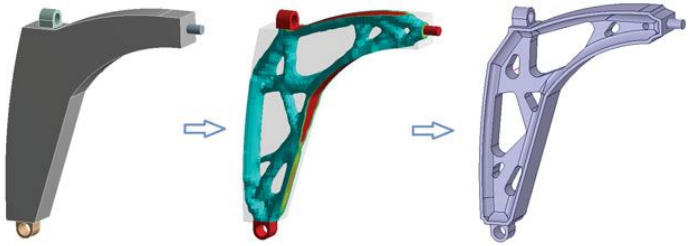
香港中文大學
The Chinese University of Hong Kong

MAEG5160: Design for Additive Manufacturing

Lecture 6: Topology Optimization (TO) by distribution of isotropic material



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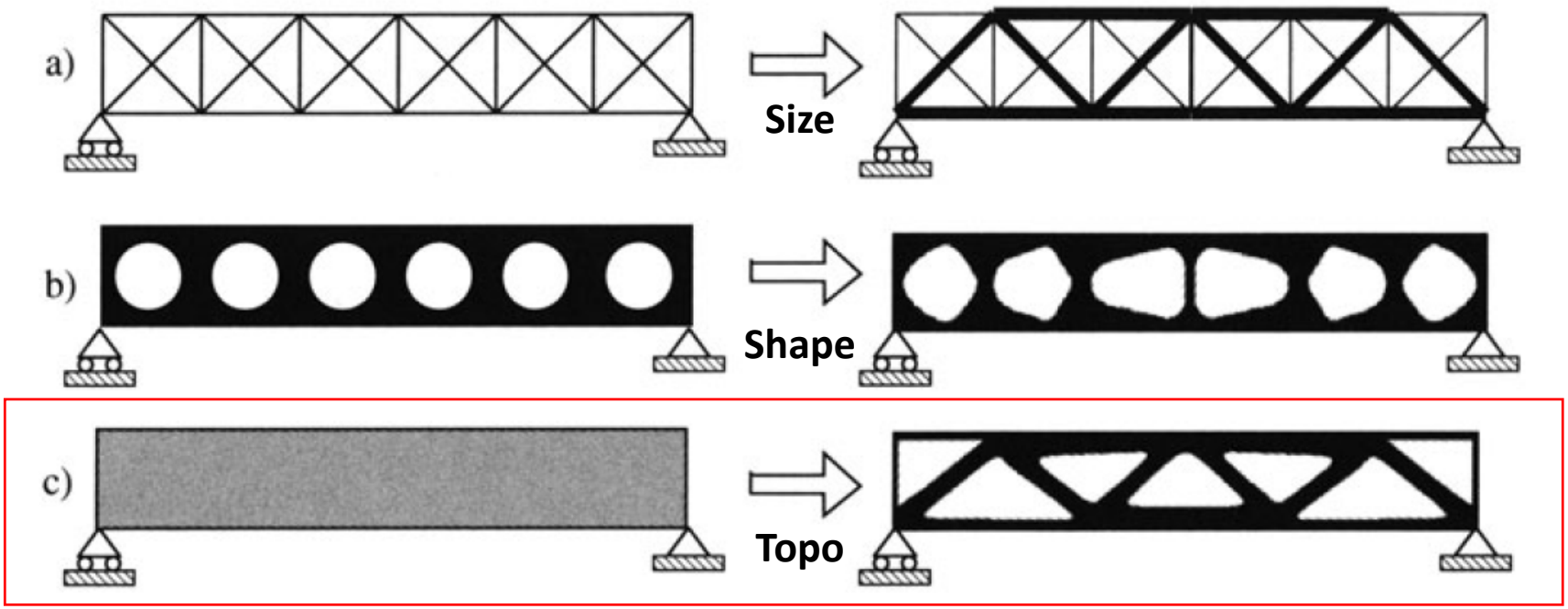
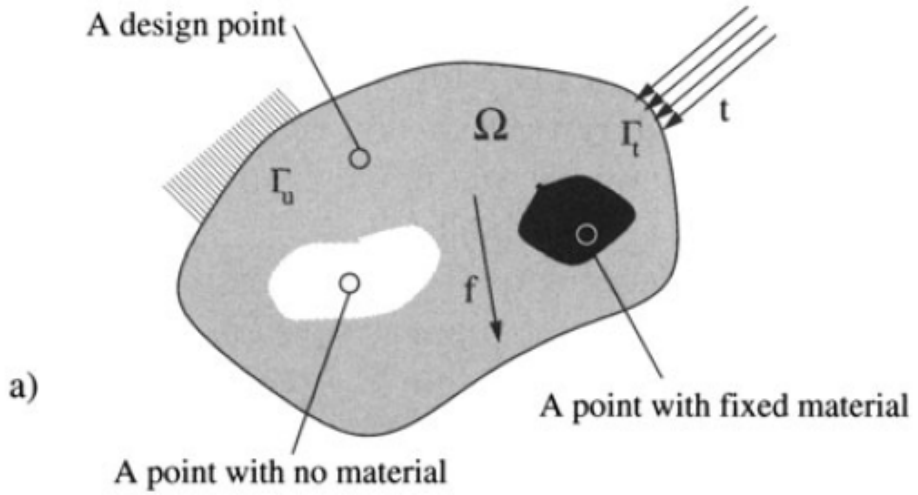
Topology Optimization (TO) by distribution of isotropic material

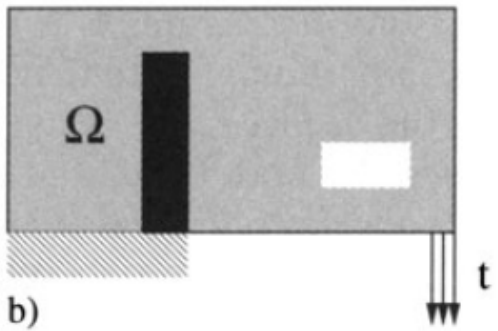
Recall: Three types of design optimization: size, shape and topology



Topology Optimization (TO) by distribution of isotropic material

1. Problem formation and parametrization of design





The generalized topology design problem of finding the optimal material distribution in a two-dimensional domain

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Introducing the energy bilinear form (i.e., the internal virtual work of an elastic body at the equilibrium *u* and for an arbitrary virtual displacement *v*)

$$a(u,v) = \int_{\Omega} E_{ijkl}(x)\varepsilon_{ij}(u)\varepsilon_{kl}(v)\mathrm{d}\Omega$$

with linearized strains $\varepsilon_{ij}(u) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$ and the load energy linear form

$$l(u) = \int_{\Omega} fu\mathrm{d}\Omega + \int_{\Gamma_T} tu\mathrm{d}s$$

the minimum compliance (maximum global stiffness) problem takes the form

$$\begin{aligned} &\min_{u\in U, E} \; l(u) \\ &\text{s.t.} : a_E(u,v) = l(v), \quad \text{for all } v \in U \\ &\qquad E \in \mathsf{E}_{\mathrm{ad}} \, . \end{aligned}$$

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Discretize the problem using finite elements. It is here important to note that there are *two* fields of interest, namely both the displacement u and the stiffness E. If we use the same finite element mesh for both fields, and discretize E as constant in each element,

$$\begin{aligned} &\min_{\mathbf{u},E_e} \mathbf{f}^T\mathbf{u} \\ &\text{s.t.} : \mathbf{K}(E_e)\mathbf{u} = \mathbf{f} \ , \\ &\quad E_e \in \mathsf{E}_{\text{ad}} \ . \end{aligned}$$

Here $\mathbf{u}$ and $\mathbf{f}$ are the displacement and load vectors, respectively. The stiffness matrix $\mathbf{K}$ depends on the stiffness E_e in element e, numbered as $e = 1, \ldots, N$, and we can write $\mathbf{K}$ in the form

$$\mathbf{K} = \sum_{e=1}^{N} \mathbf{K}_e\left(E_e\right)$$

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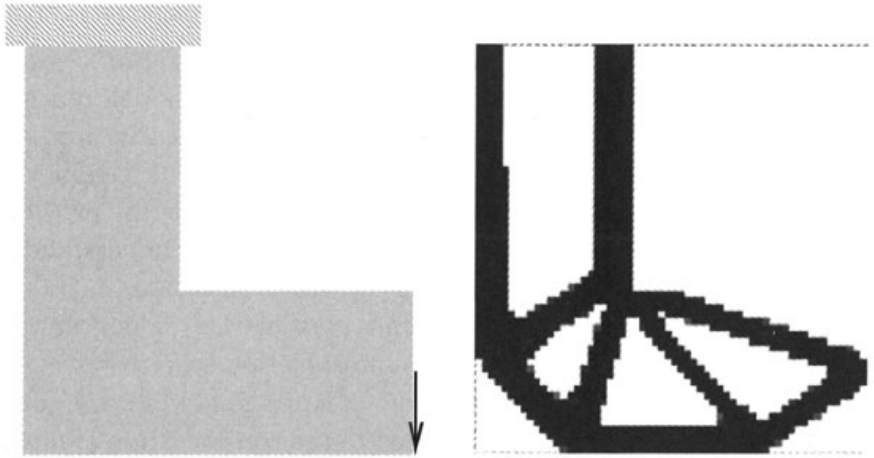
In the design of the topology of a structure we are interested in the determination of the optimal placement of a given isotropic material in space, i.e., we should determine which points of space should be material points and which points should remain void (no material). That is, we think of the geometric representation of a structure as similar to a black-white rendering of an image. In discrete form this then corresponds to a black-white raster representation of the geometry, with "pixels" (or "voxels") given by the finite element discretization. Restricting our spatial extension to the reference domain Ω we are thus seeking to determine the optimal subset Ω_{mat} of material points.

$$E_{ijkl} = 1_{\Omega^{\text{mat}}} E^0_{ijkl}, \; 1_{\Omega^{\text{mat}}} = \begin{cases} 1 \text{ if } x \in \Omega^{\text{mat}} \\ 0 \text{ if } x \in \Omega \setminus \Omega^{\text{mat}} \end{cases},$$

$$\int_\Omega 1_{\Omega^{\text{mat}}} \mathrm{d}\Omega = \text{Vol}(\Omega^{\text{mat}}) \leq V \; .$$



A black-and-white minimum compliance design for a loaded knee structure obtained with the SIMP interpolation scheme. The discretization is 60 by 60 elements and the material volume is limited to 47% of the design domain

Topology Optimization (TO) by distribution of isotropic material

The most commonly used approach to solve this problem is to replace the integer variables with continuous variables and then introduce some form of penalty that steers the solution to discrete 0-1 values. The design problem for the fixed domain is then formulated as a sizing problem by modifying the stiffness matrix so that it depends continuously on a function which is interpreted as a density of material. This function is then the design variable. The requirement is that the optimization results in designs consisting almost entirely of regions of material or no material. This means that intermediate values of this artificial density function should be penalized in a manner analogous to other continuous optimization approximations of 0-1 problems. One possibility which has proven very popular and extremely efficient is the so-called penalized, proportional stiffness model (the SIMP-model)

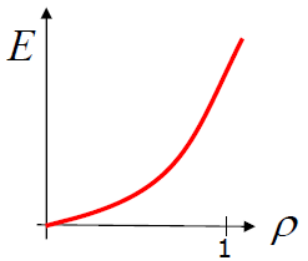
$$E_{ijkl}(x) = \rho(x)^p E^0_{ijkl}, \quad p > 1 ,$$

$$\int_\Omega \rho(x)\mathrm{d}\Omega \le V; \quad 0 \le \rho(x) \le 1, \quad x \in \Omega$$

$$E_{ijkl}(\rho = 0) = 0, \qquad E_{ijkl}(\rho = 1) = E^0_{ijkl}$$

by specifying a value of p higher than one makes it "uneconomical“ to have intermediate densities in the optimal design. Thus the penalization is achieved without the use of any explicit penalization scheme. For problems where the volume constraint is active, experience shows that optimization does actually result in such designs if one chooses p sufficiently big (in order to obtain true "0-1" designs, $p > 3$ is usually required)

Stiffness interpolation:



$$E(\rho_e) = E_1 + \rho_e^p (E_2 - E_1)$$

$$p > 1$$

Topology Optimization (TO) by distribution of isotropic material

by specifying a value of p higher than one makes it "uneconomical“ to have intermediate densities in the optimal design. Thus the penalization is achieved without the use of any explicit penalization scheme. For problems where the volume constraint is active, experience shows that optimization does actually result in such designs if one chooses p sufficiently big (in order to obtain true "0-1" designs, $p > 3$ is usually required)

the SIMP model can indeed be considered as a material model if the power p satisfies that:

$$p \geq \max\left\{\frac{2}{1-\nu^0}, \frac{4}{1+\nu^0}\right\} \quad (\text{in } 2-\text{D})$$

$$p \geq \max\left\{15\frac{1-\nu^0}{7-5\nu^0}, \frac{3}{2}\frac{1-\nu^0}{1-2\nu^0}\right\} \quad (\text{in } 3-\text{D})$$

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2. Solution methods

2.1 Conditions of optimality

The use of an interpolation scheme like SIMP allows us to convert the optimal topology problem into a *sizing* problem on a *fixed* domain. Compared to many traditional sizing problems for, e.g., frames and built-up structures of plates, stringers, etc., the present problem differs in that the number of design variables is typically very large (the number of design parameters and the number of analysis variables is of the same order of magnitude). Thus efficiency of the optimization procedure is crucial and one typically has to adopt optimization settings that trade number of constraints for number of design variables.

In the following we shall derive the necessary conditions of optimality for the density of the minimum compliance design problem that employs the SIMP interpolation scheme. The key is to devise iterative methods which, for a previously computed design and its associated displacements, update the design variables at each point (or rather at each element of a finite element discretization) independently from the updates at other points, based on the necessary conditions of optimality.

$$
\begin{aligned}
&\min_{u\in U,\rho}\ l(u)\\
&\text{s.t.}: a_E(u,v) = l(v), \quad \text{for all } v \in U\ ,\\
&\qquad E_{ijkl}(x) = \rho(x)^p E^0_{ijkl}\ ,\\
&\qquad \int_\Omega \rho(x)\mathrm{d}\Omega \le V; \quad 0 < \rho_{\min} \le \rho \le 1\ .
\end{aligned}
$$

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Note that we here have introduced a lower bound ρ_{min} on the density in order to prevent any possible singularity of the equilibrium problem. In typical applications we set $\rho_{min} = 10^{-3}$

In mathematical optimization, the method of Lagrange multipliers is a strategy for finding the local maxima and minima of a function subject to equality constraints (i.e., subject to the condition that one or more equations have to be satisfied exactly by the chosen values of the variables). The basic idea is to convert a constrained problem into a form such that the derivative test of an unconstrained problem can still be applied. The relationship between the gradient of the function and gradients of the constraints rather naturally leads to a reformulation of the original problem, known as the Lagrangian function.

The method can be summarized as follows: in order to find the maximum or minimum of a function $f(x)$ subjected to the equality constraint $g(x) = 0$

form the Lagrangian function

$$L(x, \lambda) = f(x) - \lambda g(x)$$

and find the stationary points of L, considered as a function (x) of and the Lagrange multiplier λ . The solution corresponding to the original constrained optimization is always a saddle point of the Lagrangian function.

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With Lagrange multipliers $\Lambda, \lambda^-(x), \lambda^+(x)$ for the constraints the necessary conditions for optimality for the sizing variable ρ are a subset of the stationarity conditions for the Lagrange function

$$\mathcal{L} = l(u) - \left\{ a_E(u, \bar{u}) - l(\bar{u}) \right\} + \Lambda \left(\int_\Omega \rho(x) \mathrm{d}\Omega - V \right) +$$
$$\int_\Omega \lambda^+(x)(\rho(x) - 1)\mathrm{d}\Omega + \int_\Omega \lambda^-(x)(\rho_{\min} - \rho(x))\mathrm{d}\Omega \,,$$

where $\bar{u}$ is the Lagrange multiplier for the equilibrium constraint. Note that $\bar{u}$ belongs to the set U of kinematically admissible displacement fields. Under the assumption that $\rho \geq \rho_{\min} > 0$ (so that displacement fields are unique), the conditions for optimality with respect to variations of the displacement field u give that $\bar{u} = u$ while the condition for ρ becomes:

$$\frac{\partial E_{ijkl}}{\partial \rho} \varepsilon_{ij}(u) \varepsilon_{kl}(u) = \Lambda + \lambda^+ - \lambda^- \,,$$

with the switching conditions

$$\lambda^- \geq 0, \ \lambda^+ \geq 0, \ \lambda^-(\rho_{\min} - \rho(x)) = 0, \ \lambda^+(\rho(x) - 1) = 0 \,.$$

For intermediate densities ($\rho_{\min} < \rho < 1$) the conditions (1.9), can be written as

$$p\rho(x)^{p-1} E^0_{ijkl} \varepsilon_{ij}(u) \varepsilon_{kl}(u) = \Lambda \,, \qquad (1.11)$$

Topology Optimization (TO) by distribution of isotropic material

$$\rho_{K+1} = \begin{cases} \max\{(1-\zeta)\rho_K, \rho_{\min}\} & \text{if } \rho_K B_K^\eta \le \max\{(1-\zeta)\rho_K, \rho_{\min}\}\,, \\ \min\{(1+\zeta)\rho_K, 1\} & \text{if } \min\{(1+\zeta)\rho_K, 1\} \le \rho_K B_K^\eta\,, \\ \rho_K B_K^\eta & \text{otherwise}\,. \end{cases} \tag{1.12}$$

Here ρ_K denotes the value of the density variable at iteration step K , and B_K is given by the expression

$$B_K = \Lambda_K^{-1} p \rho(x)^{p-1} E^0_{ijkl} \varepsilon_{ij}(u_K) \varepsilon_{kl}(u_K)$$

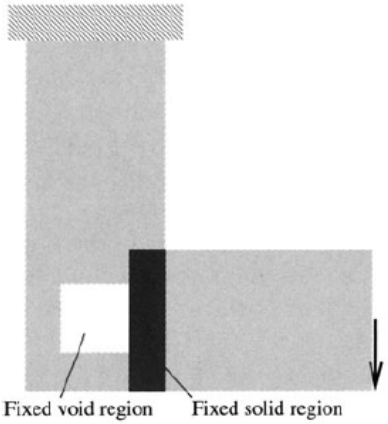
where u_K is the displacement field at at the iteration step K, determined from the equilibrium equation and dependent on ρ_K. Note that a (local) optimum is reached if $B_K = 1$ for densities ($\rho_{\min} < \rho < 1$). The update scheme (1.12) adds material to areas with a specific strain energy that is higher than Λ (that is, when $B_K > 1$) and removes it if the energy is below this value; this only takes place if the update does not violate the bounds on ρ. From integrating (1.11) one can see that Λ is proportional (by a factor p) to the average strain energy density of the part of the structure that is given by intermediate values of the density.

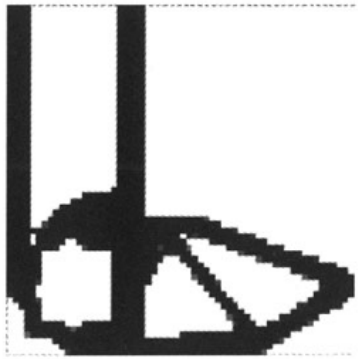
Topology Optimization (TO) by distribution of isotropic material

The variable η in (1.12) is a tuning parameter and ζ a move limit. Both η and ζ controls the changes that can happen at each iteration step and they can be made adjustable for efficiency of the method. Note that the update ρ_{K+1} depends on the present value of the Lagrange multiplier Λ, and thus Λ should be adjusted in an inner iteration loop in order to satisfy the active volume constraint. It is readily seen that the volume of the updated values of the densities is a continuous and decreasing function of the multiplier Λ. Moreover, the volume is strictly decreasing in the interesting intervals, where the bounds on the densities are not active in all points (elements of a FEM discretization). This means that we can uniquely determine the value of Λ, using a bisection method or a Newton method. The values of η and ζ are chosen by experiment, in order to obtain a suitable rapid and stable convergence of the iteration scheme. A typical useful value of η and ζ is 0.5 and 0.2, respectively.

Topology Optimization (TO) by distribution of isotropic material

2.2 Implementation of the Optimality Criteria (OC) method





Computational procedure

Pre-processing of geometry and loading:

- Choose a suitable reference domain (the ground structure) that allows for the definition of surface tractions, fixed boundaries, etc.
- Choose the parts of the reference domain that should be designed, and what parts of the ground structure that should be left as solid domains or voids
- Construct a finite element mesh for the ground structure. This mesh should be fine enough in order to describe the structure in a reasonable resolution bit-map representation. Also, the mesh should make it possible to define the a priori given areas of the structure by assigning fixed design variables to such areas. The mesh is unchanged through-out the design process.
- Construct finite element spaces for the independent fields of displacements and the design variables.

Topology Optimization (TO) by distribution of isotropic material

Optimization:
Compute the optimal distribution over the reference domain of the design variable ρ. The optimization uses a displacement based finite element analysis and the optimality update criteria scheme for the density. The structure of the algorithm is:

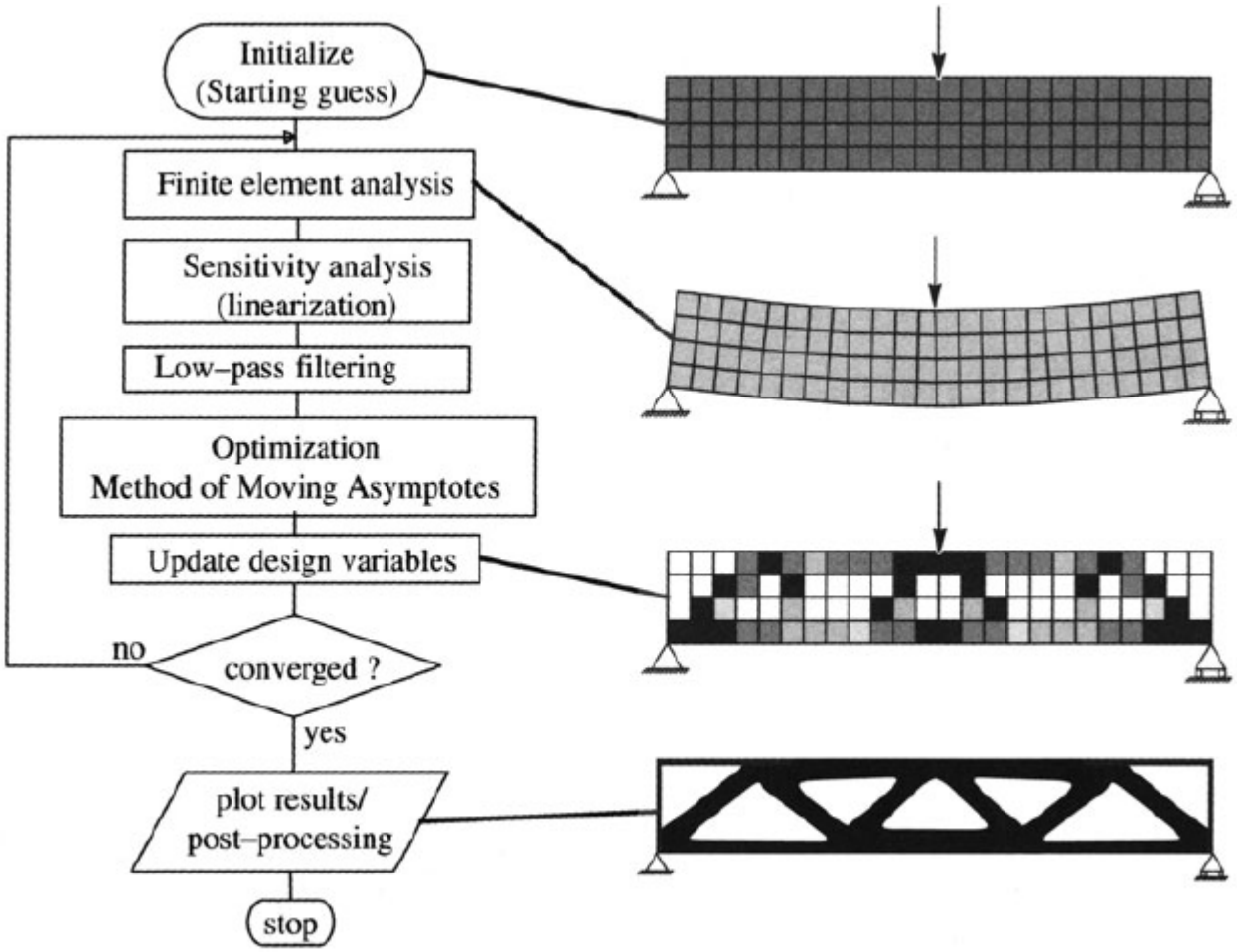
- Make initial design, e.g., homogeneous distribution of material. The iterative part of the algorithm is then:
- For this distribution of density, compute by the finite element method the resulting displacements and strains.
- Compute the compliance of this design. If only marginal improvement (in compliance) over last design, stop the iterations. Else, continue. For detailed studies, stop when necessary conditions of optimality are satisfied.
- Compute the update of the density variable, based on the scheme shown in section 1.2.1. This step also consists of an inner iteration loop for finding the value of the Lagrange multiplier Λ for the volume constraint.
- Repeat the iteration loop.

For a case where there are parts of the structure which are fixed (as solid and/or void) the updating of the design variables should only be invoked for the areas of the ground structure which are being redesigned (reinforced).

Post-processing of results:

- Interpret the optimal distribution of material as defining a shape, for example in the sense of a CAD representation.

Topology Optimization (TO) by distribution of isotropic material



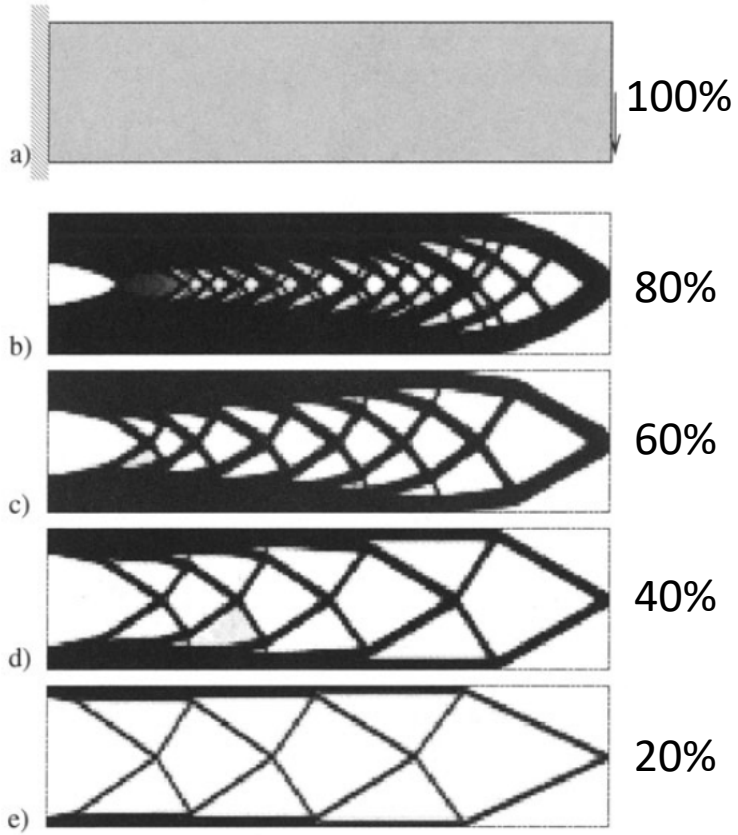
MATLAB® codes for minimum compliance problems [99-line Matlab code]

https://www.topopt.mek.dtu.dk/apps-and-software

Topology Optimization (TO) by distribution of isotropic material

2.3 Sensitivity analysis and mathematical programming methods

The use of mathematical programming algorithms for solving problems in structural optimization is well established and described in detail in the literature, for sizing as well as shape design problems. The standard procedure is to consider the design problem as an optimization problem in the design variables *only*, and with the displacement field regarded as a function of these design variables. The displacement fields are given *implicitly* in terms of the design variables through the equilibrium equation and finding the derivatives of the displacements with respect to the design variables is termed *sensitivity Analysis.*



Topology Optimization (TO) by distribution of isotropic material

Sensitivity analysis In order to complement the presentation of the optimality criteria method, we will here work with the FEM form of the minimum compliance problem

When solving this by a mathematical programming algorithm we first rewrite the problem as a problem in the design variables only:

$$\begin{aligned} &\min_{\rho_e} \; c(\rho_e) \\ &\text{s.t.} : \sum_{e=1}^{N} v_e \rho_e \leq V, \quad 0 < \rho_{\min} \leq \rho_e \leq 1, \quad e = 1, \ldots, N \; , \end{aligned} \tag{1.15}$$

where the equilibrium equation is considered as part of a function-call:

$$c(\rho_e) = \mathbf{f}^T \mathbf{u} \; , \quad \text{where } \mathbf{u} \text{ solves : } \quad \sum_{e=1}^{N} \rho_e^p \mathbf{K}_e \mathbf{u} = \mathbf{f} \; .$$

Topology Optimization (TO) by distribution of isotropic material

When gradients are required by the optimization algorithm employed to solve (1.15), these are easily derived for the objectives and constraints involving only ρ. For functions that depend on the displacements also, derivatives can be obtained by the chain-rule. These expressions will then contain derivatives of the displacement, which in turn can be obtained by taking the derivative of the equilibrium equation $\mathbf{Ku} = \mathbf{f}$. In topology design we typically work with a moderate number of constraints, so the most effective method for calculating derivatives is to use the *adjoint* method, where the derivatives of the displacement are not calculated explicitly. For the minimum compliance problem (1.15) at hand we rewrite the function $c(\rho)$ by adding the zero function:

$$c(\rho) = \mathbf{f}^T\mathbf{u} - \tilde{\mathbf{u}}^T\left(\mathbf{Ku} - \mathbf{f}\right) \ ,$$

where $\tilde{\mathbf{u}}$ is any arbitrary, but *fixed* real vector. From this, after rearrangement of terms, we obtain that

$$\frac{\partial c}{\partial \rho_e} = \left(\mathbf{f}^T - \tilde{\mathbf{u}}^T\mathbf{K}\right)\frac{\partial \mathbf{u}}{\partial \rho_e} - \tilde{\mathbf{u}}^T\frac{\partial \mathbf{K}}{\partial \rho_e}\mathbf{u} \ .$$

This can in turn be written as

$$\frac{\partial c}{\partial \rho_e} = -\tilde{\mathbf{u}}^T\frac{\partial \mathbf{K}}{\partial \rho_e}\mathbf{u} \ ,$$

when $\tilde{\mathbf{u}}$ satisfies the adjoint equation:

$$\mathbf{f}^T - \tilde{\mathbf{u}}^T\mathbf{K} = 0$$

Topology Optimization (TO) by distribution of isotropic material

This latter equation is in the form of an equilibrium equation and for compliance we see that we obtain directly that $\tilde{\mathbf{u}} = \mathbf{u}$ (normally the adjoint equation requires additional computations). Moreover, the form of the stiffness means that the derivatives of the compliance $c(\rho)$ for problem (1.15) i particularly simple form:

$$\frac{\partial c}{\partial \rho_e} = -p\rho_e^{p-1}\mathbf{u}^T\mathbf{K}_e\mathbf{u}\,. \tag{1.17}$$

Thus derivatives for the minimum compliance problem are extremely easy to compute. Also, one notices that the derivative is "localized" in the sense that the derivative only involves information at the element level; however, there is an effect from other design variables hidden in the displacement $\mathbf{u}$. Finally, we see that the sensitivity is negative for all elements, so physical intuition is confirmed in that additional material in any element decreases compliance, that is, makes the structure stiffer.

Topology Optimization (TO) by distribution of isotropic material

The Method of Moving Asymptotes (MMA) and its "mother" method CONLIN are mathematical programming algorithms well suited for topology design. They are in nature similar to methods like Sequential Linear Programming (SLP) and Sequential Quadratic Programming (SQP) for solving smooth, non-linear optimization problems, in the sense that they work with a sequence of simpler approximate subproblems of given type. For MMA and CONLIN these subproblems are separable and convex and are constructed based on sensitivity information at the current iteration point as well as some iteration history. At each iteration point this subproblem is solved by for example a dual method or by an interior point algorithm (primal-dual algorithm) , and the solution to the subproblem is then used as the next design in the iterative procedure.

In MMA the approximation of a function F of n real variables $\mathbf{x} = (x_1, \ldots, x_n)$ around a given iteration point $\mathbf{x}^0$ has the form

$$F(\mathbf{x}) \approx F(\mathbf{x}^0) + \sum_{i=1}^{n} \left(\frac{r_i}{U_i - x_i} + \frac{s_i}{x_i - L_i} \right) ,$$

where the numbers r_i, s_i are chosen as

$$\text{if } \frac{\partial F}{\partial x_i}(x^0) > 0 \text{ then } r_i = \left(U_i - x_i^0\right)^2 \frac{\partial F}{\partial x_i}(x^0) \quad \text{and} \quad s_i = 0 ,$$

$$\text{if } \frac{\partial F}{\partial x_i}(x^0) < 0 \text{ then } r_i = 0 \quad \text{and} \quad s_i = -\left(x_i^0 - L_i\right)^2 \frac{\partial F}{\partial x_i}(x^0) ,$$

Topology Optimization (TO) by distribution of isotropic material

and where, loosely speaking, the positive numbers *Ui, Li* control the range for which the approximation of F can generate reasonable answers for our optimization problem (the parameters *Ui, Li* give vertical asymptotes for the approximations of F and is the source of the name of the algorithm). In the optimization algorithm, the values of *Ui , Li* for each function of the problem are updated in each iteration, depending on the iteration history so far. A central aspect of MMA and CONLIN is the use of such separable and convex approximations. The former property means that the necessary conditions of optimality of the subproblems do not couple the primary variables (the design variables) while the convexity means that dual methods or primal-dual methods can be used. Together this has an immense effect on reducing the computational effort needed to solve the subproblems, especially for problems with only a few constraints.

We found in (1.17) that the sensitivity of compliance is negative for any element density ρ_e.

Thus an MMA approximation of the compliance gives a subproblem after iteration step K in the form

$$\min_{\rho_e} \left\{ c(\rho^K) - \sum_{e=1}^{N} \frac{\left(\rho_e^K - L_e\right)^2}{\rho_e - L_e} \frac{\partial c}{\partial \rho_e}(\rho^K) \right\}$$

$$\text{s.t.} : \sum_{e=1}^{N} v_e \rho_e \leq V, \quad 0 < \rho_{\min} \leq \rho_e \leq 1, \quad e = 1, \ldots, N \, .$$

Topology Optimization (TO) by distribution of isotropic material

Solving this problem by a dual method now involves steps similar to the ones performed in section 1.2.1 for the optimality criteria method. First one minimizes the Lagrange functional

$$\mathcal{L} = c(\rho^K) - \sum_{e=1}^{N} \frac{\left(\rho_e^K - L_e\right)^2}{\rho_e - L_e} \frac{\partial c}{\partial \rho_e}(\rho^K) + \Lambda\left(\sum_{e=1}^{N} v_e \rho_e - V\right)$$

with respect to densities satisfying $\rho_{\min} \leq \rho_e \leq 1$, $e = 1, \ldots, N$. Using convexity and that $\mathcal{L}$ is separable, this optimization can easily be performed, element by element. For the case where $L_e = 0$ this results in exactly the optimality criteria update scheme given in (1.12), with move limit $\zeta = \infty$ and tuning parameter $\eta = 0.5$. The second step of the dual method is to maximize the resulting functional with respect to Λ, and as for the optimality criteria method this corresponds to adjusting the value of Λ so that the update scheme gives a density $\rho^{(K+1)}$ that satisfies the volume constraint. In the actual implementation of MMA, one chooses the asymptote parameters L_e more cleverly, improving speed of convergence.

Topology Optimization (TO) by distribution of isotropic material

2.4 Implementation - the general concept

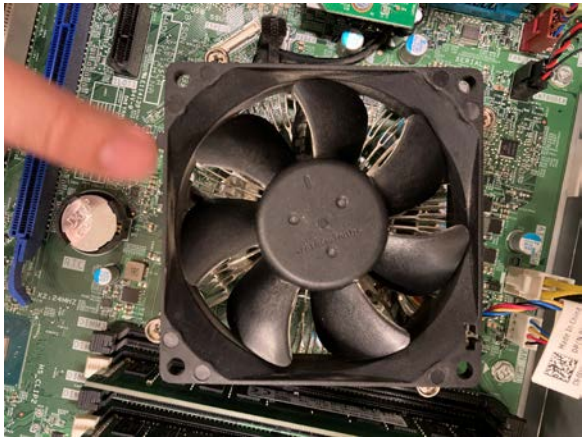
The use of mathematical programming techniques does not change the general flow of a topology design procedure. Thus, compared to the optimality criteria based method for topology design described in section 1.2.2, it only influences the optimization step of the scheme. This iterative loop becomes:

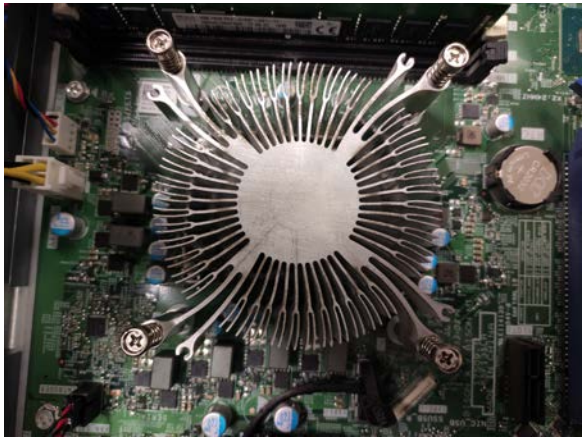
Optimization with, for example, MMA:

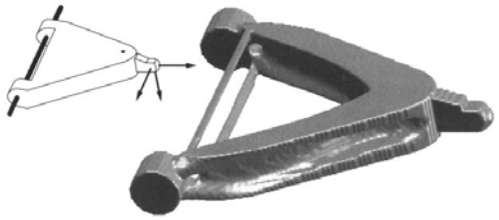
- Make initial design, e.g., homogeneous distribution of material. The iterative part of the algorithm is then:
- For this distribution of density, compute by the finite element method the resulting displacements.
- Compute the compliance of this design and the associated sensitivity with respect to design changes. If only marginal improvement (in compliance) over last design, stop the iterations. Else, continue.
- Compute the update of the density variable, based on the MMA approximate subproblem solved by a dual or a primal-dual method.
- Repeat the iteration loop.

Topology Optimization (TO) by distribution of isotropic material

It is here important to underline that for the minimum compliance problem the by far most time-consuming part of the computations is spent on solving the equilibrium equations report this share as up to 97%, in a parallel implementation). Thus it is critical for large problems, especially in 3-D, to improve on the efficiency of the analysis capability. Here the utilization of homogeneous meshes on rectangular or box-like domains is useful , as it removes the necessity for the repeated computation of local stiffness matrices. Also, the use of iterative solvers is useful in large scale problems, and may be required for storage reasons. The ultimate tool is to use vector computations and parallel computing.







Thank you for your attention