Computational design of mechanical metamaterials

Silvia Bonfanti[1,2], Stefan Hiemer[1,3,4], Raja Zulkarnain[1], Roberto Guerra[1], Michael Zaiser[3,*], and Stefano Zapperi[1,4,‡]

[1]Center for Complexity and Biosystems, Department of Physics "Aldo Pontremoli", University of Milan, Via Celoria 16, 20133 Milano, Italy
[2]NOMATEN Centre of Excellence, National Center for Nuclear Research, ul. A. Soltana 7, 05-400 Swierk/Otwock, Poland
[3]Institute of Materials Simulation, Department of Materials Science Science and Engineering, Friedrich-Alexander-University Erlangen-Nuremberg, Dr.-Mack-Str. 77, 90762, Fürth, Germany
[4]CNR – Consiglio Nazionale delle Ricerche, Istituto di Chimica della Materia Condensata e di Tecnologie per l'Energia, Via R. Cozzi 53, 20125 Milano, Italy
[*]e-mail: michael.zaiser@fau.de
[‡]e-mail: stefano.zapperi@unimi.it

ABSTRACT

The geometry of mechanical metamaterials is specially designed to achieve peculiar functions, either in terms of remarkable mechanical properties or in terms of programmed mechanisms or responses. In the past few years, metamaterial design was empowered by computational tools that allowed to overcome limitations of human intuition. Leveraging efficient optimization algorithms and computational physics models, it is now possible to explore vast design spaces, achieving new material functionalities with unprecedented performance. In this perspective, we present our viewpoint on the state of the art of computational metamaterials design, discussing recent advances in topology optimization and machine learning design with respect to challenges in additive manufacturing.

Key points:

- Mechanical metamaterials are traditionally designed based on the replication of elementary mechanisms.
- Topology optimization and machine learning can be used to extend the possibilities of metamaterials design.
- Computational design should be constrained to meet the specifications of additive manufacturing methods.
- Well-curated public databases of mechanical metamaterial structures would be needed as a tool and for designers.

Website summary: A perspective on computational approaches to the design of mechanical metamaterials discussing mechanism based design, topology optimization, machine learning and the challenges for additive-manufactured metamaterial structures.

1 Introduction

Mechanical metamaterials (MM) are artificial materials designed to display peculiar mechanical properties or programmed response thanks to a careful optimization of their geometrical features[1,2]. Examples include auxetic metamaterials displaying negative Poisson's ratio [3–8], breaking force reciprocity[9] or exhibiting pre-programmed mechanical responses under compression[10–12]. The traditional strategy employed to design MM is based on the periodic replication of unit cells which produce the desired response[1] This design strategy starts from the identification of a basic mechanism, such as beam buckling, in a simple element which is then used as a building block for the unit cells. To render this approach efficient, several analytical approaches can be used as tools to guide intuition[1] and to restrict the design space to fulfill requirements such as mechanical stability. For instance in truss networks, Maxwell's stability criterion can guide the design by ensuring that the arrangement of trusses and nodes meets basic stability requirements[13]. Of equal importance are basic microstructure parameters such as the relative density of the MM relative to the solid material from which it is constructed. It is well established that simple scaling laws determine how changes in microstructure parameters affect the overall mechanical performance of the material[14]: Structures with high connectivity tend to show stretching-dominated behavior, characterized by a linear relationship between the effective elastic modulus and the relative density, while less connected structures tend to produce bending-dominated behavior characterized by power-law relationships. Intermediate disordered structures can sometimes fall in between these two limits[15].

Human guided heuristic design has identified and exploited a wide range of MM mechanisms, and combined them to generate more complex characteristics. Important classes of MM designed in this manner include i) programmable metamaterials, designed to exhibit highly adaptive spatial structures sometimes inspired by origami and kirigami[1,16]; ii) chiral MM, providing mechanisms to transform linear into rotational motion[17,18] (for potential applications see[19]); iii) auxetic metamaterials, which contract along the lateral direction under compression[3–7,20] and iv) hierarchical metamaterials, exhibiting a multi-scale organization to achieve multi-functionality and multi-stability[21,22].

Mechanism-based design is limited by the intuition of human designers who may find it increasingly difficult to invent structures of ever increasing complexity with well-defined, possibly multiple mechanical functionalities. Computational methods can help to overcome this limitation by automating the design process, allowing for the solution of precisely formulated design problems, to generate optimal solutions that elude manual design. In this perspective, we discuss recent advances in computational metamaterials design, highlighting the constraints posed by additive manufacturing.

2 Metamaterials design by optimization methods

A broad class of computational methods used to optimize structures so that they maximize specific target properties, such as strength, flexibility or weight reduction, may be summarized under the label topology optimization (TO)[23,24].

In TO, the objective is to determine the optimal way to distribute the material within a given geometry, using a material with specific characteristics, subjected to prescribed governing equations as well as considering initial/boundary conditions. The optimal arrangement of filled and empty elements is found by iteratively improving an objective function subjected to constraints, resolving the ensuing physical problem often using the finite element method (FEM).

In *continuous* optimization approaches such as solid isotropic material with penalization (SIMP) [25–27], the requirement of having filled/empty elements is relaxed to allow for continuous densities, varying from zero (=empty) to one (=filled). The original objective function is then reformulated by introducing penalties to push the densities to zero or one while still enforcing optimal performance. Naive applications with constrained optimization and low-order elements result in checkerboard artifacts (Fig. 1(a)) and designs with a mesh-dependent length scale, rendering convergence impossible[28–30]. Smoothing filters, as used in image processing, applied to gradients or densities[31–34], eliminate checkerboards and decouple the final design scale from mesh details, rendering it dependent only on the filter size (compare Figures 1(b),1(c) and 1(d). Common optimization algorithms include optimality criteria method[35], method of moving asymptotes[36], and sequential linear/quadratic programming[23]. The typical SIMP workflow involves: i) solution of the physical problem via FEM, ii) computation of density gradients, iii) filter application, iv) density update via a gradient optimization scheme, v) repetition of the previous steps until converged and vi) postprocessing to ensure a manufacturable design. Continuous alternatives to SIMP include phase-field[37–39] and level-set methods[40–43]. Phase-field methods exhibit slower convergence, while level-set methods require more sophisticated regularization procedures compared to SIMP[24,43].

Discrete optimization approaches can be subdivided into randomized and deterministic methods. Examples of random algorithms include simulated annealing[47–49], differential evolution[50,51], and genetic algorithms[52,53]. The optimization begins with an initial guess, generates a new structure through a random process, compares the figure of merit of old and new design and applies an acceptance criterion, repeated until converged. Evolutionary Structural Optimization (ESO) and Bi-directional ESO use instead deterministic evolution rules, respectively removing "inefficient" material[54,55] or adding and deleting material at each iteration[56,57]. An advantage of discrete approaches is that they enable the treatment of non-smooth problems, and of non-connected design spaces[58]. Another advantage, although still debated, is the possibility to efficiently find global minima, i.e. optimal performance in a given design space, which can be difficult for gradient-based continuous methods when multiple local optima are present[59]. The main limitation of discrete methods is their unfavorable computational scaling with the number of design variables, leading to the use of coarse meshes, reducing the physical accuracy and therefore limiting the achievable performance due to the lack of finely detailed structures. Mixed discrete/continuous formulations can be useful for truss-based optimization as they circumvent the need to optimize in a predefined lattice or to connect all nodes to each other[60].

Compliant mechanisms are flexible structures which transmit force and motion[61] without the need of joints and hinges, thus reducing parts, assembly steps, and the need for lubrication. In this context, the design objectives are maximizing or controlling input/output ratio (displacement, energy or force), and movement path considering constraints like limited radius of action or external resistance[23,31]. Special filters[62,63] and constraints[64–68] have been developed to avoid stress concentrations and numerical artifacts. Design of compliant mechanisms has been generalized beyond purely mechanical functionalities to multiphysics problems like thermal microactuators[69], electro-thermal microactuators[70] and MEMS devices[71,72]. Bi-stable compliant mechanisms - structures that have two stable equilibrium configurations - are applied in smart applications and soft robotics due to their simplicity and stability[73–75]. Discrete methods based on beam elements have been used to design compliant mechanisms such as MM actuators implementing vertical-horizontal motion transfer[48] (Fig. 2(a)(b)), pliers mechanisms[48] and twist-compression transformations[49] (Fig. 2(c)(d)). For an overview specifically dedicated to design of compliant mechanisms we refer the reader to a review by Zhu et al.[61].

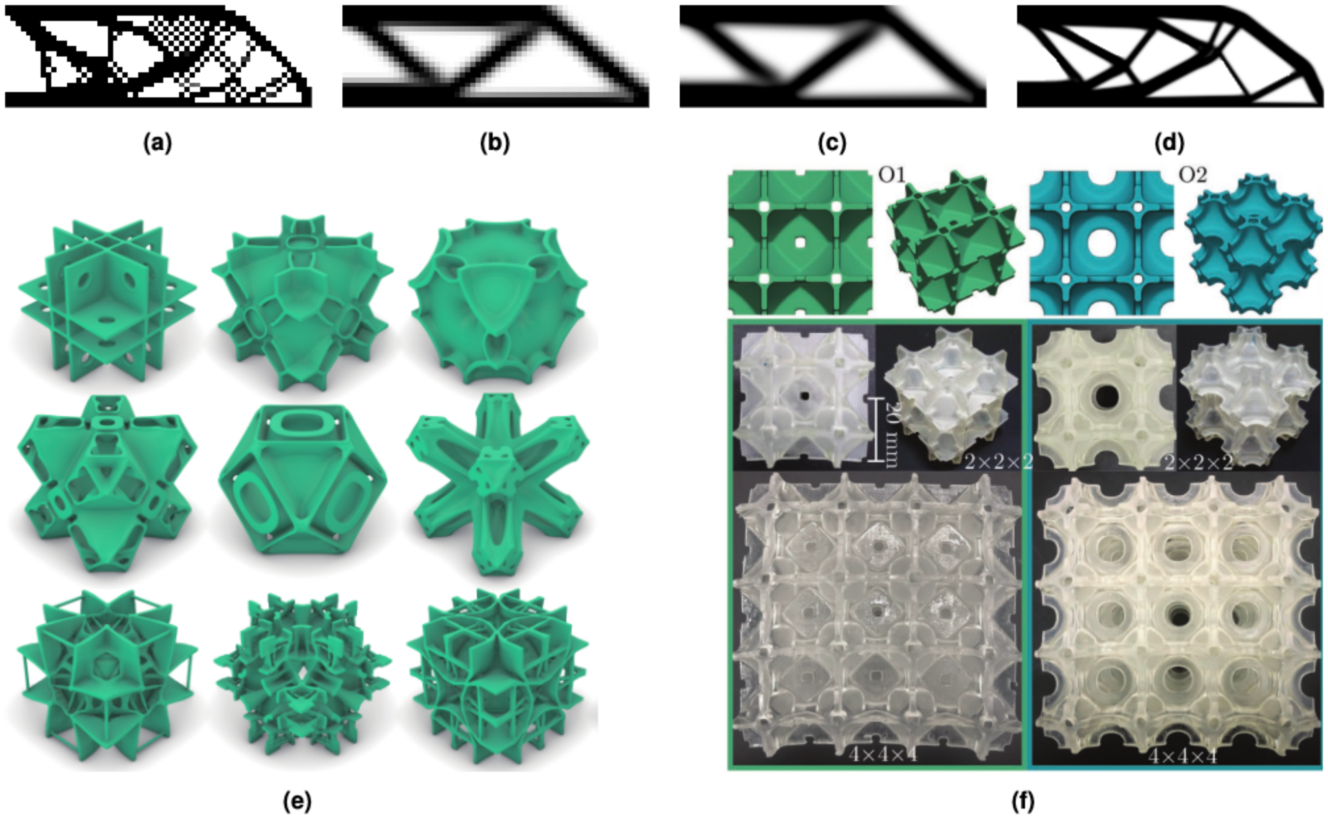

Figure 1. Metamaterials generated by continuous optimization (a)-(d) Example of a continuous optimization problem with different filter settings and mesh sizes[44] obtained from https://www.topopt.mek.dtu.dk/apps-and-software: (a) no filter and checkerboard artifacts, (b) sensitivity filtering for a 60x20 elements mesh and filter size 4 % of the beam length, (c) same settings as previously but 240x80 mesh, (d) 240x80 mesh but filter radius set to 2.4 element lengths; (e) maximization of bulk (top row) and shear modulus (middle row) as well as minimization of Poisson's ratio (bottom row) for different initial density guesses taken from Ref.[45], (f) microstructure for maximum Young's modulus (O1) and trade-off between buckling strength and Young's modulus (O2) taken from[46].

While homogenization maps a small scale geometry to macroscopic properties, *inverse homogenization* reverses this process to find microstructure geometries matching a desired set of effective properties[6,7]. Linear inverse homogenization is numerically highly efficient and enables highly detailed metamaterials (Fig. 1(e))[45]. A cheaper alternative to FEM approaches are models using rigid rods moving freely at nodes[76] to describe deformation behaviour[77,78] especially for auxetic designs[79]. Wang[80] explored the trade-off between Young's modulus and buckling strength, showing that in a multi-objective optimization scheme the Young's modulus decreased to a range of 79% to 58% compared to a stiffness-optimized closed-cell plate material while uniaxial buckling strength improved by two to eight times. Another application of TO created nonhierarchical designs (Fig. 1(f)) with stiffness surpassing both traditional truss and plate microstructures[46]. Furthermore, materials with Poisson's ratio values varying between -0.8 and 0.8 have been discovered which maintain this property over a wide strain range up to 20%[81].

Inverse homogenization allows for customization and optimization of material microstructures towards meeting homogenized properties, while topology optimization seeks the best distribution of a material with given properties to meet a desired macroscopic behavior under prescribed boundary conditions. Integrating macro- and microstructural optimization through *multiscale* topology optimization seeks to combine both approaches and to enable the search for optimal materials across multiple length scales. Techniques can be classified into two approaches: i) take a microstructure characterized by a limited set of geometrical and/or composition parameters as typically done in traditional composite design, and optimize these in view of obtaining local effective properties that best match a macroscale design, ii) optimize the macroscale by SIMP and the microscale with inverse homogenization[82,83]. Examples of the first method include structures with predefined stress responses obtained by tuning microstructures consisting of small rectangular holes in a bulk material[84], or stiffness-optimal[85,86] laminate patterns[25]. A revival of this approach has been caused by methods coined as de-homogenization[87–89] which project the macro-scale

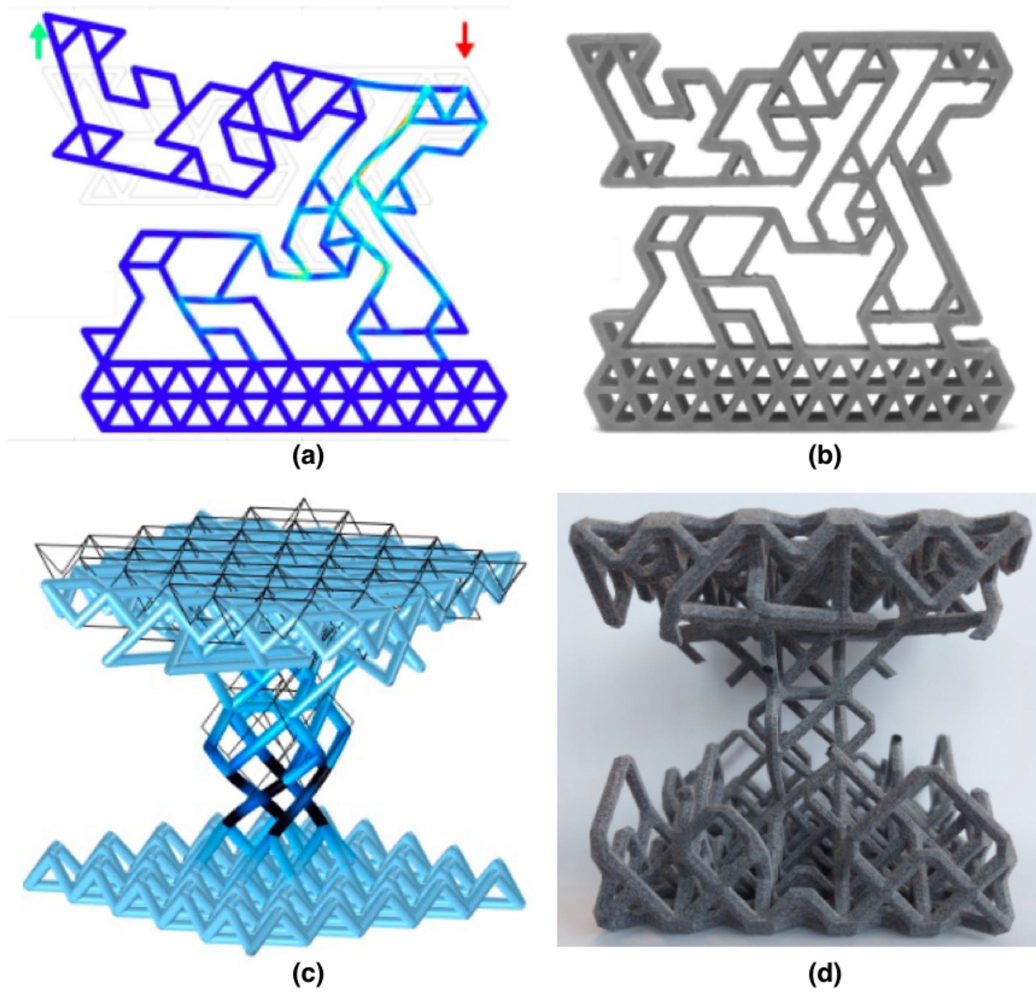

Figure 2. Flexible metamaterials obtained through discrete optimization. A two-dimensional realization implementing transfer from vertical to horizontal motion (a) is obtained by discrete optimization and then (b) realized experimentally by additive manufacturing (from[48]). A three-dimensional example implementing compression-induced rotation is reported in panels (c) and (d) (from[49]).

microstructure parameters smoothly to finer scales as a postprocessing step of the macroscale TO. For this purpose, standard techniques from numerical mathematics[89,90] and image processing/graphics rendering[91–93] have been applied for 3D[90,92] and 2D multiple loading problems[94]. When opting for unit cells created by inverse homogenization, special care must be taken as the cells must be able to rotate to align with principal stresses[95], change domain shape and be compatible/connected to transmit load, aspects which are not considered in textbook inverse homogenization[23].

The optimization methods discussed above can in principle produce structures that are impossible to realize experimentally by additive manufacturing (AM) which is increasingly used in metamaterials due to its flexibility and design freedom. Manufacturability is a problem that strongly depends on the specific nature of the AM process, and dealing with the resulting optimization constraints has given rise to a significant research activity. A literature search highlights the effort devoted to computational optimization methods across various additive manufacturing (AM) techniques (Figure 3). The majority of papers published on the subject focus on Powder Bed Fusion (359 papers) and Material Extrusion (142 papers), owing to their relevance in industrial and commercial applications. Vat Photopolymerization (61 papers) and Directed Energy Deposition (29 papers) are also considered, but to a lesser extent. Binder Jetting (10 papers) and Material Jetting (8 papers) are so far rarely studied in the context of optimization.

Simulating AM processes in their entirety is challenging due to their inherent multiscale character and the multitude of phenomena involved. Most often, this problem is attacked by formulating constraints resulting from the envisaged manufacturing process and including these within the optimization scheme, either through generic geometry considerations or by simplified physical process models to keep the computational expense in check.

Manufacturing constraints may concern both geometry and microstructure. Geometrical constraints may arise, for example, from the fact that most AM methods use layer-by-layer fabrication which imposes minimum feature sizes and may not permit to produce geometries with overhangs. To deal with such constraints, one can enforce a minimum geometric feature size based on generic assumptions about process resolution (e.g., printing nozzle size)[96] or ensure manufacturability of overhanging structures by limiting the overhang angles[97,98], combined with additional constraints to prevent undeirable features such as downward-facing cones or sawtooth patterns. Another approach involves employing a simplified geometric process model, based on the principle that printable structures must be supported by underlying elements with sufficient density[99–101].

In powder based AM techniques, further limitations come from voids in which powder remains trapped. One can avoid voids entirely by defining and solving auxiliary problems like nonlinear heat conduction[102] or discrete particle diffusion[103] where virtual heat/particles are inserted into void regions which must then be able to escape to yield a printable design. Spectral graph theory[104] offers an alternative pathway to void identification. Auxiliar approaches can also be used to create excavation holes[105,106] or the voids can be tolerated under the condition that they are self-supported[107]. Material anisotropy due to build orientation[108] or deposition orientation[109] can be included via a generic anisotropic stiffness tensor.

Simple geometry considerations are, however, not capable of capturing effects like overheating, residual stresses and other phenomena that depend on the physics of the manufacturing process. To avoid the unsustainable computational effort of dealing with a full physical description in conjunction with an optimization task, simplified process models may be used. One of the easiest adaptations is to mimic the layer-by-layer process in terms of sequential activation of element layers[110]. For the detection of overheating a slab model has been developed where the structure is segmented into overlapping slabs whose top represents a heat source simulating the behavior of a laser while the bottom serves as a heat sink[111,112] and solutions of the static heat conduction equation are used to estimate temperature profiles. Others try to circumvent the need for thermo-mechanical coupling through the use of semi-empirical schemes to infer residual strains via the inherent strain method[113] or one of its modifications (e.g.[114]) in order to reduce part distortions and residual stresses[115]. Simplified models may also be used to describe the dependency of microstructure on thermal history. For instance, it was proposed to estimate mechanical properties of steel based on the time spent in a critical heating and cooling cycle within a temperature range between 500° C and 800° C[116]. A more detailed technical discussion of these issues can be found in[117]. We note that such highly simplified models of process-microstructure-property relationships have strong limitations. They can help to ensure that the as-manufactured material indeed has properties close to those assumed in the optimization process, but much more detailed process models may be needed if one wants to exploit the inherent spatial variability of AM process parameters, such as beam intensity and profile[118], scanning velocity and hatching strategy[119], as well as the facility of manufacturing compositionally graded parts[120], in order to optimize material performance by co-designing geometry *and* microstructure[121].

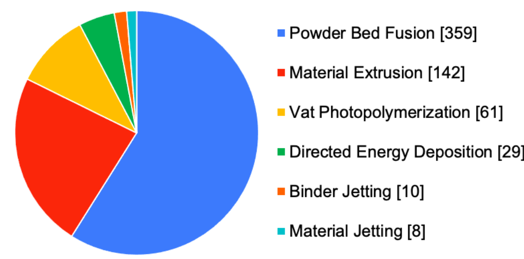

Figure 3. Chart of the number of papers in the literature, in brackets, for different AM processes.

3 Machine-learning assisted metamaterials design

Recent years have witnessed an explosive growth of the use of machine learning (ML) im metamaterials design. It is therefore important to take a critical look at ML based MM design, highlighting improvements and limitations when compared to more traditional optimization strategies. We can classify ML design solutions into the following categories which are a modified subset of the review by Woldseth *et al.*[122]: direct design, design acceleration, dimensionality reduction and post-processing. Other classification schemes exist and have been mentioned in other review papers[123–125].

In the category *direct design*, the process begins with a set of desired outcomes e.g. material properties or an output force and infers the optimal design backwards. Mao *et al.*[126] present an approach capable of systematically generating 2D metamaterials with extreme stiffness, using generative adversarial networks (GANs) trained on millions of randomly generated structures[44]. Kollmann and coworkers instead use a convolutional neural network (CNN) to predict the optimal metamaterial design on a 128×128 mesh trained on data generated by TO (see Fig. 4(a)). Their model is based on the volume fraction used for the volume constraint, and an identifier that specifies whether the bulk/shear modulus (or Poisson's ratio) should be maximised (or minimized), with a dataset of 30000 samples[127].

Several computational challenges are associated with *direct design* ML. To generate reliable designs, the algorithm should be trained on many and diverse examples able to capture a wide range of variations[122], but obtaining enough data to train ML is extremely difficult especially for large samples because each optimized sample requires a full TO process. If training is carried out on randomly generated samples, on the other hand, these have a very low probability to represent or approximate optimum solutions for any particular problem. Furthermore, inverse homogenization is non-unique and starting guess sensitive[95], therefore the ML model has to solve a non unique task.

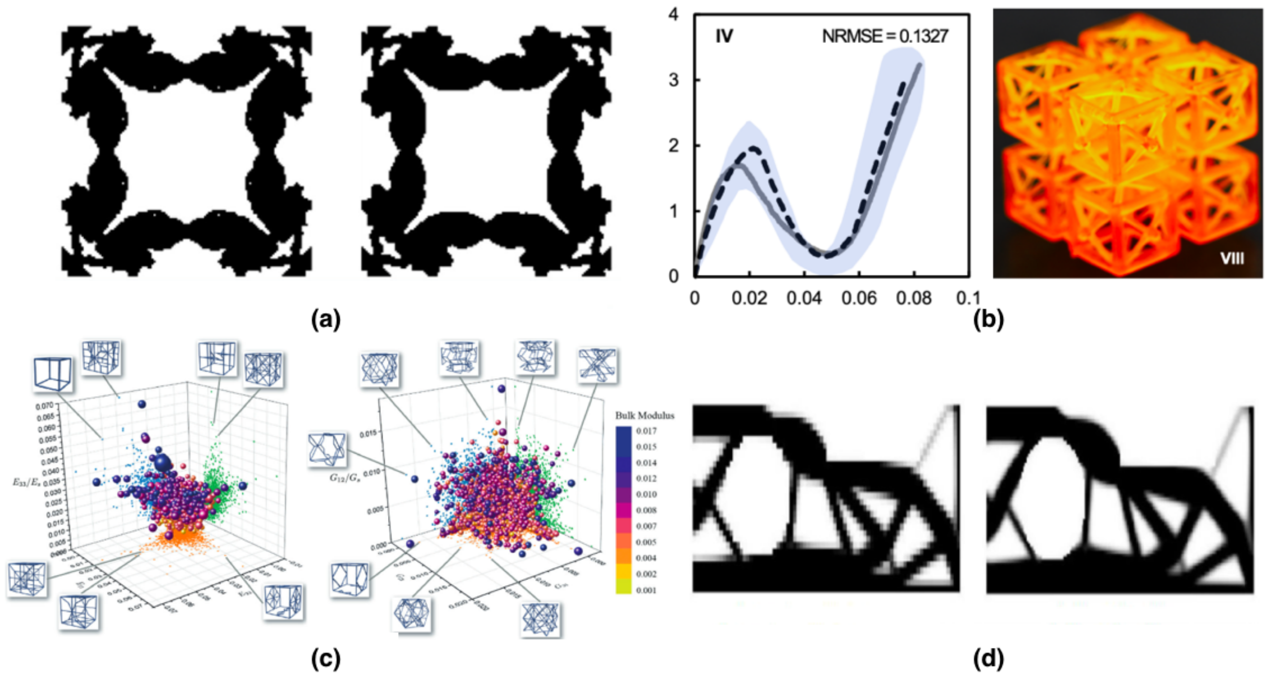

Figure 4. Example of use of ML for the design of mechanical metamaterial for different purposes. (a) Direct design example: ground truth (left) and predicted (right) design minimizing Poisson's ratio[127]. (b) Design acceleration: Target stress-strain curve and corresponding printed metamaterial[128]. (c) Dimensionality reduction: truss database showing effective directional Young's moduli (left) and shear moduli (right) along the three principal cubic directions and projections, adapted from[129]. (d) Post-processing from optimized low resolution (left) to high (right)[130].

For achieving the aim of *design acceleration*, two research directions have been followed to reduce the computational cost: i) reduction of the number of iterations needed to obtain a final design, ii) replacement of simulations and/or property calculations by ML predictions. For the first goal, two main strategies have been used: to either map an intermediate design to its converged result via image-to-image prediction of the full[131] or segmented design[132], or to interpret the iterative optimization as a time series extrapolation task[133], where the density evolution of elements during the initial stage of the TO process is used by a deep belief network to predict a near-final outcome which may then be 'polished' by performing another round of TO steps, cutting out the majority of TO calculations in the process. The first approach however is inherently mesh dependent and quite expensive as it again needs a full finite element simulation to generate one independent design sample. The latter approach can become efficient but, for problems of considerable size, the DBN training process may be lengthy and const intensive in term of samples, and the need for training sets to encompass entire DO trajectories of large samples might cause memory issues. Furthermore, non regular meshes may not fit into common image/movie based ML approaches, so one is again confined to specific types and sizes of meshes.

A second method consists in using a ML predictor to replace the physical model. Two examples where this approach has been used are Deng *et al.*[134] and Ha and coworkers[128], who tailor the stress-strain response of periodic meta materials to match desired nonlinear stress-strain curves, as shown in Fig. 4(b). In these two studies, unit cells with a prescribed set of topologies and a limited number of design parameters are periodically replicated and the ML is used to choose design topologies and parameters that match a desired response. Both Deng *et al.*[134] and Ha *et al.*[128] only represent proof-of-concept studies: The former only comprises 16 degrees of freedom to optimize a periodic metamaterial whose unit cell conists of four hinged quadrilaterals, using a training set of 7500 samples. In the second case we are dealing with periodic beam networks with cubic unit cells, the model has three degrees of freedom and is parameterized on a dataset of 1212 samples. In both cases it is arguable whether the use of the ML algorithms is cost effective, since the low dimensionality of the design spaces should allow for efficient direct optimization. d

Bonfanti *et al.* highlighted these issues when replacing optimization based on a discrete model with linear and angular springs with a deep neural network trained on images of truss based-MM [48]. While the algorithm was performing well in the validation set it required a vast amount of discrete element calculations to annotate the dataset, rendering the overall scheme cost ineffective. An advantage could only come from transfer learning, if training on a small scale structures could be generalized to design larger scale structures that are harder to simulate[48].

Dimensionality Reduction is usually achieved by implementing an information bottleneck into the ML model. The network is trained to construct the structure using the reduced variables and with the structure-response inference based on the bottleneck representation. This reduced representation, called latent space, can serve different purposes. It can act as a biasing procedure, as it is expected that the designs generated in this latent space carry properties similar to their trained counterparts. Greminger *et al.* train GANs on manufacturable parts to project the SIMP densities into a space that that is expected to guarantee manufacturable designs, and over which TO then is performed[135]. An approach for designing visually appealing wheels was proposed by Oh *et al.* who used GANs trained on images to propose an initial design as starting point for TO to combine aesthetics and mechanical requirements[136]. Another application of dimensionality reduction has been to find a reduced representation of the design space of truss metamaterials which is inherently discrete and high dimensional, mapping this on a continuous latent space of lower dimensionality and then carrying out TO on the reduced space[129], see Fig. 4(c)).

Post-processing refers to the modification of the geometry *after* an initial optimization. An example is downscaling, which refines solutions obtained on coarse meshes to approximate the results obtained with computationally more expensive finer meshes. In downscaling optimization with ML, efforts include enhancing image resolution from low to high, eliminating the need for computationally demanding calculations. In References[137] and[130], the authors convert a coarse mesh design, or overlapping slabs of it in the form of grayscale images, into more refined high-resolution meshes, reducing the computation time (see Fig. 4(d)). A limitation of this approach is that TO is length scale dependent, which is enforced by the regularization filter. This means that the downscaled design is restricted by the resolution of the coarse mesh. Dehomogenization suffers from the same problem, but it compensates by using internal variables that encode the microstructures across different scales. A interesting example for ML postprocessors is a dehomogenization network by Elingaard and collaborators where the network is trained solely on synthetic geometric patterns, not generated by TO. This makes the method independent of the physical details like domain, boundary conditions, and so on[138]. This approach has by now been outperformed by other dehomogenization approaches Ref.[93], but still demonstrates that ML can be a useful complement to TO approaches.

4 Conclusion and perspectives

In this review, we have discussed current trends in the design of MM. The advent of efficient algorithm and the availability of increasingly powerful computational resources is reshaping metamaterial research, traditionally based on trial and error, into a more systematic exploration of an expanding design space. Algorithms can now be used to predict the most suitable geometry needed to achieve a given mechanical function, overcoming many limitations of traditional human-based design. While human imagination is now expanded thanks to the use computational methods, major challenges still remain, such as a more detailed incorporation into the design process of physical aspects related to the manufacturing. In most of the outlined design approaches, material properties are assumed as given, but in reality, the material microstructure - which determines the material properties - results from a manufacturing process where local process history strongly depends on the geometry of the manufactured part. In current approaches to MM design, such interdependencies are undesirable complications which limit design accuracy. However, targeted spatio-temporal manipulation of manufacturing process parameters in order to vary the local composition, crystallography, phase and/or defect microstructure of AM samples to achieve superior overall properties may be the next frontier in MM design. Beyond design and optimization of geometry, 3D printing of microstructures requires the simultaneous consideration of sample geometry, process-microstructure and microstructure-property relations. Availability of predictive models either based upon a clear physical understanding of microstructures and processes, or upon data analysis of extensive repositories of process-microstructure-property data, is an essential prerequisite for this next step. Microstructure is also essential for stimulus-responsive metamaterials. This holds for materials with intrinsic functionalities such as ferroelectric, piezoelectric and ferromagnetic materials, where microstructure needs to be considered and manipulated on the domain level, and shape memory alloys where martensitic microstructure dominates functionality. Even more important is microstructure for multifunctional AM composites that rely on embedded functional micro-and nanoparticles to transfer functionalities to a matrix material. In such composites, both the spatial arrangement and the functional state of the embedded particles create additional design degrees of freedom that can be manipulated either during or after the manufacturing process by appropriate thermal, electromagnetic or mechanical fields (field assisted AM[139]). For such materials, co-design of metamaterial geometry and metamaterial microstructure is mandatory to achieve optimal performance, and the development of appropriate design methodologies may be an essential task controlling progress in the field of multifunctional metamaterials.

Looking still further ahead, an intriguing future roadmap may be based the development of metamaterials that can learn and adapt by themselves[140]. This idea finds a parallel in the electronic realm, as shown by Dillavou and coworkers[141] with nonlinear electronic metamaterials. Their work, involving self-adjusting transistor-based networks, highlights the possibilities for emergent learning. This breakthrough in electronic metamaterials could inspire similar advancements in the MM sector, bridging the gap between both domains and leveraging the principles of neuromorphic computing and autonomous adaptation.

It is also important to discuss potential pitfalls that can occur when using computational methods to design MM. In TO, applications with moderate element numbers ($\leq 10^6$), simple constitutive laws and problem statements can already be solved by a standard personal computer where structures comprised by to 10^8 elements can be comfortably designed with the use of a single GPU[45]. However, future optimization tasks may be much more complex, and there may be an increasing need to rely on data analytic approaches to quantify concepts like manufacturability and aesthetics[136]. However, availability of training data and transferability of results between different training scenarios remain crucial problems. Creating up to millions of training samples to solve small problems is uneconomical and unecological, as is creating data purely for the purpose of training a single ML algorithm. To be useful, published data must be adequately curated even if they are mere byproducts of more interesting endeavours. To fulfill the current need of well curated training data, it would be desirable to create a public repository devoted to metamaterials, akin to NOMAD[142] in the context of quantum chemistry, where researchers could upload their structures and properties as source for future ML efforts. At the same time, journal editors and reviewers should enforce open data policies[143] and mandatory upload to such databases, as it is now routinely done in the case of genomic data.

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6 References

References

1. Bertoldi, K., Vitelli, V., Christensen, J. & Van Hecke, M. Flexible mechanical metamaterials. *Nat. Rev. Mater.* **2**, 1–11 (2017).
2. Xia, X., Spadaccini, C. M. & Greer, J. R. Responsive materials architected in space and time. *Nat. Rev. Mater.* **7**, 683–701 (2022).
3. Lakes, R. Foam structures with a negative poisson's ratio. *Science* **235**, 1038–1040 (1987).
4. Lakes, R. Deformation mechanisms in negative poisson's ratio materials: structural aspects. *J. materials science* **26**, 2287–2292 (1991).
5. Milton, G. W. Composite materials with poisson's ratios close to—1. *J. Mech. Phys. Solids* **40**, 1105–1137 (1992).
6. Sigmund, O. Materials with prescribed constitutive parameters: an inverse homogenization problem. *Int. J. Solids Struct.* **31**, 2313–2329 (1994).
7. Sigmund, O. Tailoring materials with prescribed elastic properties. *Mech. materials* **20**, 351–368 (1995).
8. Evans, K. E. & Alderson, A. Auxetic materials: functional materials and structures from lateral thinking! *Adv. materials* **12**, 617–628 (2000).
9. Coulais, C., Kettenis, C. & van Hecke, M. A characteristic length scale causes anomalous size effects and boundary programmability in mechanical metamaterials. *Nat. Phys.* **14**, 40–44, DOI: 10.1038/nphys4269 (2017).
10. Florijn, B., Coulais, C. & van Hecke, M. Programmable mechanical metamaterials. *Phys. review letters* **113**, 175503 (2014).
11. Florijn, B., Coulais, C. & van Hecke, M. Programmable mechanical metamaterials: the role of geometry. *Soft matter* **12**, 8736–8743 (2016).
12. Rayneau-Kirkhope, D. J. & Dias, M. A. Recipes for selecting failure modes in 2-d lattices. *Extrem. Mech. Lett.* **9**, 11–20 (2016).
13. Gibson, L. J., Ashby, M. F. & Harley, B. A. *Cellular materials in nature and medicine* (Cambridge University Press, 2010).

14. Ashby, M. F. The properties of foams and lattices. *Philos. Transactions Royal Soc. A: Math. Phys. Eng. Sci.* **364**, 15–30 (2006).

15. Rayneau-Kirkhope, D., Bonfanti, S. & Zapperi, S. Density scaling in the mechanics of a disordered mechanical meta-material. *Appl. Phys. Lett.* **114** (2019).

16. Lin, X. *et al.* Mechanical fourier transform for programmable metamaterials. *Proc. Natl. Acad. Sci.* **120**, e2305380120 (2023).

17. Frenzel, T., Kadic, M. & Wegener, M. Three-dimensional mechanical metamaterials with a twist. *Science* **358**, 1072–1074 (2017).

18. Fernandez-Corbaton, I. *et al.* New twists of 3d chiral metamaterials. *Adv. Mater.* **31**, 1807742 (2019).

19. Wu, W. *et al.* Mechanical design and multifunctional applications of chiral mechanical metamaterials: A review. *Mater. & design* **180**, 107950 (2019).

20. Bertoldi, K., Reis, P. M., Willshaw, S. & Mullin, T. Negative poisson's ratio behavior induced by an elastic instability. *Adv. materials* **22**, 361–366 (2010).

21. Zhang, H., Wu, J., Fang, D. & Zhang, Y. Hierarchical mechanical metamaterials built with scalable tristable elements for ternary logic operation and amplitude modulation. *Sci. Adv.* **7**, eabf1966 (2021).

22. Zhang, X. *et al.* Kirigami-based metastructures with programmable multistability. *Proc. Natl. Acad. Sci.* **119**, e2117649119 (2022).

23. Bendsoe, M. P. & Sigmund, O. *Topology optimization: theory, methods, and applications* (Springer Science & Business Media, 2003).

24. Sigmund, O. & Maute, K. Topology optimization approaches: A comparative review. *Struct. multidisciplinary optimization* **48**, 1031–1055 (2013).

25. Bendsøe, M. P. Optimal shape design as a material distribution problem. *Struct. optimization* **1**, 193–202 (1989).

26. Zhou, M. & Rozvany, G. The coc algorithm, part ii: Topological, geometrical and generalized shape optimization. *Comput. methods applied mechanics engineering* **89**, 309–336 (1991).

27. Mlejnek, H.-P. & Schirrmacher, R. An engineer's approach to optimal material distribution and shape finding. *Comput. methods applied mechanics engineering* **106**, 1–26 (1993).

28. Diaz, A. & Sigmund, O. Checkerboard patterns in layout optimization. *Struct. optimization* **10**, 40–45 (1995).

29. Jog, C. S. & Haber, R. B. Stability of finite element models for distributed-parameter optimization and topology design. *Comput. methods applied mechanics engineering* **130**, 203–226 (1996).

30. Sigmund, O. & Petersson, J. Numerical instabilities in topology optimization: a survey on procedures dealing with checkerboards, mesh-dependencies and local minima. *Struct. optimization* **16**, 68–75 (1998).

31. Sigmund, O. On the design of compliant mechanisms using topology optimization. *J. Struct. Mech.* **25**, 493–524 (1997).

32. Bourdin, B. Filters in topology optimization. *Int. journal for numerical methods engineering* **50**, 2143–2158 (2001).

33. Bruns, T. E. & Tortorelli, D. A. Topology optimization of non-linear elastic structures and compliant mechanisms. *Comput. methods applied mechanics engineering* **190**, 3443–3459 (2001).

34. Lazarov, B. S. & Sigmund, O. Filters in topology optimization based on helmholtz-type differential equations. *Int. J. for Numer. Methods Eng.* **86**, 765–781 (2011).

35. Prager, W. & Taylor, J. E. Problems of optimal structural design. (1968).

36. Svanberg, K. The method of moving asymptotes—a new method for structural optimization. *Int. journal for numerical methods engineering* **24**, 359–373 (1987).

37. Bourdin, B. & Chambolle, A. Design-dependent loads in topology optimization. *ESAIM: Control. Optimisation Calc. Var.* **9**, 19–48 (2003).

38. Wang, M. Y. & Zhou, S. Phase field: a variational method for structural topology optimization. *Comput. Model. Eng Sci* **6**, 547–566 (2004).

39. Garcke, H., Lam, K. F., Nürnberg, R. & Signori, A. Overhang penalization in additive manufacturing via phase field structural topology optimization with anisotropic energies. *Appl. Math. & Optim.* **87**, 44 (2023).

40. Osher, S. & Sethian, J. A. Fronts propagating with curvature-dependent speed: Algorithms based on hamilton-jacobi formulations. *J. computational physics* **79**, 12–49 (1988).

41. Sethian, J. A. & Wiegmann, A. Structural boundary design via level set and immersed interface methods. *J. computational physics* **163**, 489–528 (2000).

42. Allaire, G., Gournay, F. d., Jouve, F. & Toader, A.-M. Structural optimization using topological and shape sensitivity via a level set method. *Control. cybernetics* **34**, 59–80 (2005).

43. Van Dijk, N. P., Maute, K., Langelaar, M. & Van Keulen, F. Level-set methods for structural topology optimization: a review. *Struct. Multidiscip. Optim.* **48**, 437–472 (2013).

44. Andreassen, E., Clausen, A., Schevenels, M., Lazarov, B. S. & Sigmund, O. Efficient topology optimization in matlab using 88 lines of code. *Struct. Multidiscip. Optim.* **43**, 1–16 (2011).

45. Zhang, D., Zhai, X., Liu, L. & Fu, X.-M. An optimized, easy-to-use, open-source gpu solver for large-scale inverse homogenization problems. *Struct. Multidiscip. Optim.* **66**, 207 (2023).

46. Wang, F., Brøns, M. & Sigmund, O. Non-hierarchical architected materials with extreme stiffness and strength. *Adv. Funct. Mater.* **33**, 2211561 (2023).

47. Shim, P. Y. & Manoochehri, S. Generating optimal configurations in structural design using simulated annealing. *Int. journal for numerical methods engineering* **40**, 1053–1069 (1997).

48. Bonfanti, S., Guerra, R., Font-Clos, F., Rayneau-Kirkhope, D. & Zapperi, S. Automatic design of mechanical metamaterial actuators. *Nat. communications* **11**, 4162 (2020).

49. Beretta, L. *et al.* Automatic design of chiral mechanical metamaterials. *APL Mater.* **9**, 101112 (2021).

50. Wu, C.-Y. & Tseng, K.-Y. Topology optimization of structures using modified binary differential evolution. *Struct. Multidiscip. Optim.* **42**, 939–953 (2010).

51. Kitayama, S., Arakawa, M. & Yamazaki, K. Differential evolution as the global optimization technique and its application to structural optimization. *Appl. Soft Comput.* **11**, 3792–3803 (2011).

52. Madeira, J. A., Pina, H. & Rodrigues, H. Ga topology optimization using random keys for tree encoding of structures. *Struct. Multidiscip. Optim.* **40**, 227–240 (2010).

53. Zhang, J. & Yanagimoto, J. Density-based topology optimization integrated with genetic algorithm for optimizing formability and bending stiffness of 3d printed cfrp core sandwich sheets. *Compos. Part B: Eng.* **225**, 109248 (2021).

54. Mattheck, C. & Burkhardt, S. A new method of structural shape optimization based on biological growth. *Int. J. Fatigue* **12**, 185–190 (1990).

55. Xie, Y. M. & Steven, G. P. A simple evolutionary procedure for structural optimization. *Comput. & structures* **49**, 885–896 (1993).

56. Querin, O. M., Steven, G. P. & Xie, Y. M. Evolutionary structural optimisation (eso) using a bidirectional algorithm. *Eng. computations* **15**, 1031–1048 (1998).

57. Young, V., Querin, O. M., Steven, G. & Xie, Y. 3d and multiple load case bi-directional evolutionary structural optimization (beso). *Struct. optimization* **18**, 183–192 (1999).

58. Sigmund, O. On the usefulness of non-gradient approaches in topology optimization. *Struct. Multidiscip. Optim.* **43**, 589–596 (2011).

59. Zhang, S. & Norato, J. A. Finding better local optima in topology optimization via tunneling. In *International Design Engineering Technical Conferences and Computers and Information in Engineering Conference*, vol. 51760, V02BT03A014 (American Society of Mechanical Engineers, 2018).

60. Martinez, P., Marti, P. & Querin, O. Growth method for size, topology, and geometry optimization of truss structures. *Struct. Multidiscip. Optim.* **33**, 13–26 (2007).

61. Zhu, B. *et al.* Design of compliant mechanisms using continuum topology optimization: A review. *Mech. Mach. Theory* **143**, 103622 (2020).

62. Yoon, G., Kim, Y., Bendsøe, M. P. & Sigmund, O. Hinge-free topology optimization with embedded translation-invariant differentiable wavelet shrinkage. *Struct. Multidiscip. Optim.* **27**, 139–150 (2004).

63. Luo, Z., Chen, L., Yang, J., Zhang, Y. & Abdel-Malek, K. Compliant mechanism design using multi-objective topology optimization scheme of continuum structures. *Struct. Multidiscip. Optim.* **30**, 142–154 (2005).

64. Poulsen, T. A. A simple scheme to prevent checkerboard patterns and one-node connected hinges in topology optimization. *Struct. Multidiscip. Optim.* **24**, 396–399 (2002).

65. Zhang, W., Zhong, W. & Guo, X. An explicit length scale control approach in simp-based topology optimization. *Comput. Methods Appl. Mech. Eng.* **282**, 71–86 (2014).

66. Poulsen, T. A. A new scheme for imposing a minimum length scale in topology optimization. *Int. J. for Numer. Methods Eng.* **57**, 741–760 (2003).

67. Seltmann, S. & Hasse, A. Topology optimization of compliant mechanisms with distributed compliance (hinge-free compliant mechanisms) by using stiffness and adaptive volume constraints instead of stress constraints. *Mech. Mach. Theory* **180**, 105133 (2023).

68. de Assis Pereira, A. & Cardoso, E. L. On the influence of local and global stress constraint and filtering radius on the design of hinge-free compliant mechanisms. *Struct. Multidiscip. Optim.* **58**, 641–655 (2018).

69. Jonsmann, J., Sigmund, O. & Bouwstra, S. Compliant thermal microactuators. *Sensors Actuators A: Phys.* **76**, 463–469 (1999).

70. Jonsmann, J., Sigmund, O. & Bouwstra, S. Compliant electro-thermal microactuators. In *Technical Digest. IEEE International MEMS 99 Conference. Twelfth IEEE International Conference on Micro Electro Mechanical Systems (Cat. No. 99CH36291)*, 588–593 (IEEE, 1999).

71. Sigmund, O. Design of multiphysics actuators using topology optimization–part i: One-material structures. *Comput. methods applied mechanics engineering* **190**, 6577–6604 (2001).

72. Sigmund, O. Design of multiphysics actuators using topology optimization–part ii: Two-material structures. *Comput. methods applied mechanics engineering* **190**, 6605–6627 (2001).

73. Bruns, T. & Sigmund, O. Toward the topology design of mechanisms that exhibit snap-through behavior. *Comput. Methods Appl. Mech. Eng.* **193**, 3973–4000 (2004).

74. Prasad, J. & Diaz, A. Synthesis of bistable periodic structures using topology optimization and a genetic algorithm. (2006).

75. Ohsaki, M. *et al.* Enumeration of optimal pin-jointed bistable compliant mechanisms with non-crossing members. *Struct. Multidiscip. Optim.* **37**, 645–651 (2009).

76. Laman, G. On graphs and rigidity of plane skeletal structures. *J. Eng. mathematics* **4**, 331–340 (1970).

77. Roth, B. Rigid and flexible frameworks. *The Am. Math. Mon.* **88**, 6–21 (1981).

78. Borcea, C. S. & Streinu, I. Periodic frameworks and flexibility. *Proc. Royal Soc. A: Math. Phys. Eng. Sci.* **466**, 2633–2649 (2010).

79. Mitschke, H. *et al.* Finding auxetic frameworks in periodic tessellations. *Adv. Mater.* **23**, 2669–2674 (2011).

80. Wang, F. & Sigmund, O. 3d architected isotropic materials with tunable stiffness and buckling strength. *J. Mech. Phys. Solids* **152**, 104415 (2021).

81. Clausen, A., Wang, F., Jensen, J. S., Sigmund, O. & Lewis, J. A. Topology optimized architectures with programmable poisson's ratio over large deformations. *Adv. Mater* **27**, 5523–5527 (2015).

82. Rodrigues, H., Guedes, J. M. & Bendsoe, M. P. Hierarchical optimization of material and structure. *Struct. Multidiscip. Optim.* **24**, 1–10 (2002).

83. Coelho, P. G., Fernandes, P. R., Guedes, J. M. & Rodrigues, H. C. A hierarchical model for concurrent material and topology optimisation of three-dimensional structures. *Struct. Multidiscip. Optim.* **35**, 107–115 (2008).

84. Bendsøe, M. P. & Kikuchi, N. Generating optimal topologies in structural design using a homogenization method. *Comput. methods applied mechanics engineering* **71**, 197–224 (1988).

85. Avellaneda, M. Optimal bounds and microgeometries for elastic two-phase composites. *SIAM J. on Appl. Math.* **47**, 1216–1228 (1987).

86. Francfort, G. A. & Murat, F. Homogenization and optimal bounds in linear elasticity. *Arch. for Ration. mechanics Analysis* **94**, 307–334 (1986).

87. Pantz, O. & Trabelsi, K. A post-treatment of the homogenization method for shape optimization. *SIAM J. on Control. Optim.* **47**, 1380–1398 (2008).

88. Pantz, O. & Trabelsi, K. Construction of minimization sequences for shape optimization. In *2010 15th International Conference on Methods and Models in Automation and Robotics*, 278–283 (IEEE, 2010).

89. Allaire, G., Geoffroy-Donders, P. & Pantz, O. Topology optimization of modulated and oriented periodic microstructures by the homogenization method. *Comput. & Math. with Appl.* **78**, 2197–2229 (2019).

90. Geoffroy-Donders, P., Allaire, G. & Pantz, O. 3-d topology optimization of modulated and oriented periodic microstructures by the homogenization method. *J. Comput. Phys.* **401**, 108994 (2020).

91. Groen, J. P. & Sigmund, O. Homogenization-based topology optimization for high-resolution manufacturable microstructures. *Int. J. for Numer. Methods Eng.* **113**, 1148–1163 (2018).

92. Groen, J. P., Stutz, F. C., Aage, N., Bærentzen, J. A. & Sigmund, O. De-homogenization of optimal multi-scale 3d topologies. *Comput. Methods Appl. Mech. Eng.* **364**, 112979 (2020).

93. Woldseth, R. V., Bærentzen, J. A. & Sigmund, O. Phasor noise for dehomogenisation in 2d multiscale topology optimisation. *Comput. Methods Appl. Mech. Eng.* **418**, 116551 (2024).

94. Jensen, P. D. L., Sigmund, O. & Groen, J. P. De-homogenization of optimal 2d topologies for multiple loading cases. *Comput. Methods Appl. Mech. Eng.* **399**, 115426 (2022).

95. Träff, E., Sigmund, O. & Groen, J. Simple single-scale microstructures based on optimal rank-3 laminates. *Struct. Multidiscip. Optim.* **59**, 1021–1031 (2019).

96. Lazarov, B. S., Wang, F. & Sigmund, O. Length scale and manufacturability in density-based topology optimization. *Arch. Appl. Mech.* **86**, 189–218 (2016).

97. Qian, X. Undercut and overhang angle control in topology optimization: a density gradient based integral approach. *Int. J. for Numer. Methods Eng.* **111**, 247–272 (2017).

98. Zhang, K., Cheng, G. & Xu, L. Topology optimization considering overhang constraint in additive manufacturing. *Comput. & Struct.* **212**, 86–100 (2019).

99. Gaynor, A. T. & Guest, J. K. Topology optimization considering overhang constraints: Eliminating sacrificial support material in additive manufacturing through design. *Struct. Multidiscip. Optim.* **54**, 1157–1172 (2016).

100. Langelaar, M. Topology optimization for additive manufacturing with controllable support structure costs. In *7th European Congress on Computational Methods in Applied Sciences and Engineering*, 3689–3699 (National Technical University of Athens (NTUA), Greece, 2016).

101. Langelaar, M. An additive manufacturing filter for topology optimization of print-ready designs. *Struct. multidisciplinary optimization* **55**, 871–883 (2017).

102. Luo, Y., Sigmund, O., Li, Q. & Liu, S. Additive manufacturing oriented topology optimization of structures with self-supported enclosed voids. *Comput. Methods Appl. Mech. Eng.* **372**, 113385 (2020).

103. Sabiston, G. & Kim, I. Y. Void region restriction for additive manufacturing via a diffusion physics approach. *Int. J. for Numer. Methods Eng.* **121**, 4347–4373 (2020).

104. Donoso, A., Aranda, E. & Ruiz, D. A new approach based on spectral graph theory to avoiding enclosed holes in topology optimization. *Comput. Methods Appl. Mech. Eng.* **393**, 114769 (2022).

105. Gaynor, A. T. & Johnson, T. E. Eliminating occluded voids in additive manufacturing design via a projection-based topology optimization scheme. *Addit. Manuf.* **33**, 101149 (2020).

106. Xiong, Y., Yao, S., Zhao, Z.-L. & Xie, Y. M. A new approach to eliminating enclosed voids in topology optimization for additive manufacturing. *Addit. Manuf.* **32**, 101006 (2020).

107. Wang, C. Simultaneous optimization of build orientation and topology for self-supported enclosed voids in additive manufacturing. *Comput. Methods Appl. Mech. Eng.* **388**, 114227 (2022).

108. Bruggi, M., Laghi, V. & Trombetti, T. Simultaneous design of the topology and the build orientation of wire-and-arc additively manufactured structural elements. *Comput. & Struct.* **242**, 106370 (2021).

109. Mishra, V., Ayas, C., Langelaar, M. & Van Keulen, F. Simultaneous topology and deposition direction optimization for wire and arc additive manufacturing. *Manuf. Lett.* **31**, 45–51 (2022).

110. Michaleris, P. Modeling metal deposition in heat transfer analyses of additive manufacturing processes. *Finite Elem. Analysis Des.* **86**, 51–60 (2014).

111. Ranjan, R., Ayas, C., Langelaar, M. & van Keulen, F. Fast detection of heat accumulation in powder bed fusion using computationally efficient thermal models. *Materials* **13**, 4576 (2020).

112. Ranjan, R., Ayas, C., Langelaar, M. & Keulen, F. v. Controlling local overheating in topology optimization for additive manufacturing. *Struct. Multidiscip. Optim.* **65**, 162 (2022).

113. Ueda, Y., Fukuda, K., Nakacho, K. & Endo, S. A new measuring method of residual stresses with the aid of finite element method and reliability of estimated values. *J. Soc. Nav. Archit. Jpn.* **1975**, 499–507 (1975).

114. Liang, X., Cheng, L., Chen, Q., Yang, Q. & To, A. C. A modified method for estimating inherent strains from detailed process simulation for fast residual distortion prediction of single-walled structures fabricated by directed energy deposition. *Addit. Manuf.* **23**, 471–486 (2018).

115. Bihr, M. *et al.* Part and supports optimization in metal powder bed additive manufacturing using simplified process simulation. *Comput. Methods Appl. Mech. Eng.* **395**, 114975 (2022).

116. Mishra, V., Ayas, C., Langelaar, M. & van Keulen, F. On controlling microstructure through topology optimization for additive manufacturing. .

117. Bayat, M. *et al.* Holistic computational design within additive manufacturing through topology optimization combined with multiphysics multi-scale materials and process modelling. *Prog. Mater. Sci.* 101129 (2023).

118. Shi, R. *et al.* Microstructural control in metal laser powder bed fusion additive manufacturing using laser beam shaping strategy. *Acta Materialia* **184**, 284–305 (2020).

119. Saghaian, S. E. *et al.* Effect of hatch spacing and laser power on microstructure, texture, and thermomechanical properties of laser powder bed fusion (l-pbf) additively manufactured niti. *Opt. & Laser Technol.* **149**, 107680 (2022).

120. Fu, Z., Ye, J., Franke, M. & Körner, C. A novel approach for powder bed-based additive manufacturing of compositionally graded composites. *Addit. Manuf.* **56**, 102916 (2022).

121. Liu, Z. *et al.* Additive manufacturing of metals: Microstructure evolution and multistage control. *J. Mater. Sci. & Technol.* **100**, 224–236 (2022).

122. Woldseth, R. V., Aage, N., Bærentzen, J. A. & Sigmund, O. On the use of artificial neural networks in topology optimisation. *Struct. Multidiscip. Optim.* **65**, 294 (2022).

123. Shin, S., Shin, D. & Kang, N. Topology optimization via machine learning and deep learning: A review. *J. Comput. Des. Eng.* **10**, 1736–1766 (2023).

124. Zheng, X., Zhang, X., Chen, T.-T. & Watanabe, I. Deep learning in mechanical metamaterials: From prediction and generation to inverse design. *Adv. Mater.* 2302530 (2023).

125. Jiao, P., Mueller, J., Raney, J. R., Zheng, X. & Alavi, A. H. Mechanical metamaterials and beyond. *Nat. Commun.* **14**, 6004 (2023).

126. Mao, Y., He, Q. & Zhao, X. Designing complex architectured materials with generative adversarial networks. *Sci. advances* **6**, eaaz4169 (2020).

127. Kollmann, H. T., Abueidda, D. W., Koric, S., Guleryuz, E. & Sobh, N. A. Deep learning for topology optimization of 2d metamaterials. *Mater. & Des.* **196**, 109098 (2020).

128. Ha, C. S. *et al.* Rapid inverse design of metamaterials based on prescribed mechanical behavior through machine learning. *Nat. Commun.* **14**, 5765 (2023).

129. Zheng, L., Karapiperis, K., Kumar, S. & Kochmann, D. M. Unifying the design space and optimizing linear and nonlinear truss metamaterials by generative modeling. *Nat. Commun.* **14**, 7563 (2023).

130. Napier, N., Sriraman, S.-A., Tran, H. T. & James, K. A. An artificial neural network approach for generating high-resolution designs from low-resolution input in topology optimization. *J. mechanical design* **142**, 011402 (2020).

131. Sosnovik, I. & Oseledets, I. Neural networks for topology optimization. *Russ. J. Numer. Analysis Math. Model.* **34**, 215–223 (2019).

132. Joo, Y., Yu, Y. & Jang, I. G. Unit module-based convergence acceleration for topology optimization using the spatiotemporal deep neural network. *IEEE Access* **9**, 149766–149779 (2021).

133. Kallioras, N. A., Kazakis, G. & Lagaros, N. D. Accelerated topology optimization by means of deep learning. *Struct. Multidiscip. Optim.* **62**, 1185–1212 (2020).

134. Deng, B. *et al.* Inverse design of mechanical metamaterials with target nonlinear response via a neural accelerated evolution strategy. *Adv. Mater.* **34**, 2206238 (2022).

135. Greminger, M. Generative adversarial networks with synthetic training data for enforcing manufacturing constraints on topology optimization. In *International Design Engineering Technical Conferences and Computers and Information in Engineering Conference*, vol. 84003, V11AT11A005 (American Society of Mechanical Engineers, 2020).

136. Oh, S., Jung, Y., Lee, I. & Kang, N. Design automation by integrating generative adversarial networks and topology optimization. In *International design engineering technical conferences and computers and information in engineering conference*, vol. 51753, V02AT03A008 (American Society of Mechanical Engineers, 2018).

137. Wang, C., Yao, S., Wang, Z. & Hu, J. Deep super-resolution neural network for structural topology optimization. *Eng. Optim.* **53**, 2108–2121 (2021).

138. Elingaard, M. O., Aage, N., Bærentzen, J. A. & Sigmund, O. De-homogenization using convolutional neural networks. *Comput. Methods Appl. Mech. Eng.* **388**, 114197 (2022).

139. Hu, Y. Recent progress in field-assisted additive manufacturing: materials, methodologies, and applications. *Mater. Horizons* **8**, 885–911 (2021).

140. Lee, R. H., Mulder, E. A. & Hopkins, J. B. Mechanical neural networks: Architected materials that learn behaviors. *Sci. Robotics* **7**, eabq7278 (2022).

141. Dillavou, S. *et al.* Machine learning without a processor: Emergent learning in a nonlinear electronic metamaterial. *arXiv preprint arXiv:2311.00537* (2023).

142. Scheidgen, M. *et al.* Nomad: A distributed web-based platform for managing materials science research data. *J. Open Source Softw.* **8**, 5388 (2023).

143. Wilkinson, M. D. *et al.* The fair guiding principles for scientific data management and stewardship. *Sci. data* **3**, 1–9 (2016).