Title: Meta-Material Topology Optimization with Geometric Control

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Introduction:
Topology optimization is a numerical optimization method to design lightweight, superior performing mechanical structures. With the intensive development during the last few decades, topology optimization has been proven an effective and robust tool in designing mechanical structures subject to a variety of physical discipline, e.g., solid mechanics, fluid dynamics, and thermal dynamics, etc [2]. Especially with the many manufacturability-related issues being addressed [4], topology optimization has now widely been accepted for industrial applications.

Other than part scale applications, meta-material design through topology optimization has recently been focused [3,10], since extraordinary mechanical properties can be achieved such as negative Poisson's ratio and negative thermal expansion. In addition, advancement of additive manufacturing (AM) technology makes the fabrication of the designed meta-materials no longer a tough issue, as demonstrated in literature [7,8]. Even though meta-material topology optimization has demonstrated the promise, there are still key issues to be addressed to further improve the performance and enhance the manufacturability, which are specified below:

1. Manufacturability issues still exist in meta-material AM and should be carefully addressed when developing the related optimization algorithm, e.g., the structural members should have the size larger than the AM printing resolution which otherwise cannot be successfully printed. Hence, in this article, the key problem of component length scale control will be discussed and addressed.

2. To improve the fatigue resistance of the meta-material formed structure, it is better to eliminate the sharp reentrant corners which are prone of stress concentration. This issue will be addressed by constraining curvatures of the concave boundary areas, because performing stress constrained optimization at the meta-material level is non-trivial.

3. Multi-scale topology optimization is important since all the meta-material design techniques will finally be applied in the part-scale circumstance. Hence, a few part-scale design examples will be studied in this research by including the afore-mentioned geometric control techniques.

So far, SIMP (Solid Isotropic Material with Penalization), level set, and ESO (Evolutionary Structural Optimization) are the main-stream topology optimization methods. From the authors' opinion, level set method has the strongest capability in supporting geometric control since it employs the boundary contour-based structural evolution which can always capture the clear-cut structural boundary and access the related information [1,9]. Therefore, level set method will be employed in this study so that to better solve the afore-mentioned geometric control issues.
Main idea:

Level set method

Level set function $\Phi(\mathbf{X}) : \mathbb{R}^n \to \mathbb{R}$, represents any structure in the implicit form, as:

$$
\begin{align*}
\Phi(\mathbf{X}) > 0, & \quad \mathbf{X} \in \Omega/\partial\Omega \quad (1) \\
\Phi(\mathbf{X}) = 0, & \quad \mathbf{X} \in \partial\Omega \\
\Phi(\mathbf{X}) < 0, & \quad \mathbf{X} \in \Omega/\partial\Omega
\end{align*}
$$

where $\Omega$ represents the material domain, $D$ indicates the entire design domain, and thus $D/\Omega$ represents the void.

Generally, the level set field satisfies the signed distance regulation through solution of Eq. (2), where absolute of the level set value at any point represents its shortest distance to the structural boundary and the sign indicates the point to be either solid ($>0$), or void ($<0$).

$$
|\nabla \Phi(\mathbf{X})| = 1
$$

Meta-material Optimization problem

Under the level set framework, the homogenized elasticity tensor of the representative volume can be calculated by Eq. (27).

$$
\mathbf{E}_B^H = \frac{1}{|\mathcal{Y}|} \int_D \mathbf{E}_b(e^0 - \mathbf{e}(\mathbf{u}^*))(e^0 - \mathbf{e}(\mathbf{u}^*)) H(\Phi) d\Omega
$$

where, $\mathbf{E}_b$ is the elasticity tensor of the based material and $\mathbf{E}_b^H$ is the homogenized elasticity tensor. $|\mathcal{Y}|$ is the representative volume area, $e^0$ is the applied unit strain fields, e.g. $(1,0,0)$, $(0,1,0)$, and $(0,0,1)$. $\mathbf{u}^*$ is the perturbed displacement field obtained by solving Eq. (4), which is $\mathcal{Y}$-period.

$$
\int_D \mathbf{E}_b(e^0 - \mathbf{e}(\mathbf{u}^*)) \mathbf{e}(\mathbf{v}) H(\Phi) d\Omega = 0, \quad \forall \mathbf{v} \in \mathcal{U}
$$

Therefore, to design the meta-material with specified properties, the optimization problem is formulated as follows:

$$
\begin{align*}
\min & \quad J = \frac{1}{2}(\mathbf{E}_{Bij}^H - \overline{\mathbf{E}_{ij}})^2 \\
\text{s.t.} & \quad a(\mathbf{E}_b, \mathbf{u}^*, \mathbf{v}, \Phi) = l(\mathbf{v}, \Phi), \quad \forall \mathbf{v} \in \mathcal{U} \\
& \quad V = \int_D H(\Phi) d\Omega \leq V_{\text{max}} \\
& \quad a(\mathbf{E}_b, \mathbf{u}^*, \mathbf{v}, \Phi) = \int_D \mathbf{E}_b \mathbf{e}(\mathbf{u}^*) \mathbf{e}(\mathbf{v}) H(\Phi) d\Omega \\
& \quad l(\mathbf{v}, \Phi) = \int_D \mathbf{E}_b e^0 \mathbf{e}(\mathbf{v}) H(\Phi) d\Omega
\end{align*}
$$

where, $\overline{\mathbf{E}_{ij}}$ is the target value of the homogenized $\mathbf{E}_{Bij}^H$.

The Lagrange multiplier method is applied to solve the optimization problem, and the adjoint method is employed to calculate the sensitivity result, where the boundary velocities can be calculated as:

$$
V_n = - (\mathbf{E}_{Bij}^H - \overline{\mathbf{E}_{ij}}) \mathbf{E}_b(e^0 - \mathbf{e}(\mathbf{u}^*))(e^0 - \mathbf{e}(\mathbf{u}^*))
$$

Then, the boundary velocities can be put into the Hamilton-Jacobi equation to perform the design update at an iterative basis, which belongs to the standard level set framework [9].

In Fig. 1, a few meta-material topology optimization examples are demonstrated.

Component length scale control

The length scale control functional proposed in the author’s previous work [6] is adapted to realize the length scale control effect; see Eq. (7).

$$
D_T = \int_D \left\{ \left( \frac{\Phi(\mathbf{X})}{T} \right)^+ - \left( \frac{\Phi(\mathbf{X})}{T} \right)^- \right\} H(\Phi) d\Omega
$$

The notations: $(f)^+ = \max(f,0)$; $(f)^- = \min(f,0)$
where $\bar{T}$ is the upper limit of the component length scale and $\underline{T}$ is the lower limit of the component length scale.

Fig. 1: Examples of the meta-material topology optimization, (a) $E_{11} = E_{22} = 0.3$ and $V_{\max} = 0.4$, the single- and 2*2 multi-unit views, (b) $E_{11} = E_{22} = 0.5$ and $V_{\max} = 0.6$, the single- and 2*2 multi-unit views, (c) $E_{33} = 0.14$ and $V_{\max} = 0.4$, the single- and 2*2 multi-unit views (d) $E_{33} = 0.2$ and $V_{\max} = 0.6$, the single- and 2*2 multi-unit views

Fig. 2: A comparative case study, (a) result from Fig. 1d without length scale control, (b) result with component length scale control (the red dot indicates lower limit of the component length scale)

Then, the objective function in Eq. (5) is augmented into:

$$
\text{Min. } J(\Phi) = \frac{1}{2} (E_{Bij}^H - E_{ij})^2 + wD_T(\Phi)
$$

where $w$ is the weight factor.

Here, only the sensitivity result of the length scale control functional is demonstrated in Eq. (9), since the sensitivity result of the other part is already demonstrated in the last sub-section.

$$
\frac{\partial D_T}{\partial \Phi} = \int \mathcal{G} \delta(\Phi) d\Omega
$$

$$
\mathcal{G} = \left[(\Phi(x) - \bar{T})\right]^2 - \left[(\Phi(x) - \underline{T})\right]^2
$$
\[
\int_{\text{ray}_{\text{ao}}(Y) \cap \Omega} \left[ 2 \left( \Phi(Z) - \frac{T}{2} \right)^+ - 2 \left( \Phi(Z) - \frac{T}{2} \right)^- \right] dZ
\]

where \( Y \) is the boundary point, \( \text{ray}_{\text{ao}}(Y) \) is the shortest ray connecting \( Y \) to the structural skeleton, and \( Z \) is the point on the ray. The details about the sensitivity derivation and the ray concept are lengthy and thus will not be demonstrated. Interested readers can refer to [6].

The component length scale control is tested based on the Fig. 1d which includes many thin structural members, and the geometrically constrained result is demonstrated in Fig. 2b where the red dot indicates lower limit of the component length scale while no upper limit is applied. It can be clearly seen that the length scale requirement has been well satisfied.

**Curvature control to relieve stress concentration**

Under the level set framework, the boundary curvature can be easily calculated by:

\[
\kappa = \nabla \cdot n = \nabla \cdot \left( -\frac{\nabla \Phi(X)}{|\nabla \Phi(X)|} \right)
\]

So that, curvature control can be realized by adding the following constraint, where \( R \) means the radius of the curvature.

\[
\kappa(X) > -\frac{1}{R_1}, \text{ for any } X \in \partial \Omega
\]

However, it is non-trivial to calculate the sensitivity of this constraint, and thus, we inherited the idea from [5] where the curvature flow control technique is applied to address this constraint. Equation (12) demonstrates the curvature dependent velocities for mean curvature flow control, in which \( b \) is a positive constant. If \( \kappa > 0 \), the interface will move in the direction of concavity; and if \( \kappa < 0 \), the interface will move in the direction of convexity.

\[
v = -b \kappa n
\]

To satisfy the local curvature constraints, we need to re-define the constant \( b \), that:

\[
b = 0, \quad \text{if } \kappa(X) > -\frac{1}{R}
\]

\[
b > 0, \quad \text{if } \kappa(X) \leq -\frac{1}{R}
\]

Then, the Hamilton-Jacobi equation is adapted into the convection-diffusion form, which is:

\[
\Phi_t + \nabla \cdot \nabla \Phi = -b \kappa |\nabla \Phi|
\]

The curvature control is tested based on the Fig. 1b which includes many sharp reentrant corners (especially in the 2*2 view), and the geometrically constrained result is demonstrated in Fig. 3b where the red dot indicates lower limit of the radius of the curvature. It can be clearly seen that the curvature control constraint has been well addressed.

![Fig. 3: A comparative case study, (a) result from Fig. 1b without curvature control, (b) result with curvature control (the red dot indicates lower limit of the radius of the curvature).](image-url)
Conclusion:
Metal-material topology optimization is studied in this article, especially the geometric control issues including length scale control and curvature control. The specific algorithm details have been demonstrated and the effectiveness have been proved through comparative case studies.

So far, the research on meta-material topology optimization in a part-scale circumstance is still under exploration, and the related contents will be presented in the full manuscript. Also, about the already introduced geometric control techniques, more numerical examples will be demonstrated in the full manuscript.

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References: