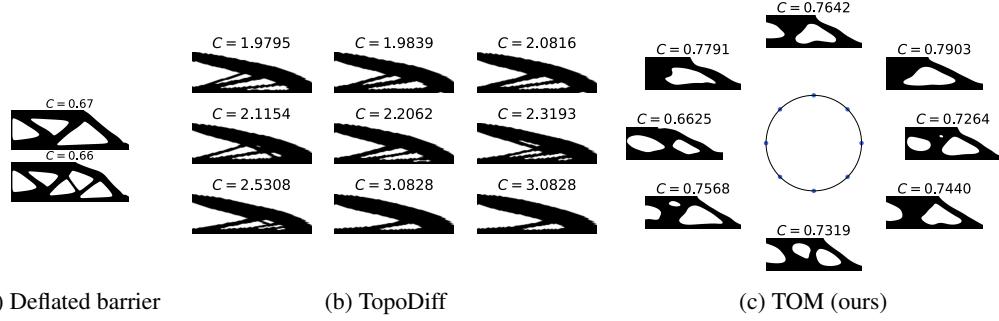


Figure 5: Solutions to the *MBB beam* problem generated by three TO methods.

158 We solve three standard TO benchmark problems comparing TOM to established classical and  
 159 data-driven methods. For all our TOM experiments, we employ the WIRE architecture [37], which  
 160 uses wavelets as activation functions. This imposes an inductive bias towards high frequencies,  
 161 while being more localized than, e.g., a sine activation [39]. We use a 2-dimensional modulation  
 162 space and sample vectors uniformly on a circle with radius  $r$ . We denote a circle centered at the  
 163 origin with radius  $r$  as the 1-sphere  $\mathcal{S}^1(r) = \{\mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x}\| = r\}$ . This 1D manifold embedded in  
 164 the 2D modulation space assures that modulation vectors are sufficiently far apart from each other  
 165 to avoid mode collapse. The radius controls the initial diversity of the shapes and is an important  
 166 hyperparameter to tune (see also Appendix A.6). At each iteration, the number of shapes  $M$  is either  
 167 9 or 25, depending on the problem. For further experimental details, see Appendix A.

168 **4.1 Problem definitions**

169 We apply our method to common linear elasticity problems [38, 19] in two and three dimensions,  
 170 namely the Messerschmitt-Bölkow-Blohm (MBB) beam, the cantilever beam, and the jet engine  
 171 bracket. Due to the symmetry of the MBB beam, we follow Papadopoulos et al. [32] and optimize  
 172 only the right half. More details and descriptions are provided in Figure 4 and Appendix D.1.

173 **4.2 Baselines**

174 The experiments compare TOM with state-of-the-art classical and data-driven approaches (see Figure  
 175 2). As previously introduced, the standard method for single shape TO is SIMP [6], for which we use  
 176 the FeniTop implementation [19] – a well-documented Python wrapper of the standard open-source  
 177 FEniCS FEM solver [3].

178 **Deflated barrier** (DB) method [32] is the state-of-the-art method for finding multiple solutions to  
 179 TO problems. DB is a sequential algorithm that cannot perform multiple solver steps in parallel. For  
 180 the jet engine bracket, a comparison to DB is omitted, given DB’s slow performance, complexity, and  
 181 hyperparameter sensitivity.

182 **TopoDiff** [25] is a state-of-the-art data-driven TO solver. It is a diffusion model trained on 33,000 TO  
 183 problem-solution pairs, discretized as  $64 \times 64$  images. Similar to DB, we could not apply TopoDiff  
 184 to the 3D benchmark problem, since neither a pretrained model nor a sufficiently large 3D TO dataset  
 185 is publicly available.

186 **4.3 Metrics**

187 **Quality.** To evaluate structural characteristics, we report compliance  $C$  and volume  $V$ . We compute  
 188 them using the open-source numerical library FEniCS [3]. For each problem, we use the same high-  
 189 resolution mesh across all methods to compute the evaluation metrics. This minimizes discretization

190 errors and prevents numerical artifacts due to the mesh dependency of the solver. Following Mazé  
 191 and Ahmed [25], we also compute the *load violation*  $LV : \Omega \mapsto \{0, 1\}$  for each solution  $\Omega$ .  $LV = 1$   
 192 only when the shape lacks material where the load is applied, resulting in high compliance.

193 **Diversity.** As a diversity measure, we use the Hill numbers  $D_q(S)$ ,  $q \in \mathbb{R}$  over a set  $S$  as introduced  
 194 by Leinster [24]. For  $q = 2$ , the Hill number corresponds to the expected dissimilarity if two  
 195 elements of a set are sampled with replacement. As a dissimilarity metric we choose the Wasserstein  
 196 distance, as it is a mathematically well-defined distance between distributions. In particular, we  
 197 use the sliced-1 Wasserstein distance approximation, a computationally cheap implementation [14].  
 198 Hence, computing the Hill number  $D_2(\Omega_{\mathcal{Z}})$  corresponds to computing the expected Wasserstein  
 199 distance:

$$\mathbb{E}[W_1] := \mathbb{E}_{\mathbf{z}_i, \mathbf{z}_j \sim p(\mathcal{Z})} [W_1(\Omega_{\mathbf{z}_i}, \Omega_{\mathbf{z}_j})]. \quad (6)$$

200 **Computational cost.** We report the wall clock time in Table 1, to give a sense of the practicality  
 201 of running each method. Additionally, we further characterize the computational cost of different  
 202 methods in Table 2.

203 **4.4 Results**

Table 1: Results on the three benchmark problems.  $C$  is the compliance.  $LVR$  is the ratio of  
 load-violating solutions. As these always result in high compliance, results marked with a \* report  
 statistics after filtering such solutions.  $V$  is the mean ( $\pm$  standard deviation) of the volumes as  
 a fraction of the available volume.  $E(W_1)$  quantifies the diversity as the expected Wasserstein-1  
 distance between solutions.  $N$  is the number of solutions for methods that produce a finite number  
 of samples. TopoDiff and TOM produce a continuous distribution that can be sampled. Last is the  
 wall-clock time to run the methods. Table 2 contains further computational characterization.

Problem	Method	$C \downarrow$	$\min(C)$	$\max(C)$	$LVR[\%] \downarrow$	$V[\%]$	$\mathbb{E}(W_1) \uparrow$	$N \uparrow$	Time[min] $\downarrow$
MBB						53.5	$\times 10^{-2}$		
	FeniTop	0.68			0	53.49	0	1	2
	DB	$0.67 \pm 0.01$	0.66	0.67	0	$53.49 \pm 0.00$	1.36	2	55.5
	TopoDiff	$2.29 \pm 0.37$	1.79	3.43	0	$51.83 \pm 0.59$	2.14		
	TOM	$0.75 \pm 0.03$	0.66	0.83	0	$55.08 \pm 1.04$	4.23		6.1
Cantilever						50.00	$\times 10^{-2}$		
	FeniTop	0.59			0	49.91	0	1	4
	DB	$0.58 \pm 0.01$	0.57	0.58	0	$49.98 \pm 0.00$	1.01	2	123
	TopoDiff*	$1.19 \pm 0.28$	0.72	1.95	87	$50.23 \pm 0.70$	2.15		
	TOM*	$0.69 \pm 0.13$	0.64	1.27	8	$49.21 \pm 0.48$	2.42		29
Bracket						7.00	$\times 10^{-2}$		
	FeniTop	0.99			0	7.16	0	1	187
	TOM	$1.31 \pm 0.01$	1.07	1.54	0	$6.86 \pm 0.09$	0.15		47

204 The quantitative results of our experiments are summarized in Table 1. Qualitatively, we show  
 205 different results in Figures 1, 5, and 6. Further quantitative and qualitative results are shown in  
 206 Appendix A.6.

207 **TOM has high quality and diversity.** Across all experiments, TOM finds diverse solutions with a  
 208 near-optimal compliance. DB has better compliance but a substantially lower diversity with a low  
 209 number of solutions ( $N = 2$ ). TopoDiff solutions are similarly diverse, but have poor compliance.  
 210 For the cantilever, we filtered  $LVR = 87\%$  of TopoDiff outputs due to load violations, whereas for  
 211 TOM 8%. Surprisingly, the high LVR of TopoDiff contradicts the  $LVR = 0\%$  reported by Mazé  
 212 and Ahmed [25]. We attribute this to the cantilever being out of distribution of TopoDiff’s training  
 213 dataset.

214 **TOM outperforms TopoDiff.** At a first glance, the TopoDiff results in Figure 1 (b) may appear visually  
 215 appealing – the shapes exhibit thin features and horizontal symmetry. However, the quantitative  
 216 examination reveals that TopoDiff produces shapes with poor compliance and high LVR, as discussed  
 217 further in Appendix A.5. In contrast, TOM achieves lower compliance, lower LVR, and greater  
 218 diversity. It is also data-free, eliminating the need for an expensive pretraining dataset. Furthermore,  
 219 TopoDiff requires around 9 seconds for inference. Although training time is not reported, it is  
 220 expected to be significantly higher due to the complex architecture, conditioning and data, as well as  
 221 training across problem instances, limiting the direct comparability of speed.

222 **TopoDiff does not amortize.** Despite being trained on 30,000 designs, TopoDiff fails to generate  
223 compliant shapes on standard TO benchmark problems. These results align with prior work Woldseth  
224 et al. [46], finding large shortcomings of purely data-driven methods.

225 **TOM is more diverse and faster than DB.** While the  
226 classical DB demonstrates higher compliance, TOM con-  
227 sistently outperforms DB in terms of diversity and wall-  
228 clock time, albeit with an increased number of solver  
229 steps. This performance advantage is primarily due  
230 to TOM’s parallel nature, contrasting with the funda-  
231 mentally sequential algorithm of DB. Additionally, the  
232 slower wall-clock time of DB can be partially attributed  
233 to its public implementation, which involves mesh re-  
234 finement during training, thereby increasing the runtime  
235 for each solver step.

236 **TOM learns a continuous space of shapes.** Due to  
237 its modulated neural field architecture, TOM enables  
238 exploring different near-optimal solutions by moving  
239 continuously in the modulation space.

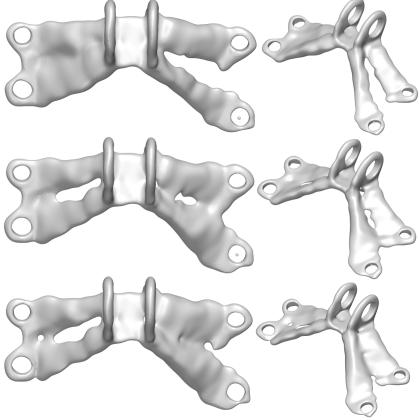
240 **TOM has surface undulations.** Qualitatively, we  
241 observe, e.g., in Figure 6, that shapes produced by  
242 TOM are wavier than DB or TopoDiff and can contain  
243 floaters (small disconnected components). Undulations  
244 and floaters are a common problem in neural TO ap-  
245 proaches [25, 30] and can be corrected with simple post-  
246 processing [41], which we demonstrate in Appendix  
247 D.3.

248 **Ablations.** We perform ablations to distill the impact of the diversity constraint, the radius of  
249 the modulation space, the SIMP penalty  $p$ , and annealing of the Heaviside filter. We find that all  
250 these components are necessary for TOM to work. Additionally, we show results for two alternative  
251 diversity metrics and demonstrate that they lead to similar conclusions. Furthermore, we ablate the  
252 uniform sampling on the circle with fixed modulation vectors. We find that this variant also leads to  
253 satisfactory results. The details are provided in Appendix A.6.

## 254 5 Conclusion

255 This paper presents topology optimization using modulated neural fields (TOM), a novel approach  
256 that addresses a limitation in traditional TO methods. By leveraging neural networks to parameterize  
257 shapes and enforcing solution diversity as an explicit constraint, TOM enables the exploration of  
258 multiple near-optimal designs. This is crucial for industrial applications, where manufacturing or  
259 aesthetic constraints often necessitate the selection of alternative designs. Our empirical results  
260 demonstrate that TOM is both effective and scalable, generating more diverse solutions than prior  
261 methods while adhering to mechanical requirements. This work opens new avenues for generative  
262 design approaches that do not rely on large datasets, addressing current limitations in engineering  
263 and design.

264 **Limitations and future work.** While TOM shows notable progress, several areas warrant further  
265 investigation to fully realize its potential. Future research could explore extending the one-dimensional  
266 modulation manifold into higher dimensions, allowing multi-axis design exploration. Notably, the  
267 mitigation of floaters and undulations requires more in-depth investigation. Additionally, more  
268 research is needed to explore different dissimilarity metrics for the diversity loss, as this could further  
269 enhance the variety of generated designs. Improving sample efficiency is also crucial for practical  
270 applications, as the current method may require significant computational resources. Promising  
271 directions include using second-order optimizers [20]. Lastly, future work could train TOM on coarse  
272 designs and subsequently refine them with classical TO methods, combining the strengths of both  
273 approaches to achieve even better results.



254 Figure 6: Three different jet engine bracket designs generated by TOM. Left: top view.  
255 Right: isometric view. Notably, all three generated designs show a similar low compliance as the single solution by the Fen-  
256 iTop baseline. These explored solutions can be further refined and post-processed by a classical pipeline.

274 **References**

275 [1] Grégoire Allaire, Charles Dapogny, and François Jouve. Shape and topology optimization. In  
276 *Handbook of numerical analysis*, volume 22, pages 1–132. Elsevier, 2021.

277 [2] Matan Atzmon and Yaron Lipman. SAL: Sign agnostic learning of shapes from raw data. In  
278 *IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, June 2020.

279 [3] Igor A. Baratta, Joseph P. Dean, Jørgen S. Dokken, Michal Habera, Jack S. Hale, Chris N.  
280 Richardson, Marie E. Rognes, Matthew W. Scroggs, Nathan Sime, and Garth N. Wells.  
281 DOLFINx: the next generation FEniCS problem solving environment. *preprint*, 2023. doi:  
282 10.5281/zenodo.1044766.

283 [4] Shamsulhaq Basir and Inanc Senocak. An adaptive augmented lagrangian method for training  
284 physics and equality constrained artificial neural networks. *arXiv preprint arXiv:2306.04904*,  
285 2023.

286 [5] Shamsulhaq Basir and Inanc Senocak. An adaptive augmented lagrangian method for training  
287 physics and equality constrained artificial neural networks. *arXiv preprint arXiv:2306.04904*,  
288 2023.

289 [6] Martin Philip Bendsøe and Noboru Kikuchi. Generating optimal topologies in structural design  
290 using a homogenization method. *Computer Methods in Applied Mechanics and Engineering*,  
291 71(2):197–224, 1988. ISSN 0045-7825. doi: [https://doi.org/10.1016/0045-7825\(88\)90086-2](https://doi.org/10.1016/0045-7825(88)90086-2).

292 [7] Arturs Berzins, Moritz Ibing, and Leif Kobbelt. Neural implicit shape editing using boundary  
293 sensitivity. In *The Eleventh International Conference on Learning Representations*. OpenRe-  
294 view.net, 2023.

295 [8] Arturs Berzins, Andreas Radler, Eric Volkmann, Sebastian Sanokowski, Sepp Hochreiter, and  
296 Johannes Brandstetter. Geometry-informed neural networks. *arXiv preprint arXiv:2402.14009*,  
297 2024.

298 [9] Mariusz Bujny, Nikola Aulig, Markus Olhofer, and Fabian Dудdeck. Learning-based topology  
299 variation in evolutionary level set topology optimization. In *Proceedings of the Genetic and  
300 Evolutionary Computation Conference, GECCO '18*, page 825–832, New York, NY, USA, 2018.  
301 Association for Computing Machinery. ISBN 9781450356183. doi: 10.1145/3205455.3205528.

302 [10] Aaditya Chandrasekhar and Krishnan Suresh. TOuNN: Topology optimization using neural  
303 networks. *Structural and Multidisciplinary Optimization*, 63(3):1135–1149, Mar 2021. ISSN  
304 1615-1488.

305 [11] Siqi Chen, Guillaume Charpiat, and Richard J Radke. Converting level set gradients to shape  
306 gradients. In *Computer Vision–ECCV 2010: 11th European Conference on Computer Vision,  
307 Heraklion, Crete, Greece, September 5–11, 2010, Proceedings, Part V 11*, pages 715–728.  
308 Springer, 2010.

309 [12] Zhiqin Chen and Hao Zhang. Learning implicit fields for generative shape modeling. In  
310 *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages  
311 5939–5948, 2019.

312 [13] Hao Deng and Albert C To. A parametric level set method for topology optimization based on  
313 deep neural network. *Journal of Mechanical Design*, 143(9):091702, 2021.

314 [14] Rémi Flamary, Nicolas Courty, Alexandre Gramfort, Mokhtar Z Alaya, Aurélie Boisbunon,  
315 Stanislas Chambon, Laetitia Chapel, Adrien Corenflos, Kilian Fatras, Nemo Fournier, et al. Pot:  
316 Python optimal transport. *Journal of Machine Learning Research*, 22(78):1–8, 2021.

317 [15] Michael Gillhofer, Hubert Ramsauer, Johannes Brandstetter, Bernhard Schäfl, and Sepp Hochre-  
318 iter. A gan based solver of black-box inverse problems. In *NeurIPS 2019 Workshop on Solving  
319 Inverse Problems with Deep Networks*, 2019.

320 [16] Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil  
321 Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial networks. *Communications  
322 of the ACM*, 63(11):139–144, 2020.

323 [17] David Ha, Andrew M. Dai, and Quoc V. Le. HyperNetworks. In *5th International Conference  
324 on Learning Representations, ICLR 2017*. OpenReview.net, 2017.

325 [18] Stephan Hoyer, Jascha Sohl-Dickstein, and Sam Greydanus. Neural reparameterization improves  
326 structural optimization. *arXiv preprint arXiv:1909.04240*, 2019.

327 [19] Yingqi Jia, Chao Wang, and Xiaojia Shelly Zhang. Fenitop: a simple fenicsx implementation for  
 328 2d and 3d topology optimization supporting parallel computing. *Structural and Multidisciplinary  
 329 Optimization*, 67(8):140, 2024.

330 [20] Anas Jnini, Flavio Vella, and Marius Zeinhofer. Gauss-newton natural gradient descent for  
 331 physics-informed computational fluid dynamics. *arXiv preprint arXiv:2402.10680*, 2024.

332 [21] Kaspar Kiis, Jared Wolfe, Gregg Wilson, David Abbott, and William Carter.  
 333 Ge jet engine bracket challenge. [https://grabcad.com/challenges/  
 334 ge-jet-engine-bracket-challenge](https://grabcad.com/challenges/ge-jet-engine-bracket-challenge), 2013. Accessed: 2024-05-22.

335 [22] Scott Kirkpatrick, C Daniel Gelatt Jr, and Mario P Vecchi. Optimization by simulated annealing.  
 336 *science*, 220(4598):671–680, 1983.

337 [23] Boyan Stefanov Lazarov and Ole Sigmund. Filters in topology optimization based on helmholtz-  
 338 type differential equations. *International journal for numerical methods in engineering*, 86(6):  
 339 765–781, 2011.

340 [24] Tom Leinster. *Entropy and diversity: the axiomatic approach*. Cambridge university press,  
 341 2021.

342 [25] François Mazé and Faez Ahmed. Diffusion models beat gans on topology optimization. In  
 343 *Proceedings of the AAAI Conference on Artificial Intelligence*, 2023.

344 [26] I. Mehta, M. Gharbi, C. Barnes, E. Shechtman, R. Ramamoorthi, and M. Chandraker. Modulated  
 345 periodic activations for generalizable local functional representations. In *2021 IEEE/CVF  
 346 International Conference on Computer Vision (ICCV)*, pages 14194–14203, Los Alamitos, CA,  
 347 USA, oct 2021. IEEE Computer Society.

348 [27] Ishit Mehta, Manmohan Chandraker, and Ravi Ramamoorthi. A level set theory for neural  
 349 implicit evolution under explicit flows. In *European Conference on Computer Vision*, pages  
 350 711–729. Springer, 2022.

351 [28] Lars Mescheder, Michael Oechsle, Michael Niemeyer, Sebastian Nowozin, and Andreas Geiger.  
 352 Occupancy networks: Learning 3d reconstruction in function space. In *Proceedings IEEE Conf.  
 353 on Computer Vision and Pattern Recognition (CVPR)*, 2019.

354 [29] Lars Mescheder, Michael Oechsle, Michael Niemeyer, Sebastian Nowozin, and Andreas Geiger.  
 355 Occupancy networks: Learning 3d reconstruction in function space. In *Proceedings of the  
 356 IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 4460–4470, 2019.

357 [30] Zhenguo Nie, Tong Lin, Haoliang Jiang, and Levent Burak Kara. Topologygan: Topology  
 358 optimization using generative adversarial networks based on physical fields over the initial  
 359 domain. *Journal of Mechanical Design*, 143(3):031715, 2021.

360 [31] Amin Heyrani Nobari, Giorgio Giannone, Lyle Regenwetter, and Faez Ahmed. Nito: Neural  
 361 implicit fields for resolution-free topology optimization. *arXiv preprint arXiv:2402.05073*,  
 362 2024.

363 [32] Ioannis PA Papadopoulos, Patrick E Farrell, and Thomas M Surowiec. Computing multiple  
 364 solutions of topology optimization problems. *SIAM Journal on Scientific Computing*, 43(3):  
 365 A1555–A1582, 2021.

366 [33] Jeong Joon Park, Peter Florence, Julian Straub, Richard Newcombe, and Steven Lovegrove.  
 367 DeepSDF: Learning continuous signed distance functions for shape representation. In *Proceed-  
 368 ings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 165–174,  
 369 2019.

370 [34] Adam Paszke, Sam Gross, Soumith Chintala, Gregory Chanan, Edward Yang, Zachary DeVito,  
 371 Zeming Lin, Alban Desmaison, Luca Antiga, and Adam Lerer. Automatic differentiation in  
 372 pytorch. In *NIPS-W*, 2017.

373 [35] Daniel Rebain, Mark J. Matthews, Kwang Moo Yi, Gopal Sharma, Dmitry Lagun, and Andrea  
 374 Tagliasacchi. Attention beats concatenation for conditioning neural fields. *Trans. Mach. Learn.  
 375 Res.*, 2023, 2022.

376 [36] Suryanarayanan Manoj Sanu, Alejandro M Aragon, and Miguel A Bessa. Neural topology  
 377 optimization: the good, the bad, and the ugly. *arXiv preprint arXiv:2407.13954*, 2024.

378 [37] Vishwanath Saragadam, Daniel LeJeune, Jasper Tan, Guha Balakrishnan, Ashok Veeraraghavan,  
 379 and Richard G Baraniuk. Wire: Wavelet implicit neural representations. In *2023 IEEE/CVF  
 380 Conference on Computer Vision and Pattern Recognition (CVPR)*, 2023.

381 [38] Ole Sigmund. Morphology-based black and white filters for topology optimization. *Structural*  
 382 *and Multidisciplinary Optimization*, 33(4-5):401–424, February 2007. ISSN 1615-147X, 1615-  
 383 1488. doi: 10.1007/s00158-006-0087-x. Number: 4-5.

384 [39] Vincent Sitzmann, Julien N.P. Martel, Alexander W. Bergman, David B. Lindell, and Gordon  
 385 Wetzstein. Implicit neural representations with periodic activation functions. In *Proc. NeurIPS*,  
 386 2020.

387 [40] Ivan Sosnovik and Ivan Oseledets. Neural networks for topology optimization. *Russian Journal*  
 388 *of Numerical Analysis and Mathematical Modelling*, 34(4):215–223, 2019.

389 [41] Subodh C Subedi, Chaman Singh Verma, and Krishnan Suresh. A review of methods for  
 390 the geometric post-processing of topology optimized models. *Journal of Computing and*  
 391 *Information Science in Engineering*, 20(6):060801, 2020.

392 [42] Damien Teney, Armand Mihai Nicolicioiu, Valentin Hartmann, and Ehsan Abbasnejad. Neural  
 393 redshift: Random networks are not random functions. In *Proceedings of the IEEE/CVF*  
 394 *Conference on Computer Vision and Pattern Recognition*, pages 4786–4796, 2024.

395 [43] Kiwon Um, Robert Brand, Yun Fei, Philipp Holl, and Nils Thuerey. Solver-in-the-Loop:  
 396 Learning from Differentiable Physics to Interact with Iterative PDE-Solvers. *Advances in*  
 397 *Neural Information Processing Systems*, 2020.

398 [44] Fan Wang, Huidong Liu, Dimitris Samaras, and Chao Chen. TopoGAN: A topology-aware  
 399 generative adversarial network. In *Proceedings of European Conference on Computer Vision*,  
 400 2020.

401 [45] Zhou Wang, Alan C Bovik, Hamid R Sheikh, and Eero P Simoncelli. Image quality assessment:  
 402 from error visibility to structural similarity. *IEEE transactions on image processing*, 13(4):  
 403 600–612, 2004.

404 [46] Rebekka V Woldseth, Niels Aage, J Andreas Bærentzen, and Ole Sigmund. On the use of artifi-  
 405 cial neural networks in topology optimisation. *Structural and Multidisciplinary Optimization*,  
 406 65(10):294, 2022.

407 [47] Daniel Yago, Juan Cante, Oriol Lloberas-Valls, and Javier Oliver. Topology optimization  
 408 methods for 3d structural problems: a comparative study. *Archives of Computational Methods*  
 409 *in Engineering*, 29(3):1525–1567, 2022.

410 [48] Jonas Zehnder, Yue Li, Stelian Coros, and Bernhard Thomaszewski. NTopo: Mesh-free topology  
 411 optimization using implicit neural representations. In M. Ranzato, A. Beygelzimer, Y. Dauphin,  
 412 P.S. Liang, and J. Wortman Vaughan, editors, *Advances in Neural Information Processing*  
 413 *Systems*, volume 34, pages 10368–10381. Curran Associates, Inc., 2021.

414 [49] Biao Zhang, Jiapeng Tang, Matthias Niessner, and Peter Wonka. 3dshape2vecset: A 3d shape  
 415 representation for neural fields and generative diffusion models. *ACM Transactions On Graphics*  
 416 (*TOG*), 42(4):1–16, 2023.

417 **A Implementation and experimental details**

418 **A.1 Algorithmic description**

419 The TOM algorithm is given in Algorithm 1. A detailed textual description is provided in the main  
 420 paper.

421 **A.2 Additional results**

422 Table 2 contains additional characterization of the main experimental results in terms of computational  
 423 resources.

424 **A.3 Model hyperparameters**

425 The most important hyperparameters are summarized in Table 3. The hyperparameters were found by  
 426 manual search with compliance and diversity as targets. The search was additionally guided by visual  
 427 inspection and interpretation of the produced shapes.

---

**Algorithm 1** TOM

---

**Input:** parameterized density  $f_\theta$ , vector of mesh points  $\mathbf{x}_i \in \mathbb{R}^{d_x}$ ,  $\beta$  and annealing factor  $\Delta_\beta$ , number of shapes per iteration  $k$ , learning rate scheduler  $\gamma(t)$ , iterations  $T$

**for**  $t = 1$  **to**  $T$  **do**

$\mathbf{z}_j \sim p(\mathcal{Z})$	{ sample modulation vectors }
$\tilde{\rho}_{z_j} \leftarrow f_\theta(\mathbf{x}_i, \mathbf{z}_j)$	{ net forward all shapes $j$ }
$\rho_j \leftarrow H(\tilde{\rho}_{z_j}, \beta)$	{ Heaviside contrast filter }
$C, V, \frac{\partial C}{\partial \rho}, \frac{\partial V}{\partial \rho} \leftarrow \text{FEM}(\rho_j)$	{ solver step }
$\frac{\partial \rho}{\partial \theta} \leftarrow \text{backward}(f_\theta, \rho_j)$	{ autodiff backward }
$\nabla_\theta C \leftarrow \frac{\partial C}{\partial \rho} \frac{\partial \rho}{\partial \theta}$	{ compliance gradient }
$\nabla_\theta V \leftarrow \lambda_V \frac{\partial C}{\partial \rho} \frac{\partial \rho}{\partial \theta}$	{ volume gradient }
$L_G \leftarrow \lambda_{\text{interface}} L_{\text{interface}} + \dots$	{ GINN constraints }
$\Delta\theta \leftarrow \text{ALM}(\nabla_\theta C, \nabla_\theta V, \nabla_\theta L_G)$	{ ALM }
$\theta \leftarrow \theta - \gamma(t) \Delta\theta$	{ parameter update }
$\beta \leftarrow \beta \Delta_\beta$	{ annealing }

**end for**

---

Table 2: Additional characterization of the main experimental results reported in Table 1, including iterations needed to converge. Each iteration consists of several FEM solver calls, which are executed in parallel for TOM, resulting in an overall faster training than the sequential DB. Lastly, we report the mesh resolution used by the FEM solver. For DB, it changes over training due to the adaptive mesh refinement, which is indicated by the initial grid  $\rightarrow$  final refined mesh size.

Problem	Method	Iterations	Total solver calls	FEM resolution
MBB	FeniTop	400	400	$180 \times 60$
	DB		3190	$50 \times 150 \rightarrow 27174$
	TopoDiff			$64 \times 64$
	TOM	400	10000	$180 \times 60$
Cantilever	FeniTop	400	400	$150 \times 100$
	DB		4922	$25 \times 37 \rightarrow 52024$
	TopoDiff*			$64 \times 64$
	TOM*	1000	25000	$150 \times 100$
Bracket	FeniTop	400	400	$104 \times 172 \times 60$
	TOM	1000	9000	$26 \times 43 \times 15$

428 **Compute.** We report additional information on the experiments and their implementation. We run  
429 all experiments on a single GPU (NVIDIA Titan V12) on a node with a Xeon Gold 6150 CPU (36  
430 Cores, 2.70GHz) and 384GB RAM. The maximum GPU memory requirements are less than 2GB for  
431 all experiments.

432 **Neural network.** For the model to effectively learn high-frequency features, it is important to use a  
433 neural network representation with a high frequency bias [39, 42]. Hence, all models were trained  
434 using the real, 1D variant of the WIRE architecture [37]. WIRE allows to adjust the frequency bias  
435 by setting the hyperparameters  $\omega_0^1$  and  $s_0$ . For this architecture, each layer consists of 2 Multi-layer  
436 perceptron (MLPs), one has a periodic activation function  $\cos(\omega_0 x)$ , the other with a gaussian  $e^{(s_0 x)^2}$ .  
437 The post-activations are then multiplied element-wise.

438 **Optimization.** The overall loss for a data point  $x$  can be expressed as  $L(x) = o(x) + \sum_i \lambda_i c_i(x)$ ,  
439 where  $o(\cdot)$  represents the objective function,  $c_i(\cdot)$  denotes the constraints, and  $\lambda_i$  are the balancing  
440 coefficients for these constraints. We employ the augmented Lagrangian method (ALM) [5] to  
441 dynamically balance the various constraints throughout the training process. Intuitively, the better a  
442 constraint  $c_i$  is satisfied, the smaller the corresponding  $\lambda_i$ . We designate the compliance loss as the  
443 objective function, which consequently remains unaffected by the balancing mechanism of ALM.  
444 Crucially, for ALM to function optimally, we scale all loss terms by a dedicated factor to ensure they

445 are approximately on the same magnitude. This adjustment is analogous to harmonizing the different  
 446 “units” of the losses (e.g., volume loss versus diversity loss).

447 **Delayed start of diversity loss for jet engine bracket.** For the jet engine bracket, we start the  
 448 chamfer discrepancy loss at an iteration where the shapes already have reasonable formed (see “start  
 449 diversity” in Table 3). Empirically, this is needed to not destroy the shapes early on. This could  
 450 have several potential reasons, including a low target volume of only 0.07 or the fact that 3D shape  
 451 optimization might be fundamentally harder. We leave further investigations to future work.

Table 3: TOM hyperparameters for different experiments.

	<b>MBB beam</b>	<b>Cantilever</b>	<b>JEB</b>
Hidden layers	32x3	32x3	64x3
$\omega_0^1$ for WIRE	10	9	18
$s_0$ for WIRE 10	10	6	
Learning rate	$5 \cdot 10^{-5}$	$5 \cdot 10^{-5}$	$10^{-3}$
Decay rate	400	200	
radius $r$	1.2	0.6	0.02
SIMP penalty $p$	3	3	1.5
$\beta$ annealing	[0, 400]	[0, 400]	[0, 400]
minimal diversity $\delta^*$	0.3	0.4	0.13
# iterations	400	1,000	1,000
# shapes per batch	25	25	9
Compliance scale	1	1	1,000
Volume scale	1	1	10
Chamfer diversity scale	1	10	10
Interface scale			2,000
Interface normal scale			1
Design region scale			1
Start diversity			350

#### 452 A.4 Reference solutions

453 We provide reference solutions to the problem settings generated by the standard TO. We use the  
 454 implementation of the SIMP method provided by the FeniTop library [19] as the classical TO baseline.  
 455 We also generate single solutions using TOM without a diversity constraint or modulation variable as  
 456 input. These single shape training runs showcase the baseline capability of TOM.  
 457 The reference solutions for MBB beam problem are shown in Figure 7, for the cantilever beam  
 458 problem in Figure 8, and for the jet engine bracket problem in Figure 9.

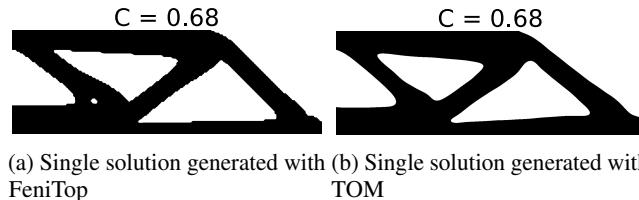
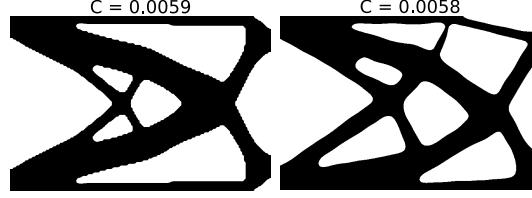


Figure 7: Reference solutions for the MBB beam problem

#### 459 A.5 Load violations in TopoDiff

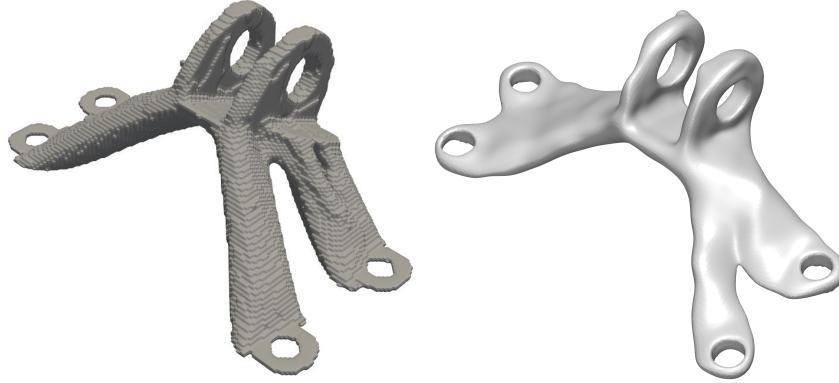
460 [25] provide a detailed evaluation of TopoDiff, including a test data set (called *level 2 test data*) with  
 461 unseen boundary conditions. They report that TopoDiff successfully generalizes to unseen boundary  
 462 conditions and produces shapes which fit these new, unseen boundaries with 100% accuracy (0%  
 463 load violations, Table 1 in [25]).

464 In the case of the 2D cantilever problem, we find that 87.2% of the shapes generated by TopoDiff  
 465 contain load violations. Our FEM solver regularizes the solve step by placing so-called ersatz material



(a) Single solution generated with FeniTop (b) Single solution generated with TOM

Figure 8: Reference solutions for the Cantilever problem



(a) Single solution generated with FeniTop (b) Single solution generated with TOM

Figure 9: Reference solutions for the jet engine bracket (JEB) problem

466 with a very low (but non-zero) density at void mesh elements. This prevents NaNs or undefined  
 467 behavior by the solver when encountering violated boundary conditions, such as no material at  
 468 loading points (load violations), see Figure 10b.

469 This results in a large jump in the compliance values, which can be seen in Figure 10a. Note that  
 470 these values are, however, unphysical and an artifact of the solver using ersatz-material instead of  
 471 void cells. Physically, the compliance is simply undefined as a force cannot be applied when no  
 472 material is present.

473 We filter out all shapes containing load violations in the results section to allow for a better comparison  
 474 and to avoid reporting compliances that are mere solver artifacts and not physically meaningful.

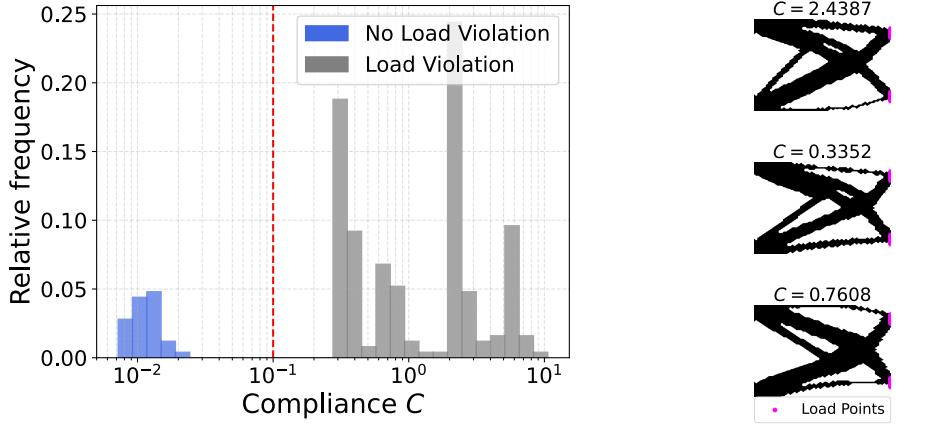
## 475 A.6 Ablations

476 To better understand the impact of different parts of TOM, we perform ablations and summarize the  
 477 results in Table 4.

478 **Diversity constraint.** We ablate the diversity loss term. While some diversity remains in the 2D case  
 479 due to the network initialization randomness, we observe complete mode collapse in 3D, illustrated  
 480 in Figure 13.

481 **Radius  $r$  of modulation space.** We highlight the choice of radius  $r$  by ablating it with a radius  
 482  $r' = \frac{1}{10}r$ . The resulting shapes are less diverse (c.f. Table 4) despite applying the diversity constraint  
 483 during training.

484 The importance of a network’s frequency bias has been highlighted by several works [39, 37].  
 485 Importantly, depending on the problem, there might be a different frequency bias necessary for the  
 486 coordinates  $\mathbf{x}$  and the modulation vectors  $\mathbf{z}$ . For the WIRE architecture we use in our experiments,  
 487 the frequency bias of the modulation is implicitly controlled by the radius  $r$ . The greater  $r$ , the greater  
 488 the diversity at initialization and convergence as suggested by Teney et al. [42].



(a) Distribution of compliance  $C$  of TopoDiff shapes. The large jump in compliance above  $10^{-1}$  is explained by forces being applied to the ersatz shapes. Shapes do not attach to all load points, leading to artifacts in the computed compliance  $C$ .

Table 4: Results for ablations on the three TO problems.

Problem	Method	$C$	$\min(C)$	$\max(C)$	$V[\%]$	$LVR[\%]$	$\mathbb{E}(W1)$	$\mathbb{E}(d_H)$	$\mathbb{E}(d_{SSIM})$
<b>MBB Beam</b>									
	Base	$0.75 \pm 0.03$	0.66	0.83	$55.08 \pm 1.04$	0.0	0.042	186.22	0.1096
	No diversity constraint	$0.76 \pm 0.02$	0.73	0.84	$54.62 \pm 1.07$	0.0	0.042	170.10	0.1124
	Radius 1/10	$0.85 \pm 0.23$	0.65	1.43	$58.55 \pm 2.63$	0.0	0.040	93.29	0.1075
	Penalty $p = 1.5$	$1.56 \pm 1.31$	0.68	5.54	$58.17 \pm 2.93$	0.0	0.043	169.28	0.1299
	Annealing	$0.89 \pm 0.25$	0.67	1.66	$59.75 \pm 1.70$	0.0	0.028	221.58	0.0917
	Fixed modulation	$0.71 \pm 0.01$	0.70	0.76	$53.49 \pm 0.32$	0.0	0.022	197.55	0.0784
<b>Cantilever</b>									
	Base	$0.69 \pm 0.13$	0.64	1.28	$49.21 \pm 0.48$	8.0	0.024	85.33	0.1799
	No diversity constraint	$0.90 \pm 0.88$	0.62	4.95	$49.63 \pm 0.61$	8.0	0.023	89.25	0.1791
	Radius 1/10	$0.92 \pm 0.07$	0.79	1.01	$49.43 \pm 2.08$	0.0	0.032	84.02	0.1186
	Penalty $p = 1.5$	$1.19 \pm 1.21$	0.54	4.97	$50.55 \pm 1.15$	12.0	0.019	69.14	0.1565
	Annealing	$0.74 \pm 0.22$	0.61	1.35	$49.53 \pm 0.33$	12.0	0.027	84.42	0.1767
	Fixed modulation	$0.82 \pm 0.26$	0.62	1.25	$48.87 \pm 0.28$	4.0	0.026	93.93	0.1848
<b>Simjeb</b>									
	Base	$0.13 \pm 0.01$	0.11	0.15	$6.86 \pm 0.09$	0.0	0.027	9.01	0.0782
	No diversity constraint	$0.11 \pm 0.01$	0.10	0.14	$7.51 \pm 0.06$	0.0	0.006	8.2	0.0687
	Radius 1/10	$0.13 \pm 0.01$	0.12	0.15	$7.35 \pm 0.02$	0.0	0.002	5.54	0.0093
	Penalty $p = 1.5$	$0.09 \pm 0.00$	0.09	0.10	$7.09 \pm 0.01$	0.0	0.010	11.33	0.0443
	Annealing	$0.60 \pm 0.19$	0.40	0.85	$6.21 \pm 0.05$	66.7	0.041	9.47	0.1024
	Fixed modulation	$0.08 \pm 0.01$	0.07	0.09	$7.64 \pm 0.04$	0.0	0.034	11.01	0.0970

489 **Sensitivity to penalty  $p$ .** As noted by prior work [36], neural reparameterization is sensitive to  
490 the penalty parameter  $p$ . For SIMP, the density is penalized with an exponent  $p$ . We ablate this  
491 parameter by setting the 2D penalty from  $p = 3$  to 1.5 and for 3D from  $p = 1.5$  to 3. Our experiments  
492 confirm that TOM is sensitive to the choice of  $p$ , as it sharpens the loss landscape. This becomes  
493 more apparent when looking at the derivative of the stiffness of a mesh element  $\frac{\partial \mathbf{K}_i(\rho_i)}{\partial \rho_i} = p \rho_i^{p-1} \mathbf{K}_i$ .  
494 E.g., for  $p = 3$  the gradient is quadratically scaled by the current density value. This implies that the  
495 higher  $p$ , the harder it is to escape local minima. We do not observe a large performance impact in  
496 the 2D experiments. However, in 3D, we observe that  $p = 3$  instead of  $p = 1.5$  leads to convergence  
497 to an undesired local minimum, illustrated in Figure 12a.

498 **Annealing is necessary for good convergence.** We find that TOM requires annealing to achieve  
499 good convergence. Figure 12b demonstrates a failed run without  $\beta$  scheduling the Heaviside function  
500 (Equation 14). The optimization fails to converge to a useful compliance value and does not fulfill  
501 the desired interface constraints.

502 **Fixed modulation vectors.** TOM uses a continuous modulation space, and in our current implemen-  
503 tation, samples modulation vectors from a circle. An interesting alternative is to keep the modulation

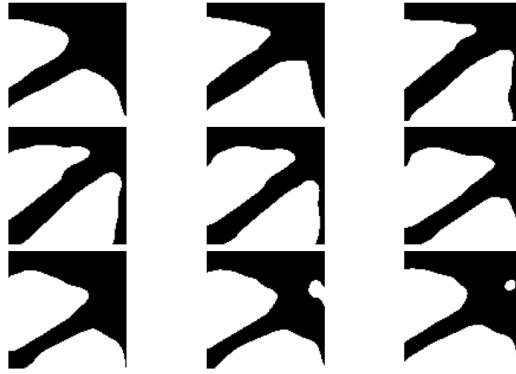


Figure 11: The cantilever ablation of the radius leads to mode collapse qualitatively.

504 vectors fixed throughout training. As shown in Table 4, the results of this variant also produce shapes  
 505 with satisfactory compliance and diversity.

506 **Alternative diversity metrics** We measure diversity via the Hill number  $D_q(S)$  over the set  $S$ , where  
 507 we choose  $q = 2$  as it is interpretable as the expected dissimilarity between two elements drawn from  
 508  $S$ . The diversity can be computed based on an arbitrary pairwise dissimilarity function. As a measure  
 509 of dissimilarity, we chose the Wasserstein distance because we consider material distributions, and  
 510 the Wasserstein distance is a distance between distributions. Also, it is a proper metric distance  
 511 satisfying the four axiomatic properties.

512 In addition to the Wasserstein-1 distance, we performed additional evaluations of the diversity based  
 513 on two other dissimilarity functions: the Hausdorff distance ( $d_H$ ) and structural dissimilarity ( $d_{SSIM}$ )  
 514 [45]. The results in Table 4 show similar results across all dissimilarity functions. Note that the  
 515 Hausdorff distance is particularly sensitive to outliers, making it less suitable for robust measurements.  
 516 Additionally, we observe that the proposed diversity metrics do not fully capture our intuition about  
 517 the variety of shapes. For instance, the radius-ablation variant of the cantilever exhibits a higher  
 518 diversity score than the base model. However, the qualitative evaluation in Figure 11 reveals mode  
 519 collapse. These shapes also exhibit poor compliance. Sanu et al. [36] demonstrated that neural  
 520 networks can more effectively explore the solution space of topology optimization (TO) problems.  
 521 We therefore hypothesize that inducing higher diversity, either at initialization or as a constraint, may  
 522 promote further exploration.

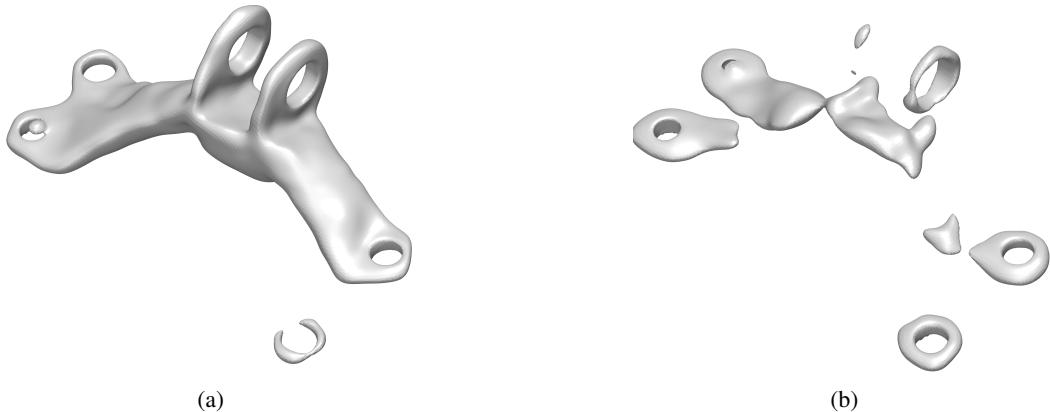


Figure 12: Ablations for penalty and  $\beta$  annealing. (a) Jet engine bracket trained with penalty  $p = 3$ .  
 (b) Jet engine bracket trained without annealing.

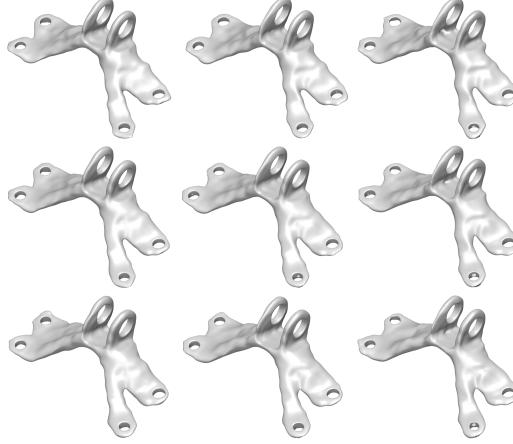


Figure 13: JEB: Training in 3D without diversity constraint results in mode collapse.

Table 5: Geometric constraints are derived from GINNs. The shape  $\Omega$  and its boundary  $\partial\Omega$  are implicitly defined by the level set  $\tau$  of the function  $f$ . The shape must reside within the *design region*  $\mathcal{E} \subseteq \mathcal{X}$  and adhere to the *interface*  $\mathcal{I} \subset \mathcal{E}$  with a specified *normal*  $\bar{n}(x)$ .

	Set constraint $c_i(\Omega)$	Function constraint	Constraint violation $c_i(f)$
Design region	$\Omega \subset \mathcal{E}$	$f(x) < \tau \forall x \notin \mathcal{E}$	$\int_{\mathcal{X} \setminus \mathcal{E}} [\max(0, f(x) - \tau)]^2 dx$
Interface	$\partial\Omega \supset \mathcal{I}$	$f(x) = \tau \forall x \in \mathcal{I}$	$\int_{\mathcal{I}} [f(x) - \tau]^2 dx$
Prescribed normal	$n(x) = \bar{n}(x) \forall x \in \mathcal{I}$	$\frac{\nabla f(x)}{\ \nabla f(x)\ } = \bar{n}(x) \forall x \in \mathcal{I}$	$\int_{\mathcal{I}} \left[ \frac{\nabla f(x)}{\ \nabla f(x)\ } - \bar{n}(x) \right]^2 dx$

## 523 B Geometric constraints

524 We formulate geometric constraints analogously to GINNs in Table 5 for density representations.  
525 There are two important differences when changing the shape representation from a signed distance  
526 function (SDF) to a density function.  
527 First, the level set  $\partial\Omega_\tau$  changes from  $\partial\Omega_\tau = \{x \in \mathbb{R}^{d_x} | f_\theta = 0\}$  to  $\partial\Omega_\tau = \{x \in \mathbb{R}^{d_x} | f_\theta = 0.5\}$ .  
528 Second, for a SDF the shape  $\Omega_{tau}$  is defined as the sub-level set  $\Omega_\tau = \{x \in \mathbb{R}^{d_x} | f_\theta \leq 0\}$ , whereas  
529 for a density it is the super-level set  $\Omega_\tau = \{x \in \mathbb{R}^{d_x} | f_\theta \geq 0\}$ .

## 530 C Diversity

### 531 C.1 Diversity on the volume

532 As noted by Berzins et al. [8], one can define a dissimilarity loss as the  $L^p$  function distance

$$d(\Omega_i, \Omega_j) = \sqrt[p]{\int_{\mathcal{X}} (f_i(x) - f_j(x))^p dx} \quad (7)$$

533 We choose  $L^1$ , to not overemphasize large differences in function values. Additionally, we show  
534 in the next paragraph that for  $L^1$  and for the extreme case where  $f(x) \in \{0, 1\}$  this is equal to the  
535 Union minus Intersection of the shapes:

$$\int_{\mathcal{X}} |f_i(x) - f_j(x)| dx = \text{Vol}(\Omega_i \cup \Omega_j) - \text{Vol}(\Omega_i \cap \Omega_j) \quad (8)$$

### 536 C.2 $L^1$ distance on neural fields resembles Union minus Intersection

537 To derive that the distance metric

$$d(\Omega_i, \Omega_j) = \sqrt[p]{\int_{\mathcal{X}} (f_i(x) - f_j(x))^p dx} \quad (9)$$

538 for  $p = 1$  and  $f_i, f_j \in \{0, 1\}$  corresponds to the union minus the intersection of the shapes, we  
539 consider the following cases:

$f_i(x)$	$f_j(x)$	$ f_i(x) - f_j(x) $
1	1	0
1	0	1
0	1	1
0	0	0

Table 6: Function distance if the function only has binary values.

540 From the table, we observe that the integrand  $|f_i(x) - f_j(x)|$  is 1 when  $x$  belongs to one shape but  
541 not the other, and 0 when  $x$  belongs to both or neither. Thus, the integral  $\int_{\mathcal{X}} |f_i(x) - f_j(x)| dx$  sums  
542 the volumes where  $x$  is in one shape but not the other, which is precisely the volume of the union of  
543  $\Omega_i$  and  $\Omega_j$  minus the volume of their intersection. It follows that

$$d(\Omega_i, \Omega_j) = \int_{\mathcal{X}} |f_i(x) - f_j(x)| dx = \text{Vol}(\Omega_i \cup \Omega_j) - \text{Vol}(\Omega_i \cap \Omega_j) \quad (10)$$

544 .

### 545 C.3 Diversity on the boundary via differentiable chamfer discrepancy

546 We continue from Equation 5:

$$\begin{aligned} \frac{\partial L}{\partial \theta} &= \frac{\partial L}{\partial x} \frac{\partial x}{\partial y} \frac{\partial y}{\partial \theta} \\ &= \frac{\partial L}{\partial x} \frac{\nabla_x f_\theta}{|\nabla_x f_\theta|^2} \frac{\partial y}{\partial \theta} \end{aligned} \quad (11)$$

547 The center term  $\frac{\nabla_x f_\theta}{|\nabla_x f_\theta|^2}$  and the last term  $\frac{\partial y}{\partial \theta}$  can be obtained via automatic differentiation. For the  
548 first term, we derive  $\frac{\partial L}{\partial x}$ , where  $L$  is the one-sided chamfer discrepancy  $\text{CD}(\partial\Omega_1, \partial\Omega_2)$ .

$$\frac{\partial}{\partial x} \text{CD}(\partial\Omega_1, \partial\Omega_2) = \frac{\partial}{\partial x} \frac{1}{|\partial\Omega_1|} \sum_{x \in \partial\Omega_1} \min_{y \in \partial\Omega_2} \|x - y\|_2 \quad (12)$$

$$= \frac{1}{|\partial\Omega_1|} \min_{y \in \partial\Omega_2} \frac{x - y}{\|x - y\|} \quad (13)$$

549 This completes the terms in the chain rule.

### 550 C.4 Finding surface points

551 We detail the algorithm to locate boundary points of implicit shapes defined by a neural density field,  
552 Algorithm 2.

553 On a high level, the algorithm first identifies points inside the boundary where neighboring points lie  
554 on opposite sides of the level set. Subsequently, it employs binary search to refine these boundary  
555 points. The process involves evaluating the neural network to determine the signed distance or density  
556 values, which are then used to iteratively narrow down the boundary points. We find that 10 binary  
557 steps suffice to reach the boundary sufficiently close.

558 For the 3D jet engine bracket, we additionally follow Berzins et al. [8] and exclude surface points  
559 which are within some  $\epsilon$  region of the interface.

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**Algorithm 2** Find Boundary Points with Binary Search

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**Input:** regular point grid  $x_i$ , level set  $l$ , neural density field  $f_\theta$ , binary search steps  $T$   
Find points  $x_i^{\text{in}} \in x_i$  for which  $f(x_i^{\text{in}}) > l$   
Find neighbor points  $(x_i^{\text{out}})_i \in x_i$  to  $x_i^{\text{in}}$   $f(x_{\text{out}}) < l$  { for 2D/3D we check 4/6 neighbors respectively}  
Refine pairs  $(x_{\text{in}}, x_{\text{out}})_i$  via  $T$  binary search steps  
Return  $((x_{\text{in}} + x_{\text{out}})/2)_i$

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560 **D Topology optimization**561 **D.1 Problem definitions**

562 **Messerschmitt-Bölkow-Blohm beam (2D).** The MBB beam is a common benchmark problem in  
563 TO and is depicted in Figure 4a. The problem describes a beam fixed on the lower right and left  
564 edges with a vertical force  $F$  applied at the center. As the problem is symmetric around  $x = L/2$ , we  
565 follow Papadopoulos et al. [32] and only optimize the right half.

566 The concrete dimensions of the beam are  $H = 1$ ,  $L = 6$ , and the force points downwards with  $F = 1$ .

567 **Cantilever beam (2D).** The cantilever beam is illustrated in Figure 4b. The problem describes a  
568 beam fixed on the left-hand side, and two forces  $F_1, F_2$  are applied on the right-hand side.  
569 The dimensions are  $H = 1$ ,  $L = 1.5$ ,  $h = 0.1$  and the forces  $F_1 = F_2 = 0.5$ .

570 **Jet engine bracket (3D).** We apply TOM to a challenging 3D task, namely the optimization of a  
571 jet engine bracket as defined by Kiis et al. [21]. The design region for this problem is enclosed by a  
572 freeform surface mesh (see Figure 4c). The load case is depicted in Figure 4c in which a diagonal  
573 force pulls in positive x and positive z direction.

574 **D.2 Smoothing and contrast filtering**

575 Filtering is a general concept in topology optimization that aims to reduce artifacts and improve  
576 convergence. *Helmholtz PDE filtering* is a smoothing filter similar to Gaussian blurring, but easier to  
577 integrate with existing finite element solvers. By solving a Helmholtz PDE, the material density  $\rho$  is  
578 smoothed to prevent checkerboard patterns, which is typical for TO [23]. *Heaviside filtering* is a  
579 type of contrast filter, which enhances the distinction between solid and void regions. The Heaviside  
580 filter function, as defined in Equation 14, equals the sigmoid function up to scaling of the input.  $\beta$  is a  
581 parameter controlling the sharpness of the transform, similar to the inverse temperature of a classical  
582 softmax (higher beta means a closer approximation to a true Heaviside step function). Note that in  
583 contrast to the Helmholtz PDE filter, the Heaviside filter is not volume preserving. Therefore, the  
584 volume constraint has to be applied to the modified output.

$$H(x, \beta) = 0.5 + \frac{\tanh(\beta(x - 0.5))}{2 \tanh(0.5\beta)} \quad (14)$$

585 **Annealing** is employed to make the continuous relaxation closer to the underlying discrete problem  
586 [22], enhancing the effectiveness of gradient-based optimization methods. Annealing gradually  
587 adjusts the sharpness of a function during the optimization. For TO, this is often done by gradually  
588 increasing the penalty  $p$  or by scheduling a sharpness filter. A common choice is the Heaviside filter  
589 as defined in Equation 14.

590 **D.3 Post-processing**

591 In general, the post-processing of TO solutions heavily depends on the downstream task and the spe-  
592 cific manufacturing requirements, e.g., additive vs subtractive manufacturing. Here, we demonstrate  
593 two simple methods to post-process TOM solutions:

594 **Method A** is a simple yet standard image-based approach that removes disconnected components  
595 (floaters) and performs morphological closing to remove small artifacts (holes).

596 **Method B** is a fine-tuning approach that performs a few iterations of classical TO updates (5% of  
597 a full run, learning rate reduced by  $\times 10$  compared to the standard FeniTop settings) on the TOM  
598 output. This approach also removes the artifacts. This illustrates how TOM extends, not competes,  
599 with classical TO.

600 We depict a version of an MBB beam with many floaters and its post-processed version in Figure 14.

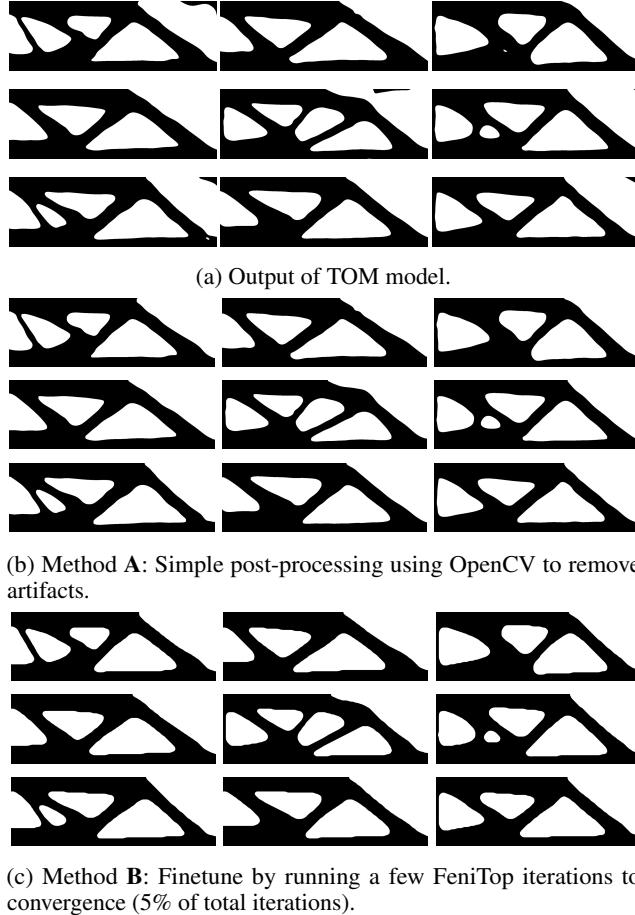


Figure 14: **Post-processing:** Showcasing 2 possible post-processing steps to remove artifacts from the TOM solutions.