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FORUM

On the usefulness of non-gradient approaches in topology optimization

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Abstract Topology optimization is a highly developed tool for structural design and is by now being extensively used in mechanical, automotive and aerospace industries throughout the world. Gradient-based topology optimization algorithms may efficiently solve fine-resolution problems with thousands and up to millions of design variables using a few hundred (finite element) function evaluations (and even less than 50 in some commercial codes). Nevertheless, non-gradient topology optimization approaches that require orders of magnitude more function evaluations for extremely low resolution examples keep appearing in the literature. This forum article discusses the practical and scientific relevance of publishing papers that use immense computational resources for solving simple problems for which there already exist efficient solution techniques.

Keywords Topology optimization · Genetic Algorithms · Stochastic optimization · Discrete optimization

1 Introduction

Since its introduction more than two decades ago the topology optimization method (Bendsøe and Kikuchi 1988; Bendsøe and Sigmund 2004) has undergone a tremendous development from being an academic exercise to being the preferred design tool for advanced mechanical, automotive and aerospace industries throughout the world. Gradient-based topology optimization techniques for continuum problems encompass the homogenization approach (Bendsøe and Kikuchi 1988), the density (SIMP) approach (Bendsøe 1989; Zhou and Rozvany 1991; Mlejnek 1992; Sigmund 2001), the level-set approach (Wang et al. 2003; Allaire et al. 2004), the evolutionary structural optimization approach (Xie and Steven 1997),[1] phase-field methods (Wang and Zhou 2004), topological derivatives (Sokołowski and Zochowski 1999) etc. The required number of function evaluations (finite element calculations) is similar for the different gradient-based approaches and typically lies in the interval between 50 and 1,000, depending on physical problem but relatively independent on number of design variables. For 2D problems discretizations using 1,000 elements is the minimum (e.g. used in the interactive topology optimization applet found at www.topopt.dtu.dk) and up to 100,000 for large-scale, fine-resolution problems, whereas discretizations in 3D problems easily reach millions of elements. Despite the use of continuous design variables in most gradient-based methods, discrete final designs can usually be obtained using penalization techniques, continuation approaches or postprocessing by thresholding and lately quite systematically using projection schemes (Guest et al. 2004; Sigmund 2007) and robust design formulations (Sigmund 2009; Wang et al. 2011b).

Despite the successful developments within gradient-based topology optimization techniques one can continuously find papers that promote optimization approaches based on random processes. Such methods encompass

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[1] Despite its name the ESO method may in fact be categorized as a gradient-based method since it uses sensitivity analysis to determine discrete design updates.

Genetic Algorithms (Balamurugan et al. 2008, 2011; Jain and Saxena 2010; Aguilar Madeira et al. 2010; Wang and Tai 2005; Zhou 2010), Artificial Immune Algorithms (Luh and Chueh 2004), Ant Colonies (Kaveh et al. 2008; Luh and Lin 2009), Particle Swarms (Luh et al. 2011), Simulated Annealing (Shim and Manoochehri 1997), Harmony Search (Lee and Geem 2004), Differential Evolution schemes (Wu and Tseng 2010) a.o. Of these approaches some actually user gradient or gradient-like information (local stresses and/or strain energy densities) to improve the search updates although most of them solely rely on objective function values. The former group encompasses some Swarm Algorithms like Ant Colonies and Particle Swarms and if combined with some kind of filtering algorithm they may actually converge to reasonable designs within an acceptable number of iterations as demonstrated by Kaveh et al. (2008). The main emphasis of the present paper is devoted to the latter group, that only uses objective function evaluations, where the reported number of evaluations typically exceeds 20,000 even for very coarsely discretized topology optimization problems. Instead of referring to specific papers, the discussion will take basis in a paper on Modified Binary Differential Evolution (MBDE) which was recently published in Structural and Multidisciplinary Optimization (Wu and Tseng 2010). Since this paper was accepted for publication in a well-esteemed international journal after a peer review process, it must be expected to represent the state-of-the-art within the field of non-gradient topology optimization approaches. However, similar results and conclusions can be drawn for the other papers referenced above.

Based on arguments from Wu and Tseng (2010) as well as the other papers referenced above, one can set up a list of the top-four arguments for using such non-gradient Topology Optimization schemes (in the following abbreviated NGTO), as opposed to Gradient-based Topology Optimization (in the following abbreviated GTO):

- NGTO uses global search and hence converges to better optima than local search GTO
- NGTO provides discrete designs (compared to grey-scale regions for GTO)
- NGTO does not need gradients and is easy to implement
- NGTO runs efficiently and scales perfectly on parallel computers

Section 2 of this forum discussion refutes each of these arguments, Section 3 lists some common arguments against NGTO, Section 4 discusses problems that may benefit from being solved by NGTO and Section 5 gives some recommendations for the future treatment of papers dealing with NGTO.

2 Arguments for non-gradient topology optimization (NGTO)

2.1 NGTO uses global search and hence converges to better optima than local search GTO

A common argument for using NGTO is that it is based on global search techniques and hence should be expected to converge towards global optima rather than local optima. Here is is important to note that global search strategies in general do not imply convergence to global optima. Whereas the convergence to a global optimum may be likely for problems with few variables, where a large part of the search space can be sampled by NGTO, it is highly unlikely that this will be the case for problems with many design variables (within reasonable computational efforts).

Theoretically, the number of combinations for a continuum-type topology optimization problem with discrete 0–1 density variables is

$$N_C = 2^N \approx 10^{0.3N}, \tag{1}$$

where N is the number of elements (design variables). With a volume equality constraint the number of combinations reduces to

$$N_{Cv} = \frac{N!}{(N-M)!\,M!}, \tag{2}$$

where M is the number of elements that are to be filled with material. However, in Table 1 it is seen that (2) approaches (1) for large N and hence the number of combinations is astronomical even with a volume constraint. Of course, a large number of realizations may be discarded before FE-analysis due to disconnectedness but the number of combinations still remains in the astronomical regime.

Case 4 in Wu and Tseng (2010) (their Fig. 22) presents the design of a cantilever beam (see Fig. 1a for geometry and boundary conditions) discretized by 24 × 12 elements and with a volume fraction constraint of 50%. For the case

Table 1 Number of combinations N_c for a topology optimization problem with N design variables and number of combinations N_{Cv} with a 50% volume fraction constraint ($M = N/2$)

N	10	20	100	144	288	10^3	10^4	10^5
N_C	1,024	$1.0 \cdot 10^6$	10^{30}	10^{43}	10^{87}	10^{301}	10^{3010}	10^{30103}
N_{Cv}	252	$1.8 \cdot 10^5$	10^{29}	10^{42}	10^{85}	10^{299}	10^{3008}	10^{30100}

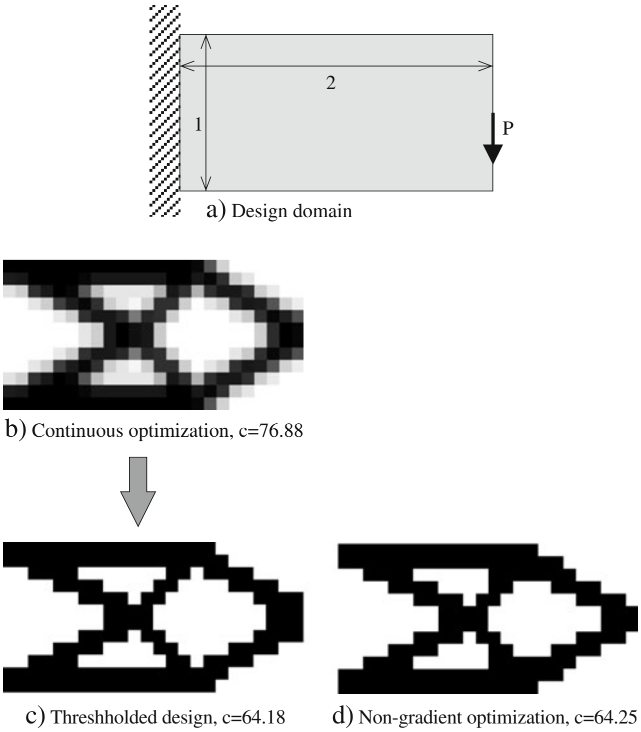

Fig. 1 **a** Design domain and boundary conditions for 2 × 1 cantilever example from Wu and Tseng (2010). Force is $P = 1$, Young's modulus 1, Poisson's ratio 0.3 and thickness = 1. **b** Optimized cantilever using density filtering (compliance $c = 76.88$). **c** Simple threshold of design from **b** resulting in a compliance of $c = 64.18$. **d** Optimized cantilever for MBDE approach by Wu and Tseng (2010) (compliance $c = 64.25$)

with no symmetry (288 design variables) they obtain a non-symmetric design with a compliance of $c = 65.79$ using 19,800 function (FE) evaluations and for the case with symmetry (144 design variables) they obtain the design shown in Fig. 1d with a compliance of $c = 64.25$ using 15,730 function evaluations.[2] From this example it is clear that already for 288 variables the state-of-the-art NGTO method does not provide a global minimum since the 288 variable case has a worse objective function value than for the symmetric 144 variable case. With more design freedom the compliance without symmetry constraint should be as good or better than for the symmetry constrained problem. Further, the author of the present paper ran the same case with a gradient-based optimality criteria solver and density filtering (Matlab code published in Andreassen et al. (2011) and available online at www.topopt.dtu.dk) with a filter size of 1.2 times the element size. After convergence the grey scale solution was simply thresholded to a 0–1 discrete design with the threshold value selected to ensure satisfaction of the volume constraint. This operation, which is illustrated in Fig. 1b and c, resulted in a discrete optimized design with a compliance value of $c = 64.18$ using only 60 function evaluations, i.e. better than the one obtained with symmetry constraint for NGTO using 15,730 evaluations.

It is interesting to note that even if gradients were not available, as could be the case when using an off-the-shelf analysis software, a finite difference-based gradient method would solve the problem more efficiently than the NGTO procedure of Wu and Tseng (2010). Assuming that the number of iterations is the same as for the case where analytical gradients are available, the finite difference-based sensitivity analysis would require $N + 1$ function evaluations pr. iteration. In the case above this would require $60 \cdot 289 = 17{,}340$ function evaluations for the non-symmetric case and only 8,700 for the symmetric case, compared to 19,800 and 15,730 for NGTO which was not able to find the better solution obtained by GTO. For finer resolutions, the number of required function evaluations for the finite-difference-based sensitivity analysis scheme is linearly dependent on the number of design variables (assuming constant number of iterations), whereas the NGTO scheme depends exponentially on the number of variables. The number of FE analyses will in both cases be almost independent on the number of extra objective or constraint function values and sensitivities to be evaluated.

From this example we can conclude

- Whereas NGTO makes use of global search techniques it is unlikely that it converges to a global optimum—not even for extremely coarse finite element discretizations that do not represent the underlying physics well
- Whereas NGTO may solve extremely coarse problems quite well, it uses two orders of magnitude more function evaluations to do so
- Whereas NGTO may solve extremely coarse problems quite well, it is obvious that it cannot solve even slightly larger problems since the number of possible combinations grows exponentially with respect to increase in design variables. A minimum discretization size of 1,000 elements has 10^{299} possible combinations compared to the 10^{42} combinations for the 144 element case in Wu and Tseng (2010), for which a global minimum was not found
- Wu and Tseng (2010) argue against GTO (the SIMP approach) due to its non-discrete, blurry boundaries with many gray elements, the requirement of good initial designs and its tendency to converge to local minima. The example above shows that none of these points are true for the considered example. Using a public

[2] Wu and Tseng (2010) report a compliance value of $c = 64.44$, however, this value was not reproducible by using the FE-solver from the 99-line Matlab code by Sigmund (2001). Exact agreement was however obtained when comparing objective values with the original examples presented in Wang and Tai (2005).

domain GTO software with standard settings followed by a simple thresholding yields a better design than the one obtained by NGTO

– For the example used by Wu and Tseng (2010) it is possible to obtain a better solution using less function evaluations when using a simple finite-difference-based sensitivity analysis scheme combined with a gradient-based optimization scheme for a coarse mesh. The number of function evaluations for this very inefficient GTO scheme depends linearly on the number of design variables whereas the NGTO schemes depend exponentially

2.2 NGTO provides discrete designs

A common argument for using NGTO is that it produces discrete, easily interpretable designs with well-defined boundaries as opposed to GTO.

Whereas it is true that NGTO produces discrete solutions, a first counterargument against this is that the extremely coarsely discretized NGTO designs represent bad finite element analysis and hence their, indeed, discrete boundary representations do not represent physics well.

There are many counter arguments to the non-discreteness of GTO solutions. First, there are GTO methods like evolutionary structural optimization and topological derivative approaches that work with discrete designs. Also some level-set approaches work with, or claim to work with, (almost) discrete design representations. Considering the density (SIMP) approach, the simplest way to obtain discrete designs is to perform a threshold after final convergence as demonstrated above, although this idea only works for problems with at most one simple constraint. An alternative heuristic way that also may result in solutions that do not satisfy length-constraints, but nevertheless works quite well in many cases and may satisfy multiple constraints, is to perform a continuation approach where the filter size is gradually diminished, ensuring final discrete designs. Lately, however, a number of systematic approaches have been published which ensure mesh-independent, discrete solutions based on Heaviside projections schemes as discussed in Guest et al. (2004), Sigmund (2007, 2009) and Wang et al. (2011b).

For some multi-physics topology optimization problems like electrostatics (Yoon and Sigmund 2008), optics (Yang et al. 2009) and optoelasticity (Gersborg and Sigmund 2011) it may be difficult to come up with interpolation schemes that produce discrete designs for GTO schemes. However, recent findings indicate that such problems may be circumvented using robust design formulations (Sigmund 2009; Wang et al. 2011a, b) and anyway, the extremely limited mesh resolutions allowed by NGTO would not be able to model the complicated physics involved in these problems correctly.

2.3 NGTO does not need gradients and is easy to implement

It is true that NGTO is easy to implement since it does not make use of gradients. Hence, NGTO may be used with any type of off-the-shelf analysis code that can return a function value for a given design. This is probably the best argument for using non-gradient optimization methods, however, as shown in Section 2.1 above, even a finite difference-based sensitivity analysis scheme will do just as well or better for coarse resolutions and much better for finer resolutions (linear versus exponential dependence on number of design variables). An implementation issue for both approaches is that they require access to the element connectivity, i.e. the NGTO scheme by Wu and Tseng (2010) needs it for resolution of connectivity issues and both NGTO and the finite difference-based GTO scheme need it for including density, sensitivity filtering or other regularization schemes.

In general it is very cheap to compute gradients for almost all linear and non-linear topology optimization problems. For compliance and other self-adjoint problems the gradients (element relative strain energy densities) come almost for free and even for most non-self-adjoint problems the added cost corresponds to the solution of one extra right hand side for the state problem. In rare cases (non-symmetric stiffness matrices or transient problems) the cost of the adjoint analysis is comparable to the direct analysis. Hence, if at all available, one should always make use of gradients for topology optimization problems. In the authors eyes, the argument that a method does not need gradient information is a disadvantage rather than an advantage when considering topology optimization problems since gradients are so cheaply obtained.

2.4 NGTO runs efficiently and scales perfectly on parallel computers

It is true that NGTO is ideally suited and scales perfectly on parallel computing facilities. However, this fact should not motivate its use. Keeping in mind that the electricity bill for running a supercomputing facility over a 3 year period equals the hardware costs, it is a waste of resources and energy to run inefficient NGTO codes when much better methods exist. Unfortunately, access to supercomputing facilities is often granted upon proof of ideal code scaling performance (i.e. doubling of processor number doubles speed). Due to the NGTO algorithms being so-called “embarrassingly parallel” such algorithms will have easier access to the facilities. Paradoxically, GTO problems that can solve huge problems with few function evaluations often encounter problems in being accepted at the same facilities since it is may be challenging to prove linear scaling of the underlying large-scale FE-code (Lazarov and Sigmund 2011).

3 Arguments against non-gradient topology optimization (NGTO)

There are several arguments against using the extremely coarse resolutions often encountered in NGTO papers.

First, people with a finite element background will rightfully argue that extremely coarse meshes are unable to represent the underlying physical problems correctly. It may be counter argued that accurate modeling is unimportant in a conceptual design phase, however, structural cross-sections should at least be modeled by a couple of elements to capture the basic physics of beam bending. For limited aspect ratios of design domains a discretization of 1,000 in 2D and 20,000 in 3D should be considered the absolute minimum. The value of 1,000 in 2D has been used in practise for almost 10 years for the web-applet found at the authors group web-page www.topopt.dtu.dk (Tcherniak and Sigmund 2001). However, for high-aspect ratio and complex geometry design domains as well as for more complex physics situations and accuracy demands, these numbers should be much higher.

Second, coarse resolutions will, at least for the pure elasticity case, not recover optimal solutions with fine scale. It is well-known that optimal stiffness design favors very fine microstructure, i.e. if allowing infinitely fine microstructure one recovers the original homogenization approach to topology optimization (Bendsøe and Kikuchi 1988). If a microstructure is not realizable, a length-scale constraint should determine the minimum feature scale—not the resolution of the finite element mesh (Petersson and Sigmund 1998). Furthermore, if one wants to compare numerical results with analytical benchmarks in the form of Michell and/or Hemp structures (Michell 1904; Hemp 1973; Lewinski et al. 1994), one should be able to optimize for fine resolutions.

To demonstrate the two aspects above, Fig. 2 shows two examples. Figure 2a shows the cantilever example from Fig. 1 but this time discretized by 200×100 elements. The absolute filter radius is the same as in Fig. 1, i.e. $200/24 \cdot 1.2 = 10$ times the element size and the same thresholding is used to obtain a discrete design at the end. The example was run with sensitivity filtering using the code from Andreassen et al. (2011) (improved in speed compared to the original version from Sigmund 2001). The resulting compliance for the grey-scale design is $c = 74.18$ and for the thresholded design it is $c = 62.58$, which was

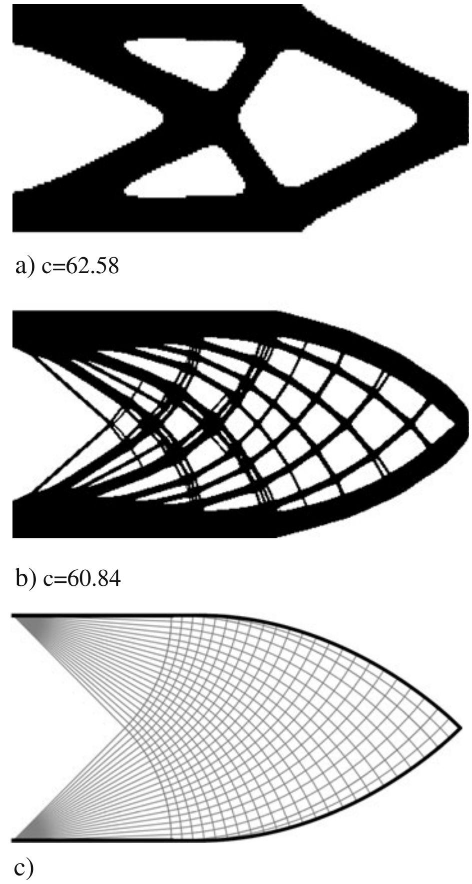

Fig. 2 Short cantilever example from Fig. 1. **a** Optimized cantilever for a 200×100 element discretization and a radius of 10 times the element size. **b** Optimized cantilever for a 400×200 element discretization for a filter size 1.5 times the element size using a continuation approach for the penalization power. **c** Optimal layout for Michell structure (from Lewinski et al. 1994; Sokol and Lewinski 2010)

obtained after 42 iterations.[3] The resulting design is seen to be topologically equal to the coarse designs from Fig. 1c and d, however, this time the boundaries are smooth and the design may almost directly be used as the blue-print for the fabrication lab. Also the FE-analysis can be trusted since all details are modeled by several elements through the cross-sections. To illustrate the benchmarking with analytical Michell-type solutions, Fig. 2b shows the result for running the same example with a mesh of 400×200 elements, a filter size of 1.5 times the element size and run with a continuation strategy that raises the penalization factor in steps of 0.1 from 1 to 3 (raised after convergence or 50 iterations) to improve the chances of approaching a solution close to the global optimum. The figure shows the design

[3] For some reason the number of iterations for the same problem solved using density filtering is an order of magnitude higher (455). The reason for this difference will be investigated in future work.

obtained after 779 iterations. The compliance for the grey-scale design is $c = 62.22$ and for the thresholded design it is $c = 60.84$, i.e. the Michell-like structure (Fig. 2b) is in this case 3% stiffer than the simple topology (Fig. 2a). The optimized design for the small filter radius resembles the analytical solution shown in Fig. 2c (Lewinski et al. 1994; Sokol and Lewinski 2010).

4 May NGTO be useful for certain problems?

The previous sections demonstrate that standard GTO methods totally outperform NGTO methods in all aspects when solving standard, minimum compliance topology optimization problems. However, there may be some special problems where GTO methods might be useful—at least when the number of design variables is limited. Examples would be applications where standard gradient methods fail. This could include problems with lots of local minima (which cannot be regularized or convexified with usual filtering techniques), disjoint design spaces or some discontinuous problems that cannot easily be smoothed. Such problems, however, are difficult to find in the literature but a few examples are discussed in the following.

An example of a non-smooth problem is the design of bi-stable compliant mechanisms (Bruns and Sigmund 2004; Prasad and Diaz 2006; Ohsaki et al. 2009). Depending on the definition of the objective function, these problems become non-differentiable and in any case they tend to cause big problems for convergence. Whereas it at present is unlikely that NGTO methods with their limited resolution will be able to solve continuum-type problems (Bruns and Sigmund 2004), it may make sense to use them for truss-like structures with limited number of design variables (Prasad and Diaz 2006), however, even for such problems there exist very efficient graph theoretical enumeration approaches (Kawamoto et al. 2004; Ohsaki et al. 2009) which may be able to solve these problems more efficiently than NGTO.

An example of non-connected design space is the optimization of photonic or phononic band gap materials (Cox and Dobson 1999; Sigmund and Jensen 2003; Halkjær et al. 2005; Sigmund and Hougaard 2008). If the optimization goal is to find the maximum relative band gap size amongst all bands, the design space becomes disjoint, i.e. it is impossible to move from the gap between bands 1 and 2 to the gap between bands 2 and 3 by continuous variation of the design variables. Due to symmetries, the number of design variables for such problems is quite low. In fact Sigmund and Hougaard (2008) performed an initial search for candidate topologies for only 16 free design variables. However, in order to avoid missing potential solutions an exhaustive search of the design space was preferred from a NGTO technique. The best coarse-mesh candidates for each band gap were subsequently refined and used as starting guesses for a standard GTO approach with fine discretization.

An example of a problem with lots of local minima which cannot be immediately regularized with usual filtering techniques is the design of atomistic structures (Dudiy and Zunger 2006). Here, it may be very difficult to find interpolation schemes that ensure convexified design spaces and hence NGTO algorithms may have a chance—also because the number of variables may be relatively limited for unit cell design problems.

A seemingly discrete and non-differentiable problem is the stacking sequence optimization for laminates. Many papers have applied NGTO for such problems (see e.g. Nagendra et al. 1996), but actually such discrete problems can often be reformulated to continuous design variables and efficiently solved using GTO (Stegmann and Lund 2005; Niu et al. 2010).

5 Recommendations

This paper has discussed the applicability of non-gradient methodologies for topology optimization. It argues that such methods are hopelessly inefficient for problems with many variables such as topology optimization. It is also demonstrated that even for extremely coarse meshes a state-of-the-art NGTO does not provide global optima. To push things to the edge: Human evolution took 5–7 million years whereas it took mankind 50–70 years to go from the first 500 flop/s vacuum tube computers to present days 2.5 petaflop/s supercomputers. Do we really want to use the tremendous technological achievement in computer hardware to mimic the tremendously slow evolutional processes as represented by non-gradient methods? From an environmental and human resource side the answer is clearly no. The electricity bill for running a supercomputer for 3 years is comparable to the original hardware costs and hence this energy should not be wasted on inefficient methods. Likewise, graduate students should not spend 3 years of their (research) life working with methods that are obviously inferior to existing methods.

Of course one should not blindly discriminate against methods that at present are inefficient. As noted in the introduction there are for example random-process-based topology optimization approaches that use gradient information to speed up convergence and may result in procedures that combine the best from two worlds.

To weed out inefficient methods but keep a door open for future developments in the field of non-gradient topology optimization methods, the author suggests that at least one of the following requirements should be fulfilled to merit publication in a serious scientific journal:

1. **Discretization:** Proposed methods should be able to handle topology optimization problems that at least are discretized by 1,000 elements and it must be proven that the method performs at least as good, and preferably much better, than a gradient-based scheme where sensitivities are computed using finite-differences. Examples must also be free of numerical anomalies like checkerboard patterns and one-node-connected elements.
2. **Problem type:** Proposed methods should deal with applications that are likely to be un-solvable with standard gradient methods.[4] This would include problems with lots of local minima (which cannot be interpolated or convexified with usual filtering techniques), disjoint design spaces or non-smooth problems where gradients cannot be calculated as discussed in Section 4.

The conclusions drawn in this paper are based on the use of non-gradient methods in continuum-type topology optimization methods, i.e. problems with thousands of design variables at the least. Other conclusions may hold for small scale problems, however, the requirement that non-gradient methods should perform better than simple finite difference-based gradient optimization schemes is generally applicable.

As the last recommendations that hold for the whole field of optimization (not only NGTO) the author suggests the following three points:

- One should never publish a result that is obviously non-optimal without discussing it. An example is the non-optimal solution without symmetry found in the paper by Wu and Tseng (2010). Sub-optimal solutions should only be shown in order to demonstrate or discuss weaknesses or short-comings of methods.
- One should never write "optimal result", "optimal solution", "optimal structure", etc. in a paper unless one can prove global optimality, as e.g. in Stolpe and Bendsøe (2010). It is much better to write "optimized result", "optimized solution", "optimized structure", etc.—then one has not promised too much.
- Due to the simple nature of compliance minimization problems (gradients always negative), almost any heuristics may solve such problems efficiently. Authors should therefore apply their algorithm to more difficult, non-self-adjoint problems (a minimum should be compliant mechanisms or stress constraints) before claiming efficiency of their approach.

[4]Claiming that GTO methods yield non-discrete, grey-scale design is not enough since these results can be easily thresholded as demonstrated in Section 2.1.

The author hopes that this Forum Discussion paper will open up a debate on the applicability of certain approaches in topology optimization and that it will contribute to ensuring the sensible use of computational, environmental and human resources in the future.

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