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Deep Learning for Additive Manufacturing-driven Topology Optimization

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Abstract

This paper investigates the potential of Deep Learning (DL) for data-driven topology optimization (TO). Unlike the rest of the literature that mainly applies DL to TO from a mechanical perspective, we developed an original approach to integrate mechanical and geometrical constraints simultaneously. Our approach takes as input the mechanical constraints (Boundary conditions, loads configuration, volume fraction) alongside the geometrical ones (total number of elements, minimum overhang, maximum length, minimum thickness) and generates a 2D design complying with these constraints. Thus, it combines the best of both mechanical (CAE) and geometrical design worlds. Conversely, geometrical design constraints are complex, not yet formalized, and contradictory between Additive Manufacturing (AM) processes, applications, and materials. Some are even descriptive, lacking a well-defined mathematical description, or are well-defined but proprietary and inaccessible. Hence, despite the synergy between AM and TO, integrating AM constraints into the TO formulation is still a hurdle. Furthermore, even when their integration is possible, TO's convergence to a solution is compromised. On the other hand, DL has proven robust in capturing geometrical and spatial correlations. Consequently, our approach solves the previously listed setbacks by aligning DL to serve Design for AM (DfAM); there is no need to identify an analytical formula for a geometrical constraint but simply a sufficient number of examples describing it, and convergence is no longer a blockade when the DL model is trained on converged designs. Our approach tailors the design's geometrical aspects with great flexibility and creativity. It reconciles design and manufacturing and accelerates the design life cycle of a part. Moreover, it can be easily updated to include additional constraints and can be implemented in the future into CAD software as a lighter and faster generative design module.

Keywords: Topology Optimization; Additive Manufacturing; Generative Design; Deep Learning.

1. Introduction

Additive manufacturing (AM) revolutionized the way products are designed and manufactured. This technology has gained significant academic and industrial interest due to its ability to create complex and customizable geometries. This characteristic of AM made it synergetic with a specific design method called topology optimization (TO). Amongst TO methods, the most prominent use density of matter as optimization variables and allows an optimal distribution of the material in a design space subject to boundary conditions, loads configuration, and a volume constraint. Despite the freedom TO and AM offer, AM requires some geometrical constraints to avoid, for example, the collapse of the part during manufacturing. Also, TO is mainly used at the conceptual design level, where it is challenging to aggregate nonlinearities (material and geometric such as buckling) and stress-related constraints. Furthermore,

the external shape is not adequately defined with TO, and geometric AM-related constraints such as overhangs cannot be easily integrated.

The following steps can summarize design for AM (DfAM), a movement to democratize design and manufacturing. First, an engineer defines the specifications of the part being designed. Second, he/she runs a TO, which proposes a specific geometry. Third, he/she re-interprets and re-draws the shape proposed by TO while implicitly considering AM constraints. Fourth, he/she tests its performance then validates the shape. Finally, he/she prints it [19]. While this cycle seems straightforward, re-interpreting TO's shape to comply with AM constraints and maintaining the initial performance intact is not. Altering TO's output compromises its initial functionality, and the designer is stuck in a loop of updating and testing the computer-aided design (CAD). Additionally, with the contradictory nature of AM constraints and the lack of standardization[12], integrating them at the conceptual level of TO can be challenging, and even when

possible, convergence to a feasible solution is not guaranteed. Accelerating DfAM's cycle is current hot research and industrial topic. We can find in the literature three general approaches to tackle the problem.

In an attempt to identify process-independent AM-based design rules, the first line of research focused on formalizing AM guidelines. Adam et al.[2] carried out several experiments over three types of processes ([2]) and formalized design rules over gap heights and widths of transitions of non-bonded elements, lengths of overhangs, positions of islands, etc. Booth et al. [9] created a one-page visual DfAM worksheet for novice AM users.

The second approach integrated specific AM constraints at TO's level. Allaire et al.[4] adapted TO to account for a minimum overhang of 45°, as it is one of the most general AM design-rule. Zhang et al.[28] considered the build orientation to reduce the need for support structures. Xu et al.[25] estimated a formulation for the hanging features and penalized the evolution of densities in the domain space accordingly. Fernández et al.[11] focused on eliminating thin features and small cavities in final optimized structures, etc.

These approaches are limited for several reasons: (1) AM constraints lack standardization [12] and are contradictory between processes, materials, and applications. For example, in a metal Powder Bed Fusion (PBF) process, support structures have a double role. They support overhanging features and help dissipate the laser heat to prevent thermal deformation or cracks due to residual stress. On the contrary, in polymer PBF, the unsintered powder material itself provides support for the overhanging features, and hence support structures are not needed [29]. (2) AM constraints are mostly geometric constraints that are, at best, approximated analytically, and integrating them into Finite-element (FE) based TO compromises its convergence and limits its freedom[28, 19]. (3) These methods are still based on FE analysis and therefore are iterative and computationally inefficient.

On the other hand, the third part used Machine Learning and Deep Learning (DL) to alleviate the computational problem of FE-TO and left the AM constraints to the shape reinterpretation phase. Some researchers partially replaced FE by substituting sensitivity analysis with neural networks (NN)[10], by using super-resolution NN to enhance the resolution of intermediate FE-TO's outputs [24], by substituting TO by a deep NN that is trained and penalized using a quality function based on FE computations[14], etc. Others opted to completely eliminate FE of TO using a PCA followed by a shallow NN [22] or directly using deep NN [1, 16] and Generative Adversarial Networks (GAN) frameworks [7, 26, 20, 18]. As previously mentioned, the latter methods did not integrate any geometrical constraints but left them to the reinterpretation phase, knowing that significant modifications might be made into the shape during this phase, and hence they accelerated only TO and not the whole DfAM cycle.

In this work, we propose, using DL, to integrate not only mechanical constraints but also geometric AM-related ones at the conceptual level. With DL's capacity to learn spatial correlations, there is no need to identify an analytical formula for a

geometrical constraint but simply a sufficient number of examples describing it.

This paper proposes a data-driven TO for AM approach (DL-AM-TO), an improved version of our previous work[5] using GMCAD[6] (a novel dataset of geometrical and mechanical 2D designs). DL-AM-TO takes as input the mechanical constraints (Boundary conditions, loads configuration, volume fraction) alongside the geometrical ones (total number of elements, minimum overhang, maximum length, minimum width) and generates a 2D design complying with these constraints. It is trained within a GAN framework.

DL-AM-TO aligns DL with DfAM. Thus, it comes to bridge the gap between the mechanical (CAE) and geometrical (CAD) worlds. Moreover, it alleviates the engineer from getting stuck in the late design phases since it is intended to generate a shape complying with mechanical and manufacturing specifications concurrently.

DL-AM-TO tailors the design's geometrical aspects with flexibility and creativity. It is a novel approach that democratizes the design and manufacturing and accelerates the design life cycle of a part. Furthermore, it can be implemented into CAD software as a lighter and faster generative design module in the future.

The major contribution of this paper is the exploration of DL to integrate at the conceptual level geometric AM-related constraints along with mechanical ones in an attempt to bridge mechanics and geometrical design into a single-phase and consequently accelerate the DfAM workflow.

The paper is organised as follows: Sections 2.1 and 2.2 provide a theoretical background on TO and GANs. Section 3 details the proposed method, DL-AM-TO's architecture and training framework. Section 4 shows and discusses the first results. Finally, section 5 summarizes this work and discusses future works.

2. Theoretical Background

2.1. Topology Optimization

Topology Optimization (TO) aims to distribute material in a design space subject to boundary conditions (BC) and loads (F) while conforming with a volume fraction constraint and a well-defined objective function. Several approaches are proposed in the literature to solve the TO problem, particularly, the level set [3], and density [8] approaches. Solid Isotropic with Material Penalization (SIMP) is the top common continuous density approach implemented in industrial design software. It uses the penalization of intermediate non-binary values of density material to converge to an optimal binary design. SIMP defines a design as a distribution of discretized square material elements e. The element-relative-density $x_i = 1/0$ represents the presence/absence of material at point i of the design domain. A common objective function in structural TO is global structural compliance. A TO problem where the objective is to minimize the compliance $c(x)$ can be written as the following:
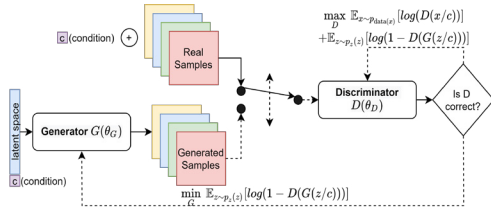
Fig. 1. Diagram of a Conditional GAN

$$min(c(x)) = U^T K U = \sum_{e=1}^{N} x_e^p u_e^T k_e u_e. \qquad (1)$$
$$s.t. \ KU = F, \ \frac{V(x)}{V0} \le f, \ 0 < x_0 \le x \le 1$$

where U and u_e are the global and element-wise displacements, F the forces vector, K and k_e are the global and element-wise stiffness matrices and N = number of elements used to discretize the design domain. x is the design variables vector i.e. the density material and x_0 the minimum relative density (non-zero to avoid singularity), p penalization power. V_0 and $V(x)$ are the design domain volume and material volume respectively and f the volume fraction.

2.2. Generative Adversarial Networks

Generative Adversarial Network (GAN)[13] is a generative method that aims to learn the data distribution. It consists of two differential networks: a generator $G(z, \theta_G)$ (the network in charge of generating new samples following the real data distribution from a latent vector z, with θ_G as the G's network parameters), and a discriminator $D(x, \theta_D)$ (a sort of a binary classifier that should distinguish real from generated data, with θ_D the D's network parameters). Each network works against the other in a minimax framework to improve the same loss function: the cross-entropy loss $L(G, D)$, hence the adversarial term. GAN's training succeeds when the discriminator stops recognizing the difference between the real p_{data} and the generated data distribution $p_{G(z)}$ i.e. $p_{G(z)} \approx p_{data}$.

In this work, the generator is conditioned on mechanical and geometrical constraints. Hence, a more adapted GAN framework is needed: the conditional GAN (cGAN) [15] (Fig.1). It extends the GAN network, enabling the generation to be oriented by a specific input condition c. In this framework, the basics of cGAN become: the conditional generator as $G((z/c), \theta_g)$, the conditional discriminator as $D((x/c), \theta_d)$ and the adversarial loss function as:

$$L(G, D) = \min_G \max_D \mathbb{E}_{x \sim p_{data}(x)}[log(D(x/c))]$$
$$+ \mathbb{E}_{z \sim p_z(z)}[log(1 - D(G(z/c)))] \qquad (2)$$

3. Deep Learning Additive Manufacturing driven Topology Optimization (DL-AM-TO)

DL-AM-TO is a novel approach where the mechanical and geometrical constraints are no longer in competition. DL-AM-TO is a generative model that takes mechanical (Boundary conditions (BC), loads (F), and the volume fraction (V)) and geometrical conditions (the minimum thickness (th_{min}), the maximum length (len_{max}), the minimum overhang (Θ_{min}), the number of bars (Nbr_{bars})) as inputs and generates a 2D structure following these constraints. It is trained within a five-discriminator-GAN [13] framework consisting of a generator (DL-AM-TO) and five discriminators: the traditional adversarial discriminator and four geometric discriminators, a bar counter, a th_{min}, len_{max} and Θ_{min} predictors (Fig.3). It is important to highlight that DL-AM-TO is an extended version of our previous work [5], where DL-AM-TO considered mechanical conditions and only the Nbr_{bars} as a geometrical one and was validated mechanically (compliance in Joules) and geometrically (comparison between the input Nbr_{bars} and generated design's Nbr_{bars}).

The four geometric constraints were chosen among the existing set of constraints as a use case to validate the proposed methodology.

3.1. Architecture

DL-AM-TO inherits the residual-convolutional encoder-decoder architecture[27] presented in our previous work[5] with one difference; the skip-connections between the outputs of encoder layers and the inputs of decoder layers were eliminated here. The traditional discriminator consists of seven down-sample convolutional layers followed by a dropout and a final fully connected layer. The geometric discriminators' network consists of a stem, an Inception/Reduction Resnet-v1-block-A, an Inception/Reduction Resnet-v1-block-B, an Inception Resnet-v1-block-C followed by an average pooling layer, a dropout layer, and a fully connected layer[1]. We would like to point out that the input of the three geometric discriminators (th_{min}, len_{max}, and Θ_{min}) consists of the 2D design only, and the bar counter's input consists of the design alongside the mechanical conditions.

3.2. Training Loss Function

The most challenging aspect of GANs is to find an equilibrium between the generator and the discriminator and avoid the dominance of one over the other. The loss function with other training parameters play an important role into stabilizing the training and condemning the phenomenon of oscillating losses. In this work, the loss function is further challenging; it has to also account for the geometrical (th_{min}, len_{max}, Θ_{min}, Nbr_{bars}) and mechanical (BC, F, V) constraints. Thus,

$$L_G = \frac{1}{6}(L_r + \lambda_{adversarial}L_{adv} + L_{Nbr_{bars}} + L_{th_{min}} + L_{len_{max}} + L_{\Theta_{min}}),$$

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[1] The stem and inception/reduction blocks used defer from the original paper [21] only by the number of input/output feature maps. However, the stem block of the len_{max} and Θ_{min} predictors consists of additional five residual layers.
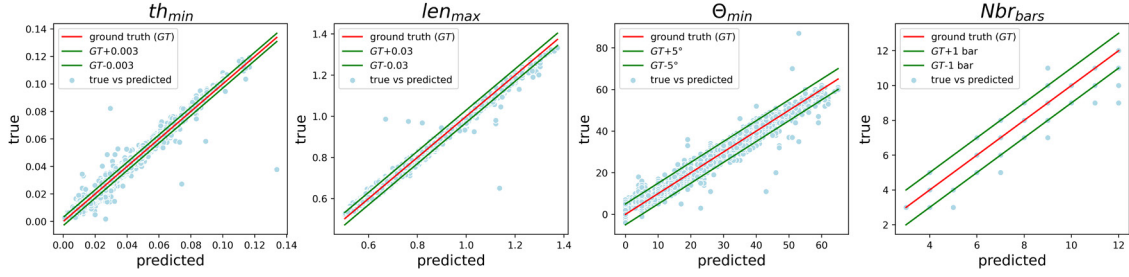
Fig. 2. Performance of geometric discriminators showing predicted vs true values of th_{min}, len_{max}, Θ_{min}, & Nbr_{bars}, from left to right respectively. The worst performant discriminator is clearly the th_{min} predictor.
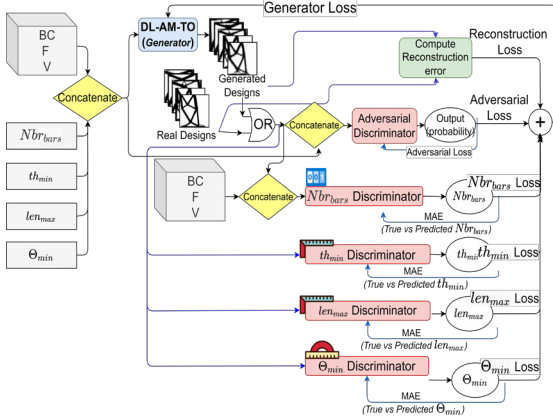

Fig. 3. Training Procedure

Fig. 4. DL-AM-TO's performance when trained with and without th_{min}.

with (1) the reconstruction loss $L_r = \frac{1}{N}\sum_{i=1}^{N}(x_i - \hat{x}_i)^2$ s.t. x_i and $\hat{x}_i$ are the real and generated 2D design and N is the batch size, (2) $\{L_c = \sum_{i=1}^{N} |c_i - \hat{c}_i|, c \in \{Nbr_{bars}, th_{min}, len_{max}, \Theta_{min}\}\}$ s.t. c and $\hat{c}$ are the input and predicted geometrical values respectively, and (3) the adversarial loss L_{adv} is the Binary Cross Entropy ($0 \leq L_{adv} \leq 100$ in PyTorch). Hence, $\lambda_{adversarial}$ was set to 0.01, so L_{adv} becomes of the same order of magnitude of all other losses varying between 0 and 1.

4. Results

This work's evaluation focuses on DL-AM-TO's performance regarding the geometrical constraints. Thus, we not only evaluate the aesthetics of the generated designs (Fig. 4) but also test DL-AM-TO 's ability to respond to geometrical changes (Figures 5, 6, 7).

4.1. Training and Test Dataset

11719 samples of GMCAD are used for training and 4405 samples for test. It consists of 2D designs (in a .png format) alongside their mechanical and geometrical constraints. GM-CAD's features are detailed in [6].

4.2. Geometric Discriminators' performance

To train the geometric discriminators, we augmented the training dataset with three rotations of 90°, 180°and 270°.
The predictive performance of the geometrical discriminators is presented in Fig. 2. In order to evaluate a predictor, an admissible error interval is set (predictions within the green lines
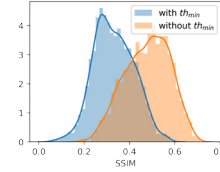
in Fig.2 are considered correct). As we can clearly see, the th_{min} predictor shows the highest number of inadmissible predictions (predictions outside the green intervals). To quantify this observation, the percentage of erroneous predictions for every geometrical discriminator is computed. We choose for the th_{min} and len_{max} the relative prediction error defined as $e_\% = \frac{|True - Predicted|}{True} \times 100$, and for the Θ_{min} and Nbr_{bars} the difference $\Delta = |True - Predicted|$. The percentage of predictions that fall within $e_{th_{min}\%} > 5\%$ is 46%, $e_{len_{max}\%} > 5\%$ is 1%, $\Delta\Theta_{min} > 5°$is 3.15% and $\Delta Nbr_{bars} > 1bar$ is 0.15%. Consequently, we can conclude that all geometric discriminators are sufficiently precise except for the th_{min} one, which needs further improvement. In fact, if we tolerate a higher error interval of 10% for th_{min}, we would end up with 29.1% of inadmissible predictions.

4.3. DL-AM-TO's performance

Figure 4 illustrates the Structural Similarity Index Measure (SSIM)[23] of the generated designs. The blue distribution corresponds to the generator (DL-AM-TO) trained with all geometric discriminators. The average SSIM is 0.33, which demonstrates, aesthetically speaking, a weak generation. As we have mentioned previously, the th_{min} discriminator is not predicting th_{min} with high precision, and hence the generator is penalized with a less informative loss, which explains DL-AM-TO's behavior. Furthermore, th_{min} is a continuous complex quantity to be treated by DL, particularly convolutional networks. We can find several designs with different minimum thicknesses that look indistinguishable in the dataset. Indeed, th_{min} is a texture feature, unlike Θ_{min}, an edge feature, where a slight variation can drastically modify the geometry, and hence the pixels' distribution. Additionally, the thickness information can be compensated with post-processing over the skeletons of the designs; we can erode/dilate skeletons to generate designs with arbitrary thicknesses.
In order to alleviate this setback, we re-train our model with-

Real Design						
Generated Design						
Real Skeleton						
Generated Skeleton						
ΔNbr_{bars}	0	0	0	0	0	0
$\Delta \Theta_{min}$	-9°	0°	-1°	+4°	+0.5°	0°
$e_{len_{max}}\%$	3.5%	2.9%	0%	7.7%	3.7%	0%
$SSIM$	0.44	0.57	0.55	0.59	0.56	0.58
$SSIM_{skeleton}$	0.7	0.73	0.63	0.76	0.75	0.66

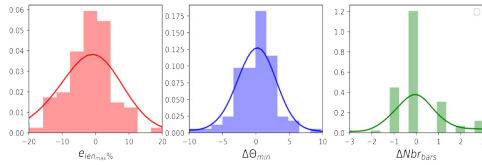Fig. 5. Comparison between the real and generated designs in their full and skeleton formats on the test set.

Fig. 6. The distribution of the geometrical metrics ($e_{len_{max}}\%$, $\Delta \Theta_{min}$, ΔNbr_{bars}) manually measured over 100 designs of the test set.

out the th_{min} variable. The generator's loss becomes $L_G = \frac{1}{5}(L_r + \lambda_{adversarial}L_{adv} + L_{Nbr_{bars}} + L_{len_{max}} + L_{\Theta_{min}})$.
As expected, SSIM was improved by 44% as illustrated by the orange distribution in Fig.4.
Figure 5 shows a sample of real versus generated designs alongside their skeletons and the geometrical metrics: ΔNbr_{bars}, $\Delta \Theta_{min}$ and $e_{len_{max}}\%$ (section 4.2). As a matter of fact, designers are more interested in the design's geometry, which is best defined by the skeletons, which explains their use here for comparison.
As we can clearly see, DL-AM-TO captures the geometrical information; $\Delta Nbr_{bars} = 0$, $\Delta \Theta_{min}$ rarely exceeds 5°, similarly, $e_{len_{max}}\%$ does not exceed 10%. Aesthetically, the generated designs' skeletons are similar to the real ones; SSIM is ≈ 0.7.
The overall geometrical performance was evaluated manually over a sample of 100 designs of the test set; in other terms, we counted the Nbr_{bars} and measured the len_{max}, and Θ_{min} manually. We define a design complying with (i) the Nbr_{bars} constraint if $\Delta Nbr_{bars} \leq 1$, (ii) the len_{max} constraint if $e_{len_{max}}\% \leq 10\%$, and (iii) the Θ_{min} constraint if $\Delta \Theta_{min} \leq 5°$. We find that 83% of the designs respect the Nbr_{bars} constraint, 76% comply with the len_{max} constraint, and 90% with the Θ_{min} constraint (Fig.6).
In order to further investigate the geometrical understanding of DL-AM-TO, we realized an experiment as shown in Fig.7. We fixed the mechanical constraints and altered one geometrical variable at a time (len_{max} and Θ_{min}). To calibrate the design's geometry, we simply need to modify the input value of the desired geometrical condition. As we can see, every time we increase len_{max}/Θ_{min}, the design's shape is modified in order to comply with this variation while always conforming with mechanical constraints (the F and BC). However, we can notice that some geometrical constraints are correlated; increasing the Θ_{min} alters the len_{max}, and at a certain value, an additional bar
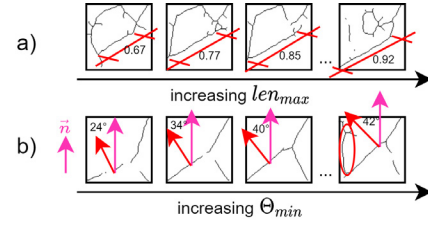

Fig. 7. DL-AM-TO's response versus increasing len_{max} & Θ_{min}. In (a), to comply with len_{max}, the skeleton's layout changes drastically with the increase of len_{max}. The same behavior is noticed with the variation of Θ_{min}, at a point where additional bars start appearing (circled in red, 4th design in (b)). *The pink arrow is the build orientation, the red arrow is the normal of the beam.*

appears (the 4th design in Fig.7b).
To sum up, DL-AM-TO captures the geometrical and mechanical constraints concurrently and responds to geometrical changes creatively; the obtained results encourage the further improvement of the model.

4.4. Discussion

DL-AM-TO's performance is tied with several criteria.
The first impact comes from the input data samples. In this work, the traditional SIMP was chosen to forward the GM-CAD dataset creation as detailed in section 3.1 of the article [6]. SIMP may not be the most performant but is the simplest and easily implemented TO algorithm (found in $\approx 70\%$ of the industrial and commercial software). Thus, the designs driving the training might not be the most optimal ones but are sufficient to validate the methodology proposed. Indeed, any new data coming from other more optimal TO algorithms can be used to train our model and improve its performance. Additionally, the mechanical conditions of GMCAD's designs are predictions of DL-models, which adds a layer of uncertainty over the input training data samples, and its impact is to be investigated in future works[6].
Moreover, It is important to highlight that the main objective here is not to create a new TO algorithm but to compensate for the difficulties faced in TO to integrate the mechanical and the geometrical conditions simultaneously at the same level via DL architectures, particularly generative networks.
In the second position comes the geometrical discriminators' performance. The better the discriminator predicts the geometrical condition, the more informative the generator's loss function is; hence, DL-AM-TO is more reliable. We note that it is trained within GAN frameworks known for their unstable oscillating losses, which explains its sensitivity to the losses delivered by its discriminators. This phenomenon is observed with the th_{min} variable; integrating the latter to the model deteriorated its performance. The th_{min} discriminator was not as precise as it should be. As a matter of fact, the image-like designs in GMCAD are CADS converted to images with computer vision filtering techniques, which can easily alter the thicknesses of the design.
Finally, the proposed method's objective is to generate one design complying with specific input geometrical conditions. However, the latter can be turned as objectives, and changing multiple conditions at a time for multiple times will generate a set of optimal Pareto front solutions.

5. Conclusion

In this work, we propose a novel DL-based approach, DL-AM-TO, to facilitate the integration of geometrical AM-related constraints into the early design phases of the DfAM cycle.

In general, in product development, mechanical and geometrical design are two separate phases for each requires different skills and, most importantly, human expertise. Integrating manufacturing constraints with conventional FE-TO methods is cumbersome, especially since many manufacturing constraints lack an analytical formulation. We address this problem and bridge the gap between the mechanical and geometrical worlds via DL generative methods. DL treats the design as an image, a distribution of density, and not like a sketch or a parametric CAD, which makes it compatible with the mechanical design phase (TO), allowing us to integrate the mechanical and geometrical constraints concurrently at the same level.

It is essential to highlight that DL is not here to replace FE and robust mechanical calculations. On the opposite, it compensates for the difficulties encountered by TO when considering geometric-manufacturing constraints at the conceptual level of design, especially since DL has demonstrated its potential in learning spatial correlations. The DL generative method, DL-AM-TO, accelerates the designer's work, for it offers a broader possibility and versatility of designs within a fraction of seconds.

In the future, further constraints will be incorporated into DL-AM-TO, including non-linear ones (buckling, thermal distortion, etc.), for the GAN framework along which DL-AM-TO is trained offers flexibility to consider as many constraints as needed. DL-AM-TO can be implemented into CAD software as a lighter and faster generative module.

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