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Multi-material topology optimization for nonlinear heat conduction with temperature-dependent properties

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ABSTRACT

With the continuous trend towards miniaturization and high power density in modern engineering systems, thermal management faces unprecedented challenges. Traditional topology optimization based on constant material property assumptions often fails to capture the inherent dependence of material properties on temperature, thereby limiting the design potential in extreme operating environments. In this work, a multi-material topology optimization (TO) framework for steady-state heat conduction considering temperature-dependent material properties (TDMPs) is proposed. By integrating nonlinear finite element analysis with the discrete material optimization (DMO) scheme, a nonlinear heat conduction TO model is constructed. Two optimization objective functions, namely, the minimization of thermal compliance and peak temperature, are investigated to address distinct thermal design requirements. The effectiveness of the proposed method is demonstrated through several two- and three-dimensional numerical examples, including complex and irregular engineering domains. A material switching mechanism is identified from the optimized results, wherein the proposed method autonomously allocates materials with high thermal conductivity based on the local temperature distribution. Furthermore, two numerical approaches are proposed to verify the correctness of the optimized results, and the optimized designs are compared with those obtained from conventional experience-based designs and other multi-material interpolation schemes. The results demonstrate that introducing multiple materials with TDMPs yields physically reasonable designs and superior performance. This observation confirms the potential of the proposed method for thermal design in multifunctional and high-temperature structures.

1. Introduction

With the increasing complexity and power density of modern engineering structures, efficient thermal management has become a critical challenge (Yang et al., 2024; Zhang & Zhang, 2024). From a microscopic perspective, particularly in electronic devices where heat dissipation directly impacts device lifespan, to the extreme environments faced by aerospace components, structural systems are often subjected to intense thermal gradients. Under such realistic operating conditions, Fourier's law of heat conduction becomes highly nonlinear, as the thermal conductivity of practical engineering materials varies significantly with temperature (Uyanna & Najafi, 2022; Retailleau et al., 2022). Consequently, designing high-performance structures that can withstand these nonlinear

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behaviors requires advanced methodologies that account for temperature-dependent material properties (TDMPs), rather than relying on the traditional simplification of constant material properties (CMPs).

Topology optimization (TO) has emerged as a powerful automated design tool, with extensive applications in fields ranging from fluid dynamics (Aage et al., 2017) to compliant mechanisms (Wu et al., 2021; Han et al., 2026b), energy-absorbing structures (Han et al., 2024), multiscale design (Sun et al., 2025), and soft robotics (Yuhn et al., 2023). Rather than relying on intuition, TO iteratively distributes highly conductive materials within a design domain to form optimal thermal pathways. This approach has successfully generated highly efficient, non-intuitive heat conduction structures, such as needle-like (Yan et al., 2018) and hair-like (Liu et al., 2022) layouts. Over the past decades, various TO frameworks have been established, including the density-based method (Ferrari & Sigmund, 2020; Sigmund, 2007), the level set method (Allaire et al., 2004; Wang et al., 2003), the evolutionary structural optimization (ESO) method (Xia et al., 2018), and the movable morphable components method (Guo et al., 2014). Among these, the density-based method is particularly favored for heat transfer problems due to its computational efficiency (Zhao et al., 2021; Yan et al., 2024). The effectiveness of this method in heat transfer design has also been demonstrated in industrial applications (Zhou et al., 2016). However, the majority of existing thermal TO studies (Zhang & Liu, 2008; Sun et al., 2024a; Ogawa et al., 2024) are still confined to the CMP assumption. Neglecting the inherent TDMPs inevitably leads to inaccurate evaluations of internal thermal resistance, resulting in sub-optimal layouts under real-world conditions.

To address this discrepancy, recent efforts have begun incorporating TDMPs into thermal TO (Tang et al., 2019; Ha et al., 2004). These investigations have demonstrated that accounting for TDMPs can improve thermal performance compared to classical CMP-based designs. However, these optimization models were primarily restricted to single-material settings and regular design domains (Tang et al., 2019; Ha et al., 2004). As reported in Ha et al. (2004), while accounting for TDMPs improves the prediction accuracy of the temperature field, it often yields only minor topological modifications compared to CMP-based designs. From a heat transfer perspective, this phenomenon occurs because modifying the temperature-dependent thermal conductivity of a single material merely alters its local thermal resistance, offering limited spatial freedom to reroute the primary heat flux pathways. To achieve highly adaptive thermal management, it is essential to expand the design space by introducing multiple materials with TDMPs. Physically, different classes of materials exhibit distinct temperature-dependent thermal-conductivity behaviors. For example, the thermal conductivity of pure metals generally decreases with rising temperature due to increased electron-phonon scattering, whereas highly alloyed metals, doped semiconductors, and certain technical ceramics can exhibit more complex, non-monotonic, or material-dependent temperature dependencies (Tanabe et al., 2003; Pop, 2010; de Faoite et al., 2012). Hence, a multi-material TO framework can leverage the material-switching mechanism for nonlinear heat conduction. This allows the optimization process to dynamically allocate highly conductive materials based on the local temperature distribution, offering significant performance gains over single-material designs.

Although multi-material interpolation schemes for TO, such as discrete material optimization (DMO) (Stegmann & Lund, 2005; Sanders et al., 2018; Han et al., 2026a), extended SIMP (Sigmund & Torquato, 1997; Li et al., 2024; Han et al., 2025), and ordered material interpolation (Zuo & Saitou, 2017; Sun et al., 2024b), are well established, their integration with TDMPs for heat conduction design remains under-explored. This gap is primarily attributed to the complexities associated with sensitivity analysis and nonlinear finite element (FE) formulations. Furthermore, incorporating TDMPs into multi-material designs introduces intersecting thermal conductivity curves across different candidate materials. Such temperature-induced crossovers pose a challenge to traditional schemes (e.g., ordered SIMP), which rely on a priori monotonic rankings of material properties. Applying such restrictive models to TDMP problems violates the physical characteristics of the materials and misleads the optimization trajectory. Therefore, a symmetric and unbiased design space, such as the DMO scheme (Stegmann & Lund, 2005; Sanders et al., 2018; Han et al., 2026a), is required to accommodate these curve intersections without predefined property ordering. However, existing DMO-based thermal optimization methods rely on the assumption of constant material properties (Ogawa et al., 2024), which restricts the available material combinations and consequently limits the design space.

Furthermore, to meet the requirements of distinct application scenarios, it is necessary to explore different objective functions. Most previous studies focus on minimizing thermal compliance, which is physically equivalent to minimizing global thermal resistance (or maximizing overall heat dissipation). However, in critical engineering applications, mitigating local hotspots to prevent thermal failure is more important than maximizing overall heat dissipation (Yan et al., 2024; Zhu et al., 2019). Thus, minimizing the peak temperature becomes a necessity. Given the highly nonlinear dependence between temperature distribution and thermal conductivities, optimizing for global heat dissipation versus local hotspot mitigation may trigger entirely different topological configurations, necessitating a comparative investigation that is currently absent in the literature.

Based on these theoretical and practical demands, we propose a multi-material topology optimization framework for nonlinear steady-state heat conduction considering TDMPs. Distinguished from conventional DMO-based approaches under the CMP assumption, the present framework incorporates the TDMPs into the DMO scheme, allowing the optimizer to freely select from candidate materials featuring distinct temperature-dependent thermal conductivities. This integration empowers the optimizer to exploit the adaptive material-switching mechanism, wherein the optimized multi-material layout is dynamically influenced by the temperature distribution. In particular, a key advantage of the proposed framework is its capability to adaptively allocate materials exhibiting different temperature-dependent thermal conductivity behaviors, such as materials whose thermal conductivity increases within a certain temperature range but decreases beyond a critical temperature. Meanwhile, two objective functions, namely, thermal compliance and peak temperature, are investigated to address different thermal management requirements. The effectiveness of the proposed method is demonstrated through two- and three-dimensional numerical examples. Furthermore, we provide two numerical approaches to verify the optimality of the designs and the physical correctness of the material-switching mechanism. The results

demonstrate that incorporating multiple materials with TDMPs yields physically reasonable layouts that outperform conventional designs.

The rest of this work is structured as follows: Section 2 presents the theoretical framework, including the nonlinear finite element formulation considering TDMPs, the DMO-based multi-material interpolation scheme, and the numerical implementation of the optimization algorithm. Subsequently, several two- and three-dimensional numerical examples are provided in Section 3 to demonstrate the effectiveness of the proposed method and to discuss the physical correctness of the multi-material design. Finally, concluding remarks and future perspectives of this work are presented in Section 4. Additionally, the detailed derivation of the sensitivity analysis and a numerical verification case are included in Appendix A.

2. Methodology

In this section, the multi-material formulation considering TDMPs and the corresponding optimization model are presented. First, the nonlinear steady-state heat conduction analysis is briefly described in Section 2.1. Subsequently, the multi-material topological representation strategy based on the DMO interpolation scheme is presented in Section 2.2. The corresponding optimization model is introduced in Section 2.3, followed by a detailed description of the numerical procedure.

2.1. Nonlinear steady-state heat conduction analysis

Assuming isotropic and temperature-dependent materials, the governing equation for nonlinear steady-state heat conduction and its boundary conditions (Tang et al., 2019) defined on the design domain Ω are expressed as

$$\begin{cases} -\nabla \cdot (k(T)\nabla T) = Q & \text{in } \Omega \\ T = \bar{T} & \text{on } \Gamma_D \\ -k(T)\nabla T \cdot \mathbf{n} = \bar{q} & \text{on } \Gamma_N, \end{cases} \quad (1)$$

where $k(T)$ and T are the temperature-dependent thermal conductivity and temperature field, respectively. Q denotes the volumetric internal thermal load. Γ_D and Γ_N ($\Gamma_D \cup \Gamma_N = \partial\Omega$, $\Gamma_D \cap \Gamma_N = \emptyset$) denote the Dirichlet and Neumann boundaries with specified temperature $\bar{T}$ and normal heat flux $\bar{q}$, respectively, and $\mathbf{n}$ is the outward unit normal vector. In this work, the Robin boundary condition is not taken into account because it may be design-dependent (Bruns, 2007; Iga et al., 2009).

By applying the chain rule of differentiation to the divergence operator in the governing equation, Eq. (1)₁ can be rewritten as

$$-k(T)\nabla^2 T - \frac{dk(T)}{dT}(\nabla T \cdot \nabla T) = Q. \quad (2)$$

This equation highlights that heat transfer is governed not only by standard heat diffusion (the first term) but also by the additional heat flux variation induced by the spatial gradient of temperature-dependent material properties (the second term). This latter term constitutes the primary source of nonlinearity in the present heat conduction problem. It should be noted that the expansion yielding Eq. (2) assumes that the thermal conductivity k depends on the temperature T locally (i.e., the Fourier-type constitutive relation $\nabla k = d_T k \nabla T$). This local, non-hysteretic assumption is effective for standard engineering materials under steady-state conditions. For specialized materials exhibiting strong nonlocal thermal behavior (Su et al., 2025) or severe hysteresis (Tan et al., 2020), this formulation would require further modification.

To solve this nonlinear problem numerically, the standard Galerkin finite element method (FEM) is employed. The continuous domain Ω is discretized into n_e finite elements, and the resulting system of nonlinear equations can be written in residual form as

$$\mathbf{R}(T) = \mathbf{Q}_{\text{int}} - \mathbf{Q}_{\text{ext}} = \mathbf{K}(T)\mathbf{T} - \mathbf{Q}_{\text{ext}} = \mathbf{0}, \quad (3)$$

where $\mathbf{R}$ is the global residual vector, $\mathbf{T}$ is the global nodal temperature vector, $\mathbf{Q}_{\text{int}}$ represents the internal equivalent heat load vector, and $\mathbf{Q}_{\text{ext}}$ is the global external thermal load vector. Here, $\mathbf{Q}_{\text{ext}}$ is assembled as follows:

$$\mathbf{Q}_{\text{ext}} = \bigcup_{e=1}^{n_e} \left[\int_{\Omega_e} \mathbf{N}^T Q dV - \int_{\Gamma_N} \mathbf{N}^T \bar{q} dA \right], \quad (4)$$

where $\mathbf{N}$ denotes the shape function. In the finite element implementation, rather than integrating a continuous volumetric source, the thermal load is directly applied as concentrated nodal loads. This is achieved by assigning a non-zero scalar value, denoted by Q_{ext} , to the corresponding degrees of freedom in the global external load vector $\mathbf{Q}_{\text{ext}}$. Here, $\bigcup$ denotes the standard finite element assembly operator. The temperature-dependent global conductivity matrix $\mathbf{K}(T)$ is assembled from the element-level conductivity matrices $\mathbf{K}_e$ as

$$\mathbf{K}(T) = \bigcup_{e=1}^{n_e} \mathbf{K}_e = \bigcup_{e=1}^{n_e} \left(k(T_e) \int_{\Omega_e} \mathbf{B}^T \mathbf{B} dV \right), \quad (5)$$

which assumes an element-wise constant conductivity $k(T_e)$ evaluated at the element-averaged temperature T_e . The effectiveness of the element-wise constant conductivity assumption is discussed in Appendix B. Here, $\mathbf{B} = \nabla \mathbf{N}$ denotes the temperature gradient

matrix. This representative temperature is computed as the arithmetic mean of the local nodal temperatures within the element, given by

$$T_e = \frac{1}{n_d} \sum_{j=1}^{n_d} T_{e,j}, \quad (6)$$

where n_d is the number of nodes per element, and $T_{e,j}$ denotes the local nodal temperature.

The root of the nonlinear residual equation in Eq. (3) is obtained using the Newton–Raphson (NR) iterative method. The relationship between two successive iterations, i and $i + 1$, is established by a first-order Taylor expansion of the residual $\mathbf{R}(\mathbf{T})$ as follows:

$$\mathbf{R}(\mathbf{T}^{(i+1)}) \approx \mathbf{R}(\mathbf{T}^{(i)}) + \frac{\partial \mathbf{R}(\mathbf{T}^{(i)})}{\partial \mathbf{T}} \Delta \mathbf{T} = \mathbf{0}, \quad (7)$$

where $\Delta \mathbf{T} = \mathbf{T}^{(i+1)} - \mathbf{T}^{(i)}$ is the temperature increment vector. The Jacobian matrix $\mathbf{J}$, often referred to as the tangent conductivity matrix in nonlinear thermal analysis, is obtained by differentiating the residual vector $\mathbf{R}$ with respect to the temperature vector $\mathbf{T}$. To avoid ambiguity in tensor operations, its components J_{IJ} are defined in index notation as

$$J_{IJ} = \frac{\partial R_I}{\partial T_J} = K_{IJ} + \sum_{K=1}^{n_{\text{dof}}} \frac{\partial K_{IK}}{\partial T_J} T_K, \quad (8)$$

where the indices I, J , and K (ranging from 1 to n_{dof}) denote the global degrees of freedom. The first term K_{IJ} represents the standard conductivity matrix component, while the second term introduces asymmetry into the tangent conductivity matrix. This is a distinctive mathematical feature arising from the temperature dependence. The partial derivative $\partial_{T_J} K_{IK}$ captures the influence of the temperature-dependent thermal conductivity on the local nodal temperature.

2.2. Multi-material formulation based on the DMO interpolation

In this work, the discrete material optimization (DMO) scheme (Stegmann & Lund, 2005) is adopted to represent m distinct candidate materials within the design domain. Compared to other multi-material interpolation schemes, such as the extended SIMP scheme (Sigmund & Torquato, 1997; Li et al., 2024) or the ordered material interpolation scheme (Zuo & Saitou, 2017; Sun et al., 2024b), the DMO scheme is particularly suitable for nonlinear heat conduction problems due to its inherent weight symmetry. This property guarantees an unbiased material selection process, ensuring that the optimizer does not artificially favor any specific material during the early stages of optimization, which is essential when materials exhibit complex and intersecting temperature-dependent properties. Furthermore, this interpolation scheme is highly compatible with diverse constitutive models, as demonstrated in Han et al. (2026a), allowing base materials with complex functional variations (e.g., temperature dependence) to be directly integrated.

To describe the multi-material distribution, the DMO scheme introduces m sets of design variables. Specifically, for each finite element e , the scalar variable $x_{e,i} \in [0, 1]$ ($i = 1, 2, \dots, m$) represents the design variable associated with the i -th candidate material. Based on the DMO scheme, the effective elemental thermal conductivity $k_e(\mathbf{w}_e, T_e)$ is interpolated as

$$k_e(\mathbf{w}_e, T_e) = \sum_{i=1}^m w_{e,i} k_i(T_e), \quad (9)$$

where $w_{e,i}$ is the penalized weight of material i in element e , and $k_i(T_e)$ is the temperature-dependent thermal conductivity associated with material i . Ideally, to achieve a physically meaningful material distribution, the resulting weights should be binary, satisfying $w_{e,i} \in \{0, 1\}$ and $\sum_{i=1}^m w_{e,i} \leq 1$.

The element-level weight $w_{e,i}$ in Eq. (9) is calculated using the DMO function, which is formulated to penalize intermediate material mixtures and drive the design variables toward a binary state, and is given by

$$w_{e,i} = \epsilon + (1 - \epsilon)(\hat{x}_{e,i})^p \prod_{\substack{j=1 \\ j \neq i}}^m (1 - \gamma_j(\hat{x}_{e,j})^p), \quad i = 1, \dots, m, \quad (10)$$

where $\hat{x}_{e,i}$ is the projected physical density variable (see Eq. (11)₂) associated with material i in element e , and ϵ represents a small positive value (e.g., 10^{-6}) assigned to the void phase (ersatz material) to prevent numerical singularities in the global conductivity matrix. Here, $p = 3$ is the penalization power used to suppress intermediate density variables. Since the material selection in the considered TO problem must be adaptively adjusted according to the local temperature distribution during the optimization process, a continuation scheme is employed. Specifically, the DMO continuation factor γ_j is gradually increased from 0 to 1 in increments of 0.2.

Simultaneously, to ensure a well-posed optimization problem and suppress numerical instabilities such as checkerboard patterns, the design variables $x_{e,i}$ are processed using standard density filtering and Heaviside projection techniques (Sigmund, 2007). The filtered density variable $\tilde{x}_{e,i}$ and the projected physical density variable $\hat{x}_{e,i}$ are successively obtained as

$$\tilde{x}_{e,i} = \frac{\sum_{j \in \mathbb{N}_e} H_{ej} v_j x_{j,i}}{\sum_{j \in \mathbb{N}_e} H_{ej} v_j}, \quad \hat{x}_{e,i} = \frac{\tanh(\beta \eta) + \tanh(\beta(\tilde{x}_{e,i} - \eta))}{\tanh(\beta \eta) + \tanh(\beta(1 - \eta))}, \quad (11)$$

where $\mathbb{N}_e$ denotes the set of neighboring elements j whose center-to-center distance $\Delta(e, j)$ from element e is less than the specified filter radius $r_{\min}$, with the weight factor defined as $H_{ej} = \max(0, r_{\min} - \Delta(e, j))$. The variable v_j is the volume of element j . The projection steepness parameter β is initialized at 1 and incremented by 1 (up to 40) whenever the relative change in the objective function between consecutive iterations falls below 0.5%. By utilizing this product-based formulation in Eq. (10), the DMO interpolation inherently treats all candidate materials symmetrically, thereby ensuring an unbiased material selection process.

Incorporating the multi-material DMO interpolation, the strong form of the governing equation in Eq. (1) for nonlinear heat conduction can be rewritten as

$$\begin{cases} -\nabla \cdot (\sum_{i=1}^m w_i k_i(T) \nabla T) = Q & \text{in } \Omega \\ T = \bar{T} & \text{on } \Gamma_D \\ -(\sum_{i=1}^m w_i k_i(T)) \nabla T \cdot \mathbf{n} = \bar{q} & \text{on } \Gamma_N. \end{cases} \quad (12)$$

Following the standard Galerkin finite element discretization, this problem is reformulated as finding the root of the nonlinear residual vector, i.e., $\mathbf{R}(\mathbf{w}, T) = \mathbf{K}(\mathbf{w}, T)T - \mathbf{Q}_{\text{ext}} = \mathbf{0}$. Here, the effective global temperature-dependent thermal conductivity matrix $\mathbf{K}(\mathbf{w}, T)$ is assembled from the elemental contributions $\mathbf{K}_e(\mathbf{w}_e, T_e)$ as

$$\mathbf{K}(\mathbf{w}, T) = \bigcup_{e=1}^{n_e} \mathbf{K}_e(\mathbf{w}_e, T_e) = \bigcup_{e=1}^{n_e} \left(\left(\sum_{i=1}^m w_{e,i} k_i(T_e) \right) \int_{\Omega_e} \mathbf{B}^T \mathbf{B} dV \right). \quad (13)$$

In this density-based TO framework, the design domain is treated as a continuous heterogeneous medium. Material interfaces are implicitly captured by the spatially varying conductivity $\mathbf{K}(\mathbf{w}, T)$. Consequently, the interfacial continuity conditions are naturally satisfied in the finite element weak form, precluding the need for explicit interface tracking. Meanwhile, when solving this discretized nonlinear system using the Newton–Raphson iterative scheme, the components of the global Jacobian matrix $\mathbf{J}$ defined in Eq. (8) must be updated to reflect the multi-material interpolation. Using index notation, the components of the global tangent conductivity matrix J_{IJ} are expressed as

$$J_{IJ} = \bigcup_{e=1}^{n_e} \left[\sum_{i=1}^m w_{e,i} K_{IJ}^{(e,i)} + \sum_{K=1}^{n_{\text{dof}}} \left(\sum_{i=1}^m w_{e,i} \frac{\partial K_{IK}^{(e,i)}}{\partial T_J} \right) T_K \right], \quad (14)$$

where the indices I , J , and K (ranging from 1 to n_{dof}) denote the global degrees of freedom. The first term inside the assembly operator represents the standard conductivity matrix component contributed by the multi-material distribution, where $K_{IJ}^{(e,i)}$ is the linear conductivity component of candidate material i in element e . Similar to the single-material derivation, the second term renders the global tangent conductivity matrix inherently asymmetric, which is a distinctive feature arising from the temperature dependence. In this work, the convergence criterion for the Newton–Raphson method is given by $\|\mathbf{R}(T)\| < 10^{-6}$.

From a numerical implementation perspective, the asymmetry of the tangent conductivity matrix introduces specific requirements for the solver strategy and affects the overall conditioning of the system. Standard symmetric iterative solvers, such as the preconditioned conjugate gradient (PCG) method, cannot be directly applied. Hence, robust solvers for non-symmetric systems must be employed, such as the biconjugate gradient stabilized (BiCGSTAB) method adopted for the 3D examples in this work to improve computational efficiency. Furthermore, artificially enforcing symmetry on the tangent conductivity matrix would deteriorate the convergence performance of the Newton–Raphson iterative scheme.

2.3. Topology optimization formulation and its numerical procedure

The objective of the topology optimization problem in this work is to determine the optimal multi-material distribution that minimizes a prescribed thermal objective function, subject to a global volume constraint and the nonlinear heat equilibrium governing equation. To this end, the mathematical formulation is expressed as

$$\begin{aligned} \min_{\mathbf{x}} \quad & c(T(\mathbf{x}), \mathbf{x}), \\ \text{s.t.} \quad & \begin{cases} \mathbf{R}(\mathbf{x}, T) = \mathbf{K}(\mathbf{w}(\mathbf{x}), T)T - \mathbf{Q}_{\text{ext}} = \mathbf{0} \quad (\text{Eq. (12)}) \\ g(\mathbf{x}) = \sum_{e=1}^{n_e} \sum_{i=1}^m \frac{\hat{x}_{e,i} v_e}{f_{\text{vol}} V_{\Omega}} - 1 \leq 0 \\ 0 \leq x_{e,i} \leq 1, \quad \forall e \in \{1, \dots, n_e\}, \quad i \in \{1, \dots, m\} \end{cases}, \end{aligned} \quad (15)$$

where $\mathbf{x} = [x_{1,1}, x_{1,2}, \dots, x_{n_e,m}]^T$ represents the vector of design variables for the m candidate materials. The objective function is denoted by $c(T(\mathbf{x}), \mathbf{x})$. The first constraint represents the nonlinear steady-state heat conduction equation derived in Section 2.2. The second constraint limits the total material usage, where v_e is the elemental volume, f_{vol} is the prescribed maximum volume fraction, and V_{Ω} is the total volume of the design domain. The design variables are bounded between 0 and 1.

In this work, two objective functions, namely thermal compliance and peak temperature, are considered to address different thermal management requirements, as defined below:

$$\begin{aligned} \text{Thermal compliance:} \quad & c_1(T, \mathbf{x}) = \mathbf{Q}_{\text{ext}}^T T, \\ \text{Peak temperature:} \quad & c_2(T, \mathbf{x}) = \left(\sum_{J=1}^{n_{\text{dof}}} T_J^{p_{\text{norm}}} \right)^{1/p_{\text{norm}}}, \end{aligned} \quad (16)$$

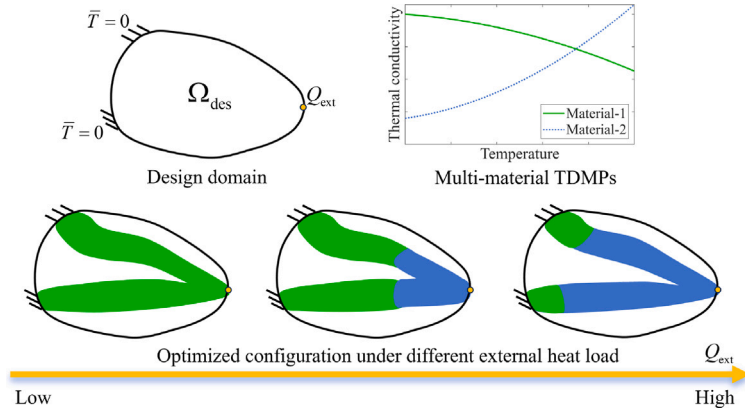


Fig. 1. Schematic illustration of the proposed multi-material topology optimization framework considering TDMPs.

Here, the first objective function, known as thermal compliance, is typically used to obtain an optimal configuration with a more uniform temperature distribution. Meanwhile, the second objective function employs the continuous p_{norm} -based aggregation function to approximate the non-differentiable maximum function ($T_{\text{max}} = \max(T)$) (Deng et al., 2022), thereby minimizing the peak temperature. Note that a smaller p_{norm} value leads to an inaccurate approximation of the true peak temperature, whereas an excessively large p_{norm} introduces severe numerical ill-conditioning and strong non-convexity, which traps gradient-based optimizers in poor local optima. To address the trade-off between approximation accuracy and optimization stability, the aggregation parameter is set to $p_{\text{norm}} = 16$ in this work based on numerical observations and discussed in Appendix C. Meanwhile, due to the inherent non-convexity of the multi-material nonlinear thermal design problem, the optimized results are also affected by the initial material distribution and the continuation schemes of the parameters (e.g., γ_j in Eq. (10) and β in Eq. (11)). To maintain the conciseness of the main text, detailed numerical discussions on these effects are provided in Appendix D.

Fig. 1 illustrates the conceptual framework of this work using a simplified design domain. The domain is subjected to a localized external heat load Q_{ext} on the right side, while the left side is prescribed with $\bar{T} = 0$. Two candidate materials with contrasting temperature-dependent behaviors are introduced to demonstrate the material-switching mechanism. The first material (depicted in green) exhibits thermal conductivity degradation with increasing temperature, representing a generic material with a negative temperature coefficient. Conversely, the second material (depicted in blue) shows a positive temperature coefficient of thermal conductivity, representing an alternative class of temperature-dependent materials. As the magnitude of the external thermal load Q_{ext} increases, the optimization method evolves both the structural configuration and the material distribution, transitioning from the material with a negative temperature coefficient to the one with a positive coefficient in high-temperature regions. This adaptive reconfiguration highlights the necessity and effectiveness of the proposed multi-material nonlinear heat conduction topology optimization method.

The optimization problem is solved using a nested iterative approach, in which the outer loop updates the design variables while the inner loop solves the nonlinear heat conduction equation. The detailed numerical procedure, illustrated in Fig. 2, is summarized as follows:

1. First, define the FE boundary conditions, specify the temperature-dependent properties for multiple materials, and initialize the design variables $\mathbf{x}$;
2. Compute the physical density variables using filtering and projection techniques, and evaluate the elemental thermal conductivity using the DMO scheme;
3. Solve the nonlinear heat conduction equation $\mathbf{R}(\mathbf{x}, T) = \mathbf{0}$ using the Newton–Raphson method. The tangent conductivity matrix is updated iteratively until the residual norm satisfies $\|\mathbf{R}\| \leq 10^{-6}$;
4. Solve the linear adjoint equation to compute the sensitivities of the objective function and constraints with respect to the design variables. The design variables $\mathbf{x}$ are then updated using the Method of Moving Asymptotes (MMA) optimizer based on the computed sensitivities. To avoid excessive changes in the design variables, a maximum step size of 0.1 is imposed;
5. Repeat steps 2–4 until the relative change in the objective function falls below a predefined tolerance and the projection parameter β reaches 40.

Remark 1. The sensitivity analysis method and its verification are not considered as novel contributions of this work and are therefore provided in Appendix A for completeness.

3. Numerical examples

In this section, four numerical examples are presented to demonstrate the effectiveness of the proposed multi-material topology optimization framework considering TDMPs. The examples cover a range of scenarios, from simple two-dimensional square design

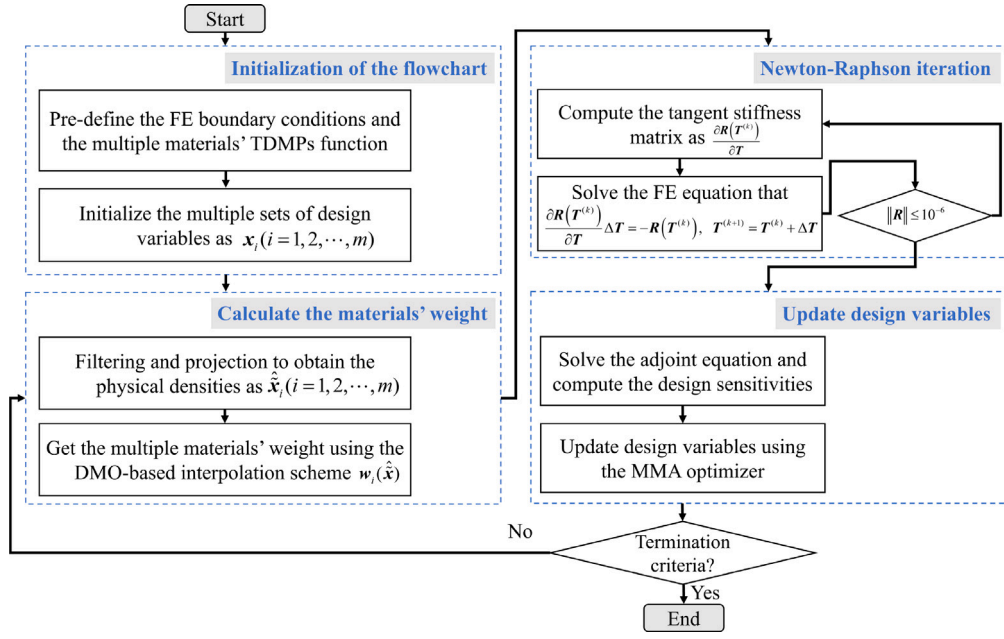


Fig. 2. Numerical procedure.

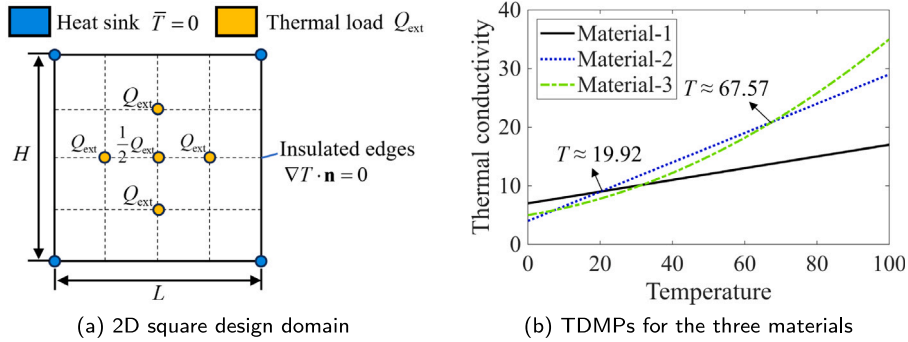


Fig. 3. Problem setup for Example 1.

domains to complex irregular geometries, including a two-dimensional suspension structure and a realistic three-dimensional engineering pipe. For generality and ease of comparison, all physical quantities and material parameters in this work are expressed in dimensionless form.

3.1. Example 1: 2D square domain

To evaluate the proposed method, a simple two-dimensional square design domain with dimensions $L = H = 1$ is considered, as illustrated in Fig. 3(a). The four corners of the design domain are prescribed as heat sinks ($\bar{T} = 0$), while the remaining external edges are assumed to be perfectly insulated ($\nabla T \cdot \mathbf{n} = 0$). To generate a non-uniform temperature field, five external thermal loads are uniformly distributed within the domain, with one located at the center having a magnitude of $Q_{\text{ext}}/2$ and four surrounding loads each with magnitude Q_{ext} .

As shown in Fig. 3(b), three materials with distinct temperature-dependent thermal conductivities are employed, distinguished by different colors. Their conductivity functions $k(T)$ are defined as

$$\left\{ \begin{array}{ll} \text{Material-1 (black):} & k_1(T) = 0.1T + 7, \quad \frac{dk_1}{dT} = 0.1 \\ \text{Material-2 (blue):} & k_2(T) = 0.25T + 4, \quad \frac{dk_2}{dT} = 0.25 \\ \text{Material-3 (green):} & k_3(T) = 2 \times 10^{-3}T^2 + 0.1T + 5, \quad \frac{dk_3}{dT} = 4 \times 10^{-3}T + 0.1 \end{array} \right. . \quad (17)$$

Table 1

Classification of material dominance ranges based on TDMPs ranking for Example 1.

Range	Temperature interval (T)	Preferred material	TDMPs ranking
1	[0, 19.92)	Material-1 (black)	$k_1(T) > \max(k_2(T), k_3(T))$
2	[19.92, 67.57)	Material-2 (blue)	$k_2(T) > \max(k_1(T), k_3(T))$
3	[67.57, ∞)	Material-3 (green)	$k_3(T) > k_2(T) > k_1(T)$

Table 2

Thermal compliance of different optimization results.

External load	Material-1 Section 3.1.1	Material-2 Section 3.1.1	Material-3 Section 3.1.1	Two materials Section 3.1.2	Three materials Section 3.1.2
$Q_{\text{ext}} = 10$	3.885×10^2	5.283×10^2	5.098×10^2	3.889×10^2	3.893×10^2
$Q_{\text{ext}} = 30$	3.168×10^3	3.504×10^3	3.735×10^3	3.161×10^3	3.162×10^3
$Q_{\text{ext}} = 180$	7.772×10^4	6.407×10^4	6.633×10^4	6.410×10^4	6.390×10^4

From the intersection points of the conductivity curves in Fig. 3(b), two transition temperatures are identified at $T \approx 19.92$ and $T \approx 67.57$. These points naturally divide the temperature range into three distinct regions. The preferred material in each region, defined as the material possessing the highest thermal conductivity, is summarized in Table 1. This theoretical segmentation provides the physical basis for the material-switching mechanism observed in the subsequent optimization results. It should be noted that this mechanism is facilitated by the application of a global volume constraint (Eq. (15)), rather than individual volume constraints for each material. The global constraint provides the topology optimization method with sufficient design freedom to allocate the optimal material based on the local temperature. In contrast, imposing separate volume constraints for each material would restrict the design space, potentially leading to sub-optimal material distributions and thereby compromising the overall performance.

In what follows, the effects of multi-material design strategies under TDMPs are investigated. The investigations are structured into three parts as follows:

1. First, optimization based on the single-material assumption is conducted to examine topological variations in a simple design domain under different TDMPs and external loads Q_{ext} ;
2. Second, multiple materials are introduced to demonstrate performance improvements and the material-switching mechanism enabled by the proposed framework;
3. Third, a visual verification approach is presented to demonstrate the physical correctness of the optimized results.

3.1.1. Single-material topology optimization under TDMPs

Before introducing the multi-material design framework, a baseline is established by examining the optimized configurations of single-material designs with temperature-dependent properties. In this subsection, topology optimization is performed separately for Material 1, Material 2, and Material 3 (as defined in Fig. 3(b)), and the objective function is defined as the minimization of thermal compliance, i.e., $c_1 = Q_{\text{ext}}^T T$. The finite element (FE) mesh is discretized into 200×200 elements, and the maximum volume fraction f_{vol} is set to 50%. To generate different levels of thermal gradients, the magnitude of the external thermal load is given as $Q_{\text{ext}} = 10$, 30, and 180.

The optimized configurations and their corresponding temperature fields are presented in Fig. 4. An important observation is that although the temperature distribution and peak values vary significantly with increasing external thermal load Q_{ext} , the optimized configurations remain nearly unchanged for each material. For instance, the designs using Material 1 at $Q_{\text{ext}} = 10$ and $Q_{\text{ext}} = 180$ exhibit negligible geometric differences, despite substantial variations in thermal conductivity. This topological invariance arises from the fundamental difference between the scalar nature of heat conduction and the tensorial nature of mechanical force transmission. In structural mechanics, nonlinearity causes internal force redistribution, effectively redirecting the load path to stiffer regions. However, in a single-material heat conduction design case, even if the thermal conductivity is temperature-dependent $k(T)$, heat flow still follows the path of least thermal resistance determined by the boundary conditions. The temperature-dependent thermal conductivity $k(T)$ primarily modifies the magnitude of local thermal resistance rather than the direction of heat flux. Consequently, the TO process tends to generate similar structures to minimize thermal compliance, even under large variations in thermal conductivity.

The objective function values (thermal compliance) for these single-material designs are listed in Fig. 4 and will be summarized later in Table 2 for comparison. The results indicate that although TO incorporating TDMPs improves predictive accuracy, it exhibits limited topological variation under the single-material assumption, even when the external thermal load varies significantly. This limitation highlights the necessity of introducing multiple materials to expand the design space and enable high-performance heat conduction design.

3.1.2. Multi-material optimization results for thermal compliance minimization

Following the single-material study, the multi-material topology optimization framework is applied to the same design domain. Two scenarios are examined: a two-material case (utilizing Materials 1 and 2) and a three-material case (utilizing Materials 1, 2,

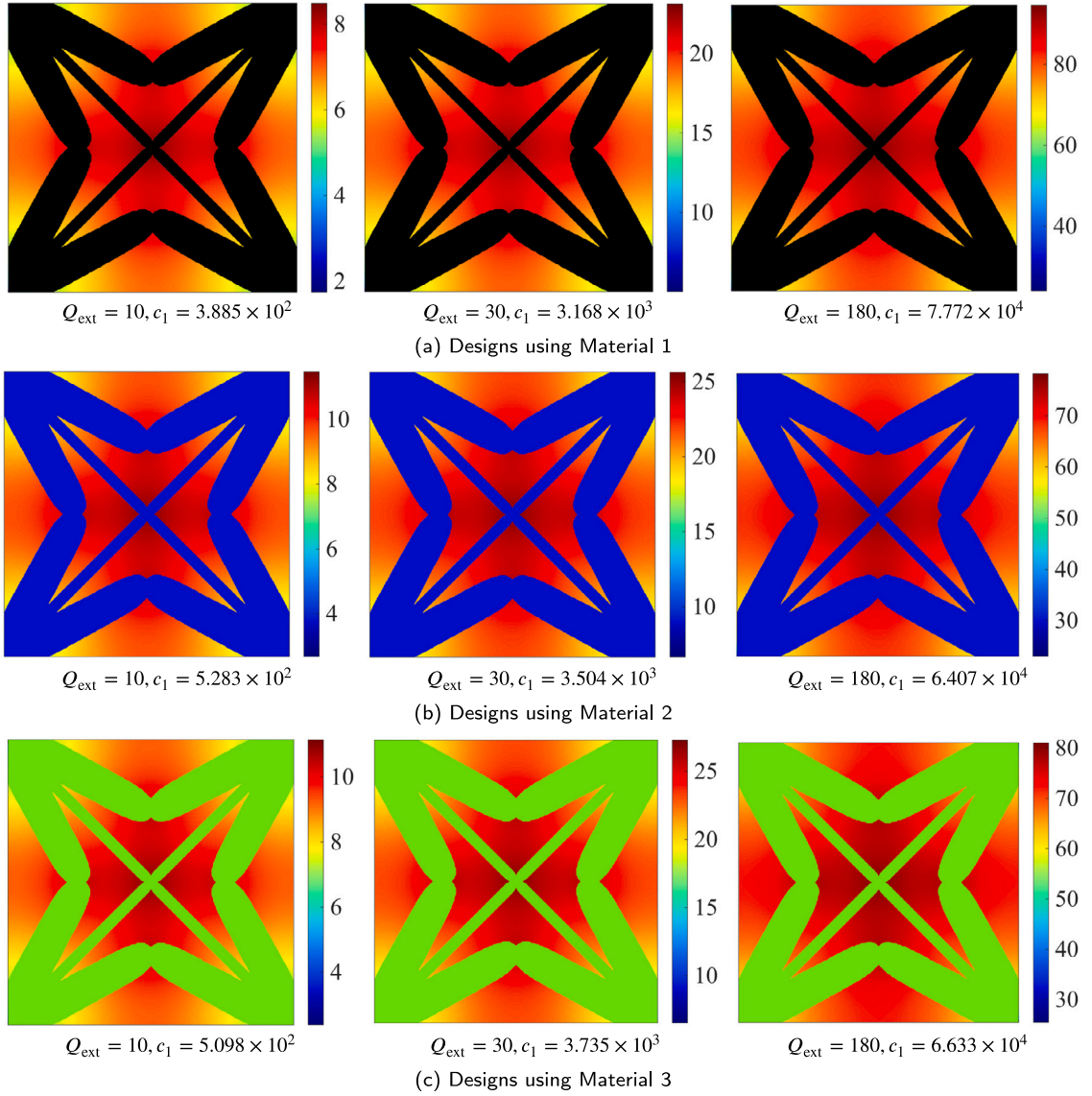


Fig. 4. Optimized topological configurations and corresponding temperature distributions for Example 1: Thermal compliance minimization (single-material assumption).

and 3). The temperature-dependent thermal conductivities of these materials are depicted in Fig. 3(b). All other parameters are kept consistent with the single-material study. Based on the theoretical dominance regions defined in Table 1, the optimizer is expected to allocate Material 1 to low-temperature regions and transition to Materials 2 or 3 in higher-temperature regions.

The optimized material distributions under external thermal loads ($Q_{\text{ext}} = 10, 30$, and 180) are presented in Fig. 5. Unlike the nearly invariant configurations observed in the single-material cases (Fig. 4), the multi-material designs exhibit a clear material-switching mechanism driven by the local temperature distribution, consistent with the theoretical dominance regions in Table 1.

For instance, under low external thermal loads ($Q_{\text{ext}} = 10, 30$), as shown in the first two columns of Fig. 5, the maximum temperature within the domain remains below the second transition point ($T \approx 67.57$). Consequently, Material 3 (green) is not utilized, as its conductivity is suboptimal within this temperature range (Ranges 1 and 2 in Table 1). This explains why the optimized configurations for the three-material case coincide with those of the two-material case under these conditions ($Q_{\text{ext}} = 10, 30$). The optimized structures primarily consist of Material 1 (black), with Material 2 (blue) appearing only in regions where the local temperature exceeds 19.92 . In contrast, when the external thermal load increases to $Q_{\text{ext}} = 180$, additional material switching is triggered. As observed in the rightmost column of Fig. 5, the high-temperature central region necessitates the use of Material 3 (green), which exhibits the highest thermal conductivity for $T > 67.57$.

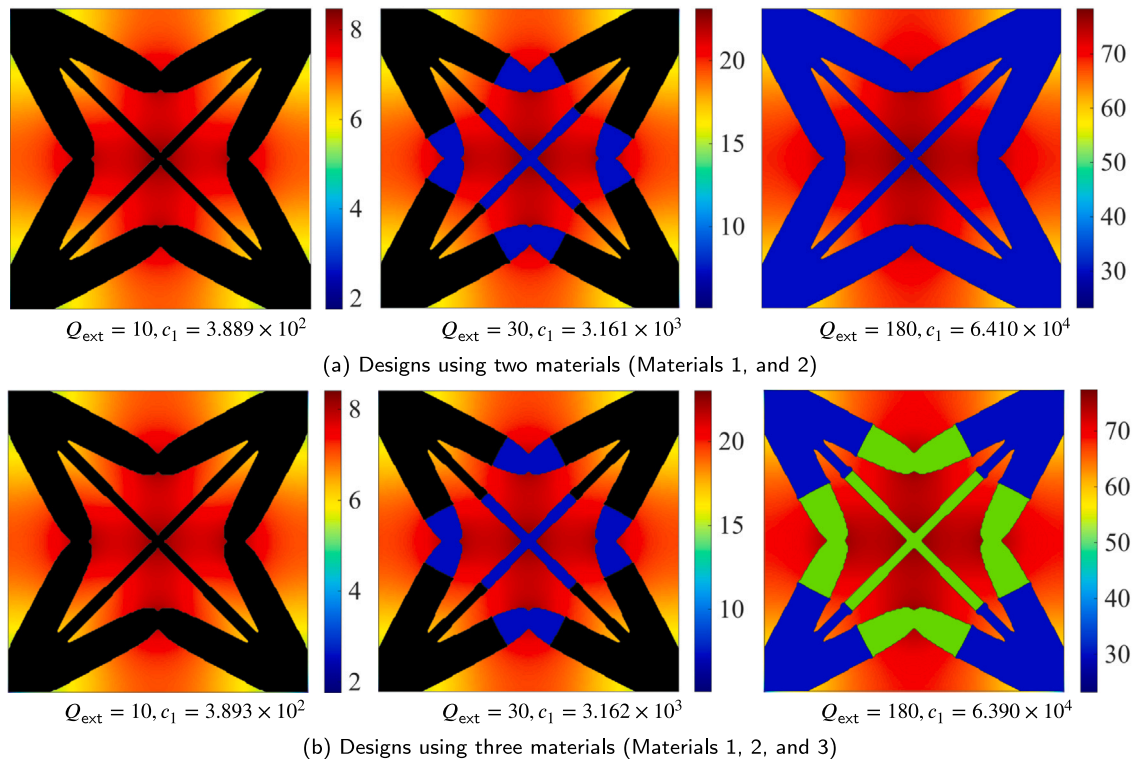


Fig. 5. Optimized topological configurations and corresponding temperature distributions for Example 1: Thermal compliance minimization (multi-material assumption).

Table 3

Performance of the optimization results by peak temperature minimization.

External load	Two-material results		Three-material results	
	Thermal compliance	Peak temperature ($T_{\max}$)	Thermal compliance	Peak temperature ($T_{\max}$)
$Q_{\text{ext}} = 10$	3.904×10^2	8.72	3.901×10^2	8.72
$Q_{\text{ext}} = 30$	3.183×10^3	23.74	3.183×10^3	23.74
$Q_{\text{ext}} = 180$	6.431×10^4	79.77	6.414×10^4	79.28

The resulting thermal compliance values are summarized in Table 2. The multi-material designs yield lower thermal compliance than the single-material baselines in Section 3.1.1. In particular, at $Q_{\text{ext}} = 180$, the inclusion of the third material further reduces thermal compliance compared to the two-material case. This reduction demonstrates the effectiveness of the material-switching mechanism in expanding the design space for high-temperature applications. Quantitatively, the proposed multi-material approach improves the objective function by up to 17.78% relative to the worst-performing single-material design (7.772×10^4 to 6.390×10^4). This improvement highlights the importance of incorporating multiple TDMP materials in topology optimization for systems subjected to large temperature variations, such as aerospace components and energy infrastructure.

3.1.3. Multi-material optimization results for peak temperature minimization

Although minimizing thermal compliance improves overall heat dissipation efficiency, practical engineering applications often require the suppression of local overheating to prevent material failure. To address this requirement, the optimization is reformulated using the p_{norm} -based aggregation of the temperature field, $c_2 = (\sum_{j=1}^{n_{\text{dof}}} T_j^{p_{\text{norm}}})^{1/p_{\text{norm}}}$, as the objective function. Furthermore, a numerical analysis of the influence of the aggregation parameter p_{norm} on the optimized configurations is provided in Appendix C.

The optimized results, presented in Fig. 6, exhibit a similar material-switching mechanism to that observed in the compliance-based designs (Fig. 5) as the external thermal load increases. To suppress peak temperatures, the optimizer redistributes high-conductivity materials (Material 2 and Material 3) toward the high-temperature central region, while the conductive branches become slightly thicker. This configuration establishes efficient thermal pathways to dissipate heat from the external load, thereby reducing the peak temperature. For comparison, the peak temperatures of the compliance-optimized designs in Fig. 5(b) under the three-material assumption are evaluated at 8.76, 23.88, and 79.42, respectively. Thus, the capability of the proposed formulation to suppress localized hotspots is demonstrated. Meanwhile, as the boundary conditions in this case are relatively simple, the decrease in peak temperature is small.

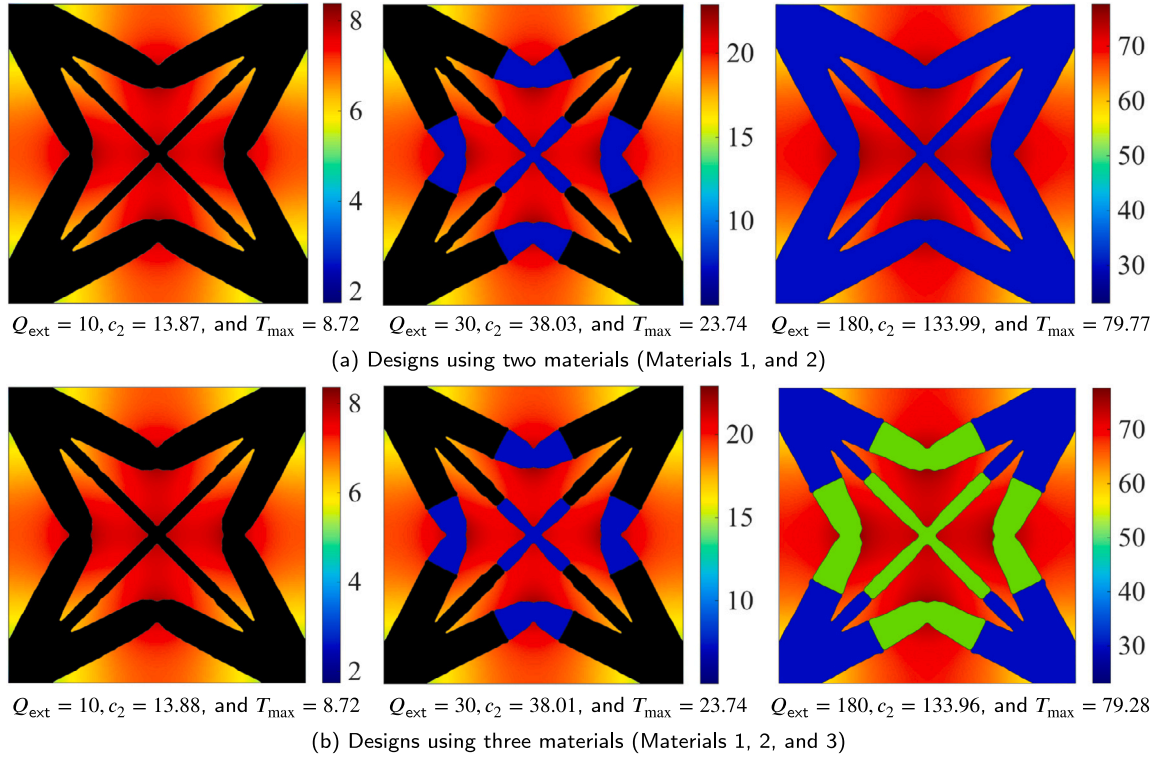


Fig. 6. Optimized topological configurations and corresponding temperature distributions for Example 1: Peak temperature minimization (p_{norm} -based aggregation).

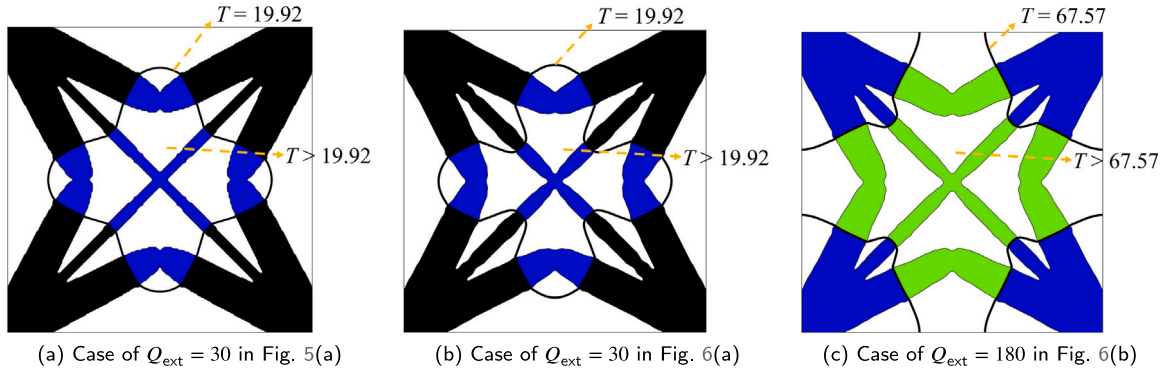


Fig. 7. Verification of the physical reasonableness of the optimized multi-material distributions by superimposing theoretical transition isotherms onto the optimized structures.

Subsequently, the optimized peak temperature and thermal compliance values are summarized in Table 3. The results indicate that this objective formulation effectively reduces the maximum temperature, although it results in a slight increase in thermal compliance. This trade-off demonstrates the flexibility of the proposed multi-material framework in tailoring designs to specific thermal management objectives.

3.1.4. Verification of the optimized multi-material design

To verify the physical correctness of the optimized multi-material distributions, a visual verification approach is proposed. The theoretical transition isotherms numerically calculated in Table 1 ($T \approx 19.92$ and $T \approx 67.57$) are superimposed onto the optimized multi-material configurations. Three representative designs from Figs. 5 and 6 are selected for this verification.

As illustrated in Fig. 7, the boundaries between different materials closely align with the theoretical transition isotherms. Specifically, the interface between Material 1 (black) and Material 2 (blue) follows the $T = 19.92$ isotherm, while the interface between Material 2 and Material 3 (green) coincides with the $T = 67.57$ isotherm. These observations provide direct numerical

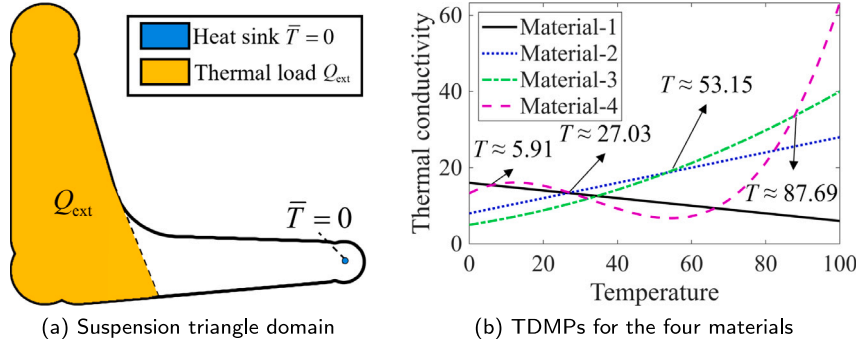


Fig. 8. Problem setup for Example 2.

Table 4

Classification of material dominance ranges based on TDMPs ranking of the four materials for Example 2.

Range	Temperature interval (T)	Preferred material	TDMPs ranking
1	$[0, 5.91)$	Material-1 (black)	$k_1(T) > \max(k_2(T), k_3(T), k_4(T))$
2	$[5.91, 27.03)$	Material-4 (pink)	$k_4(T) > \max(k_1(T), k_2(T), k_3(T))$
3	$[27.03, 53.15)$	Material-2 (blue)	$k_2(T) > \max(k_1(T), k_3(T), k_4(T))$
4	$[53.15, 87.69)$	Material-3 (green)	$k_3(T) > \max(k_1(T), k_2(T), k_4(T))$
5	$[87.69, \infty)$	Material-4 (pink)	$k_4(T) > \max(k_1(T), k_2(T), k_3(T))$

evidence that the proposed method accurately captures the local temperature distribution and activates the thermally optimal material accordingly.

3.2. Example 2: 2D suspension triangle domain

To demonstrate the applicability of the proposed framework to irregular engineering domains, a suspension triangle domain (Talışchi et al., 2012) is considered, as shown in Fig. 8(a). The domain is discretized into 77,279 elements with 78,233 degrees of freedom to ensure numerical accuracy. A uniform volumetric heat generation area is applied to the left region with intensity Q_{ext} , while the right circular region is prescribed as a heat sink with a fixed temperature ($\bar{T} = 0$).

In this example, more complex temperature-dependent material property (TDMP) functions are introduced. Firstly, these functions involving four candidate materials are depicted in Fig. 8(b) and are defined as follows:

$$\begin{cases}
 \text{Material-1 (black):} & k_1(T) = -0.1T + 16, & \frac{dk_1}{dT} = -0.1 \\
 \text{Material-2 (blue):} & k_2(T) = 0.2T + 8, & \frac{dk_2}{dT} = 0.2 \\
 \text{Material-3 (green):} & k_3(T) = 2 \times 10^{-3}T^2 + 0.15T + 5, & \frac{dk_3}{dT} = 4 \times 10^{-3}T + 0.15 \\
 \text{Material-4 (pink):} & k_4(T) = \frac{(T-20)^3}{4000} - \frac{(T-15)^2}{100} - \frac{T}{10} + 17.5, & \frac{dk_4}{dT} = \frac{3(T-20)^2}{4000} - \frac{T}{50} + \frac{1}{5}
 \end{cases} \quad (18)$$

As depicted in Fig. 8(b), Materials 1 and 2 exhibit linear degradation and enhancement trends, respectively. Material 3 shows a quadratic increase in conductivity, representing materials with a nonlinear positive temperature coefficient. In addition, Material 4 (pink) is introduced with a cubic conductivity function to represent complex materials that exhibit non-monotonic property variations. Based on the intersection points of these conductivity curves, the temperature range is divided into multiple dominance regions, as summarized in Table 4. For the four-material scenario, four distinct transition temperatures ($T \approx 5.91, 27.03, 53.15$, and 87.69) partition the temperature range into several regimes, leading to a complex competition among materials. The preferred material switches in the order of Material 1 $\rightarrow$ Material 4 $\rightarrow$ Material 2 $\rightarrow$ Material 3 $\rightarrow$ Material 4 as the temperature increases. This intricate material-switching behavior poses a significant challenge to the optimization capability of the proposed method.

Furthermore, a quantitative verification strategy is introduced to assess the physical consistency of the optimized results. A comparative study is conducted against a conventional experience-based design strategy derived from the single-material assumption. In addition, the computational cost and iteration histories are reported to evaluate the efficiency and stability of the proposed method.

3.2.1. 2D suspension triangle designs considering two materials

The optimization is first carried out for a two-material scenario (Materials 1 and 2) under a 30% volume constraint, considering two different objective functions. As presented in Fig. 9, the results under varying uniform external thermal loads ($Q_{\text{ext}} =$

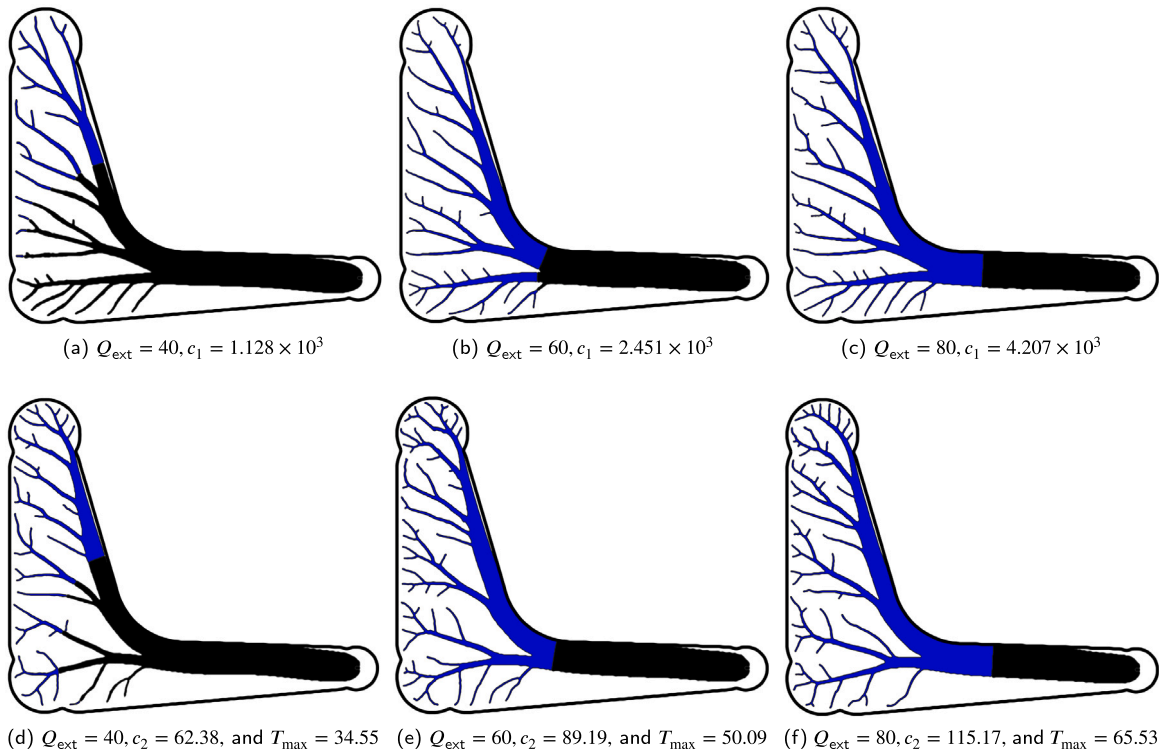


Fig. 9. Optimized suspension triangle heat conduction structure for Example 2: Under different objective functions and external loads based on the two-material assumption. ((a–c) thermal compliance minimization; (d–f) peak temperature minimization).

Table 5

Performance of optimization results considering different objective functions based on the two-material assumption.

External load	Aim at thermal compliance (Fig. 9(a–c))		Aim at peak temperature (Fig. 9(d–f))	
	Thermal compliance	Peak temperature	Thermal compliance	Peak temperature
$Q_{\text{ext}} = 40$	1.128×10^3	66.55	1.167×10^3	62.38
$Q_{\text{ext}} = 60$	2.451×10^3	93.49	2.574×10^3	89.19
$Q_{\text{ext}} = 80$	4.207×10^3	120.35	4.378×10^3	115.17

Table 6

Performances of optimization results considering different objective functions based on the four-material assumption.

External load	Aim at thermal compliance (Fig. 10(a–c))		Aim at peak temperature (Fig. 10(d–f))	
	Thermal compliance	Peak temperature (T_{max})	Thermal compliance	Peak temperature (T_{max})
$Q_{\text{ext}} = 80$	4.143×10^3	70.53	4.401×10^3	63.22
$Q_{\text{ext}} = 120$	8.458×10^3	89.39	8.728×10^3	82.05
$Q_{\text{ext}} = 160$	1.355×10^4	104.32	1.379×10^4	96.74

40, 60, 80) clearly reveal the material-switching mechanism. Specifically, high-temperature regions near the heat generation zone are progressively replaced by Material 2 as the local temperature exceeds the transition point $T \approx 27.03$. This observation highlights the necessity of accounting for TDMPs in multi-material heat conduction design.

Because the temperature field is more concentrated in the upper-left corner of the design domain, additional material is allocated in this region to effectively reduce the peak temperature, as shown in Figs. 9(d–f). To facilitate comparison, the objective function values for these optimization results are listed in Table 5. The variations in optimized configurations and their corresponding objective values indicate that the selection of the objective function should be tailored to specific engineering thermal management requirements.

3.2.2. 2D suspension triangle designs considering four materials

Subsequently, a four-material scenario is investigated to evaluate the capability of the proposed method in handling non-monotonic material preferences, as summarized in Table 4. The external volumetric thermal loads are increased to $Q_{\text{ext}} = 80, 120,$

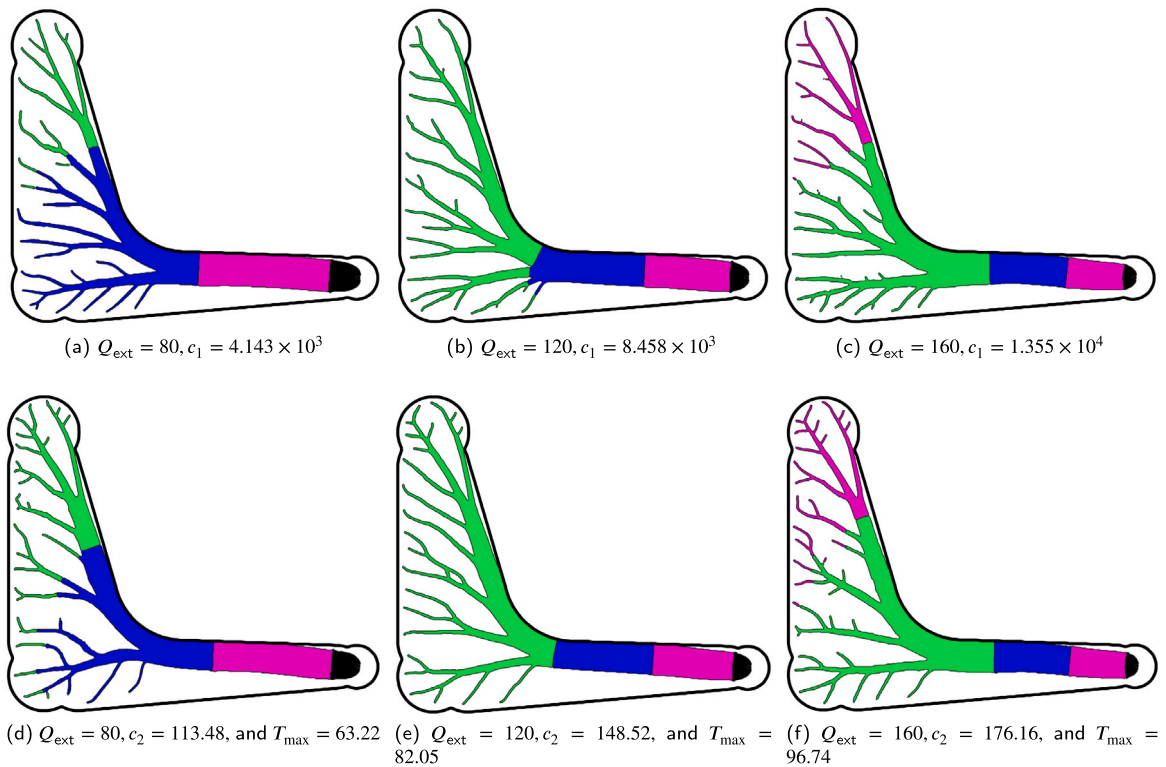


Fig. 10. Optimized suspension triangle heat conduction structure for Example 2: Under different objective functions and external loads based on the four-material assumption. ((a–c) thermal compliance minimization; (d–f) peak temperature minimization).

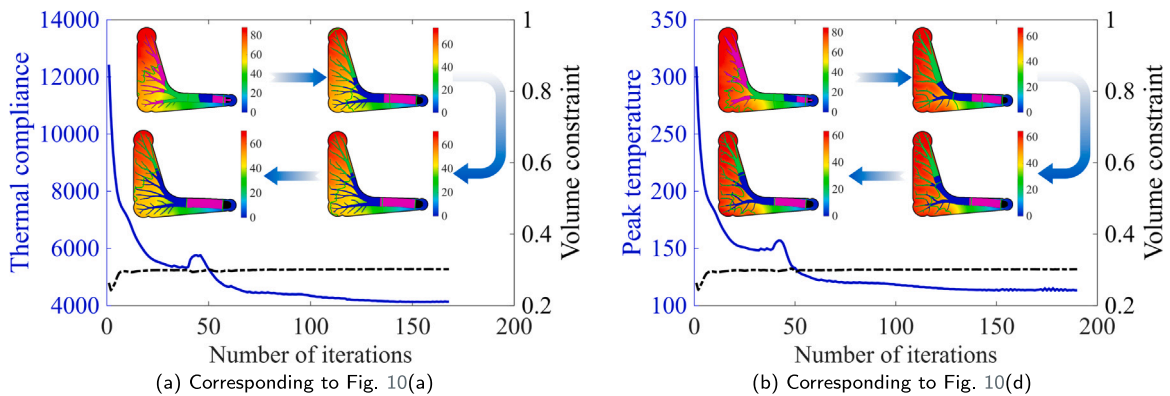


Fig. 11. Iteration histories and several intermediate configurations of the optimized suspension structure.

and 160. The optimized results are depicted in Fig. 10, showing a complex multi-material distribution. A key observation is the re-entrant appearance of Material 4 (pink). Since Material 4 exhibits the highest thermal conductivity in both the low ($T \in [5.91, 27.03]$) and high ($T > 87.69$) temperature ranges, the optimizer assigns it to both the cool peripheral region and the hot core region. These two regions are spatially separated by regions occupied by Materials 2 and 3. This result demonstrates that the proposed method can accurately capture complex, non-monotonic material preferences and allocate materials according to the local temperature field. The objective function values for these cases are summarized in Table 6 for comparison. As indicated, the peak temperature minimization formulation reduces the maximum temperature at least by 7% compared to the thermal compliance-optimized designs. Furthermore, despite the symmetric interpolation weights of the DMO scheme, the inherent non-convexity of the TO problem introduces a degree of dependence on the initial guess. A detailed investigation of this phenomenon is provided in Appendix D.

To assess the optimization stability of the proposed method, the iteration histories for the cases in Figs. 10(a) and 10(d) are shown in Fig. 11, together with several intermediate configurations at intervals of 40 iterations. The objective function decreases monotonically overall and converges within 200 iterations, with only minor fluctuations caused by the projection parameter

Table 7
Computational time of different optimization results.

Numerical example	Number of design variables	Time for FE analysis (s)	Time for sensitivity (s)	Time for updating (s)	Total optimization time (s)
Fig. 9(a)	154,558	1397.22 (82.28%)	62.59 (3.69%)	228.67 (13.47%)	1698.21
Fig. 9(d)	154,558	1452.71 (82.65%)	66.40 (3.78%)	229.01 (13.03%)	1757.76
Fig. 10(a)	309,116	2074.66 (81.25%)	61.97 (2.43%)	408.19 (15.99%)	2553.53

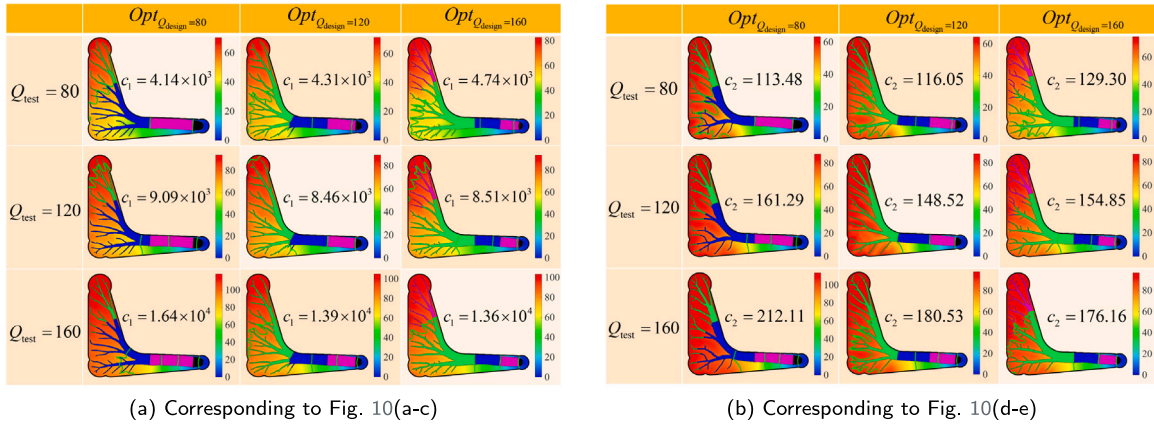


Fig. 12. Cross-validation analysis of the optimized multi-material structures; the designs optimized for specific external loads are re-evaluated under varying testing external loads.

continuation scheme, demonstrating the numerical stability of the method. Furthermore, as the temperature field evolves during the optimization process, the proposed method progressively reallocates materials in accordance with the updated temperature distribution. This observation further highlights the importance of incorporating TDMPs in topology optimization.

3.2.3. Cross-validation and computational time of the optimized result

In nonlinear topology optimization, the optimized results are highly dependent on the prescribed thermal boundary conditions. Consequently, an optimized structure is expected to exhibit optimal performance only under its specific design conditions. To quantitatively verify this optimality, a cross-validation study is conducted. The designs optimized for specific external thermal loads (Q_{design}) are re-evaluated under off-design thermal boundary conditions (Q_{test}). The resulting performance matrix and the corresponding temperature distributions with superimposed theoretical transition isotherms are visualized in Fig. 12.

As demonstrated in Fig. 12, the diagonal entries, which represent the performance under the corresponding design conditions, consistently yield the minimum objective values within each column. This observation confirms that a structure optimized for a given thermal load performs best under the same condition, while off-design usage leads to suboptimal performance. Specifically, relative to suboptimal layouts, the performance improvement reaches up to 17.07% for thermal compliance (1.64×10^4 to 1.36×10^4) and 16.95% for p_{norm} -based aggregation peak temperature (212.11 to 176.16). Furthermore, the physical consistency of these results is supported by the superimposed theoretical transition isotherms; only the diagonal designs show precise alignment between material interfaces and temperature isotherms.

In addition, the computational efficiency of the proposed framework is evaluated. The computational times for selected cases are listed in Table 7, conducted on a laptop equipped with an Intel® Core™ i9-12900H @ 2.50 GHz CPU and 32 GB of RAM. The reported time includes the finite element (FE) analysis, sensitivity analysis (via the adjoint equation), and design variable updates. Several observations can be made regarding computational efficiency. First, the computational times for different objective functions are comparable. Second, the sensitivity analysis is computationally inexpensive because the adjoint equation is linear. Third, the design variable update incurs a moderate cost due to the large number of design variables (e.g., 309,116 variables for the four-material cases). While reducing the number of design variables could further improve efficiency (Sun et al., 2024a, 2024b), this aspect is beyond the scope of the present study. Most notably, the majority of the computational cost is attributed to the Newton–Raphson (NR) iterations, since the tangent conductivity matrix and residual vector must be updated iteratively. Nevertheless, even the most complex design case requires less than one hour of computational time on a standard personal computer, demonstrating the computational efficiency of the proposed framework.

3.2.4. Comparison of the optimized result with the experience-based design

To assess the advantages of the proposed framework, a comparison is conducted with a classical experience-based design approach, as illustrated in Fig. 13. In this approach, topology optimization is first performed under the assumption of a single

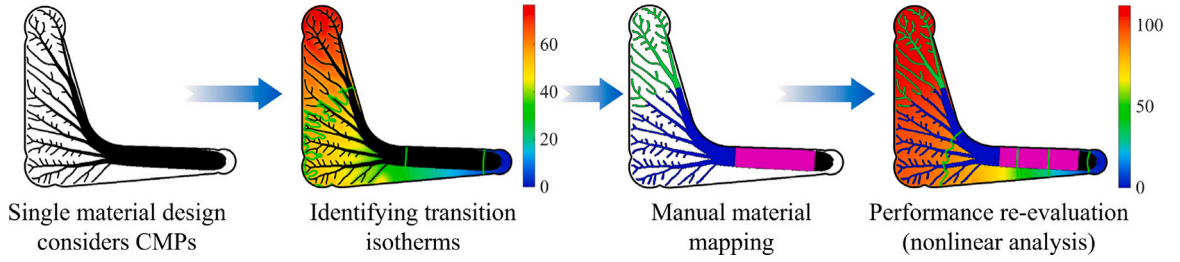


Fig. 13. Illustration of the classical experience-based design strategy used for comparison.

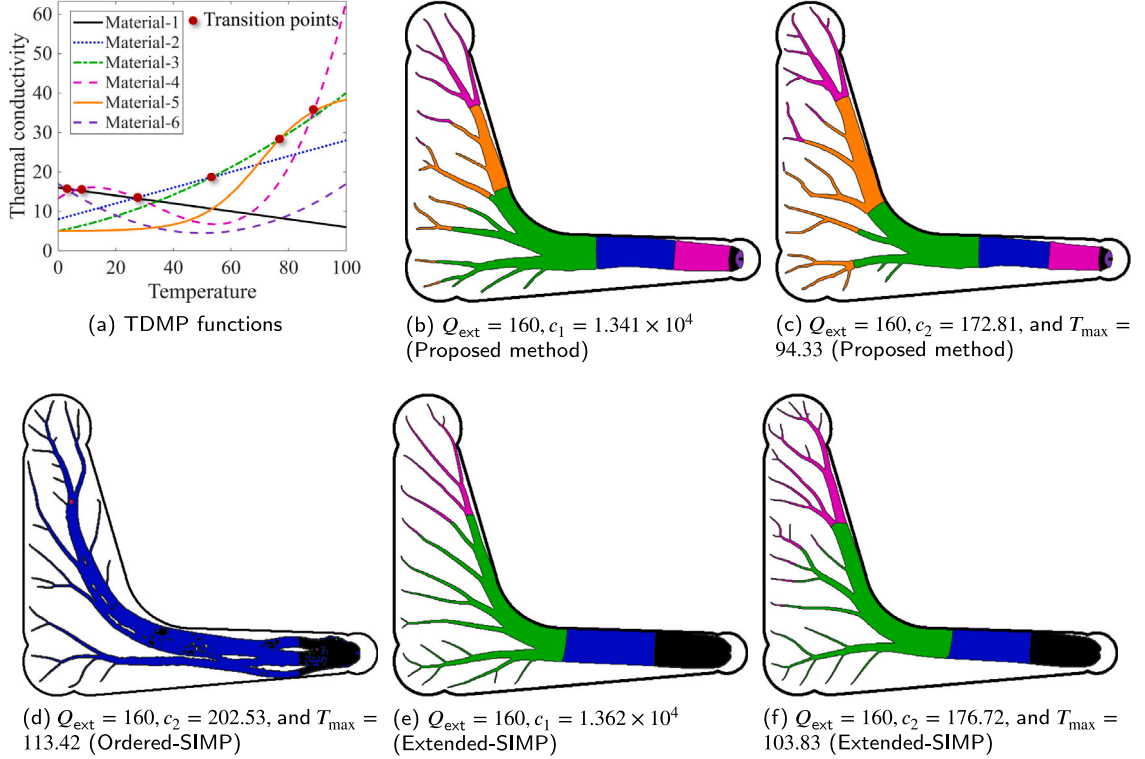


Fig. 14. Optimized suspension triangle heat conduction structure for Example 2: Under the six-material assumption, comparing different interpolation methods. ((b), (e) thermal compliance minimization; (c), (d), and (f) peak temperature minimization.)

material with constant properties ($k = 30$ and $Q_{\text{ext}} = 160$) to determine the structural layout. Subsequently, the thermal transition isotherms are identified from the resulting temperature field, and materials are manually assigned to their theoretically optimal regions defined in Table 4. Finally, the performance of this multi-material design is re-evaluated using nonlinear heat conduction analysis.

The experience-based design yields a thermal compliance of 1.781×10^4 , which is 31.5% higher than that obtained using the proposed method (1.355×10^4). Meanwhile, the re-evaluated temperature field reveals a clear misalignment between the manually assigned material interfaces and the actual transition isotherms. This discrepancy indicates that the structural layout and material distribution are strongly coupled in nonlinear heat conduction TO problems; therefore, a sequential design strategy leads to sub-optimal configurations that cannot fully exploit the design space.

Although iterative refinement guided by the material-switching mechanism could gradually improve the design, such a process would require a large number of repeated analyses to approach the performance achieved by the proposed method. Moreover, handling complex phenomena such as material re-entry, as observed in the numerical examples, would be particularly challenging within the conventional design method.

Table 8

Classification of material dominance ranges based on TDMPs ranking of the six materials for Example 2.

Range	Temperature interval (T)	Preferred material	TDMPs ranking
1	[0, 2.47)	Material-6 (purple)	$k_6(T) > \max_{j \neq 6} k_j(T)$
2	[2.47, 5.91)	Material-1 (black)	$k_1(T) > \max_{j \neq 1} k_j(T)$
3	[5.91, 27.03)	Material-4 (pink)	$k_4(T) > \max_{j \neq 4} k_j(T)$
4	[27.03, 53.15)	Material-2 (blue)	$k_2(T) > \max_{j \neq 2} k_j(T)$
5	[53.15, 77.04)	Material-3 (green)	$k_3(T) > \max_{j \neq 3} k_j(T)$
6	[77.04, 87.69)	Material-5 (orange)	$k_5(T) > \max_{j \neq 5} k_j(T)$
7	[87.69, ∞)	Material-4 (pink)	$k_4(T) > \max_{j \neq 4} k_j(T)$

3.2.5. Extension to six candidate materials and comparison with other interpolation schemes

To further demonstrate the scalability of the proposed framework and highlight the advantages of the adopted DMO scheme, the design problem is extended to six candidate materials and compared with two widely used interpolation approaches, namely, the ordered material interpolation (ordered-SIMP) and the extended multi-phase SIMP (extended-SIMP).

Two candidate materials (Materials 5 and 6) are introduced to the library of Example 2 (Fig. 14(a)), with their TDMP functions defined as

$$\begin{cases} \text{Material-5 (orange):} & k_5(T) = 5 + \frac{35}{1 + \exp(-0.1(T - 70))}, & \frac{dk_5}{dT} = \frac{3.5 \exp(-0.1(T - 70))}{(1 + \exp(-0.1(T - 70)))^2} \\ \text{Material-6 (purple):} & k_6(T) = 4.5 + 0.005(T - 50)^2, & \frac{dk_6}{dT} = 0.01(T - 50) \end{cases} \quad (19)$$

As shown in Fig. 14(a), the inclusion of these two additional materials significantly increases the complexity of the TDMP curves. The multiple intersections divide the operational temperature range into seven distinct intervals, each featuring a unique dominant material as summarized in Table 8.

Under the external thermal load $Q_{\text{ext}} = 160$, the proposed DMO-based method successfully allocates all six materials to their thermally optimal regions as presented in Figs. 14(b)–(c). This successful optimization is attributed to the symmetry of the DMO formulation, which ensures an unbiased design space and enables proper material selection in nonlinear multi-material heat conduction TO problems.

In contrast, while the ordered-SIMP method is computationally efficient since it requires only one design variable per element, it relies on predefined monotonic material ordering. Because the intersecting TDMP curves violate this assumption, the ordered-SIMP method fails to effectively utilize higher-index materials as shown in Fig. 14(d). Therefore, only the peak-temperature minimization result is reported for this method, yielding a value of 202.53, which is significantly worse than the proposed method (172.81).

Similarly, although the extended-SIMP method removes the monotonic ordering requirement, its sequential multiplication formulation introduces asymmetry. Materials positioned later in the sequence require the simultaneous activation or deactivation of multiple variables, making them difficult to select in gradient-based optimization due to reduced sensitivities. Consequently, it fails to identify the newly introduced materials and cannot capture the re-entry behavior of Material 4 (Figs. 14(e)–(f)), resulting in inferior performance.

Remark 2. Expanding to $m = 6$ linearly increases the design variables to $6 \times n_e$, leading to higher computational cost, particularly in assembling elemental conductivity matrices and updating design variables. To handle the resulting highly non-convex design space and avoid premature convergence, a more conservative continuation strategy is adopted for γ_j in Eq. (10), with a reduced step size of 0.1. Also, the DMO method may become more susceptible to local optima due to cross-penalization effects; however, similar challenges can arise in other multi-material interpolation schemes. Therefore, symmetric interpolation approaches without cross-penalization, such as UMI (Yi et al., 2023) and PU (Bui & Nguyen, 2025), may be explored in future work to further improve optimization robustness.

3.3. Example 3: 3D regular rectangular domain

To demonstrate the scalability of the proposed method, the numerical example is extended to a three-dimensional (3D) domain. A simple regular design domain with dimensions $2 \times 2 \times 3$ is considered, as illustrated in Fig. 15(a). The domain is discretized into $40 \times 40 \times 60$ voxel elements, and the volume fraction f_{vol} is prescribed as 25%. A localized external thermal load is applied to the top surface, with its magnitude sequentially increased to $Q_{\text{ext}} = 50, 55$, and 60. Four small surface regions located at the bottom corners are prescribed as heat sinks ($\bar{T} = 0$). For consistency with the 2D analysis, the candidate materials include Material 1 and Material 2 (as defined in Eq. (17) and shown in Fig. 15(b)), characterized by a transition temperature of $T \approx 19.92$. The thermal compliance, $c_1 = Q_{\text{ext}}^T T$, is adopted as the objective function.

The optimized 3D topological configurations and their corresponding material distributions are visualized in Fig. 16, where different materials are displayed separately to highlight their spatial distributions. The resulting structures form 3D branch-like configurations that efficiently channel heat flux from the top source to the bottom sinks. Similar to the 2D cases, the 3D results exhibit a material-switching mechanism driven by the vertical thermal gradient. Under a lower external thermal load ($Q_{\text{ext}} = 50$),

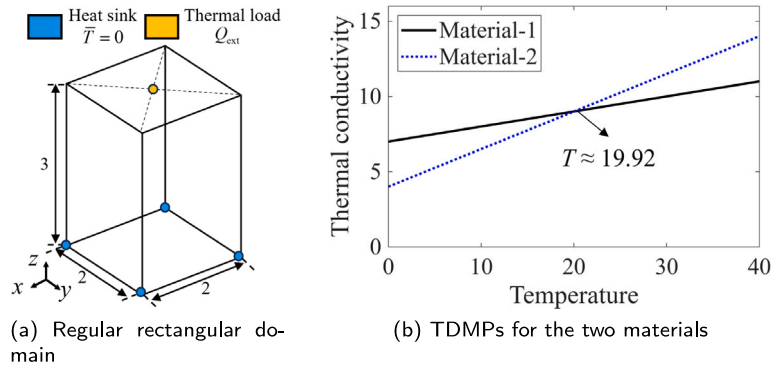
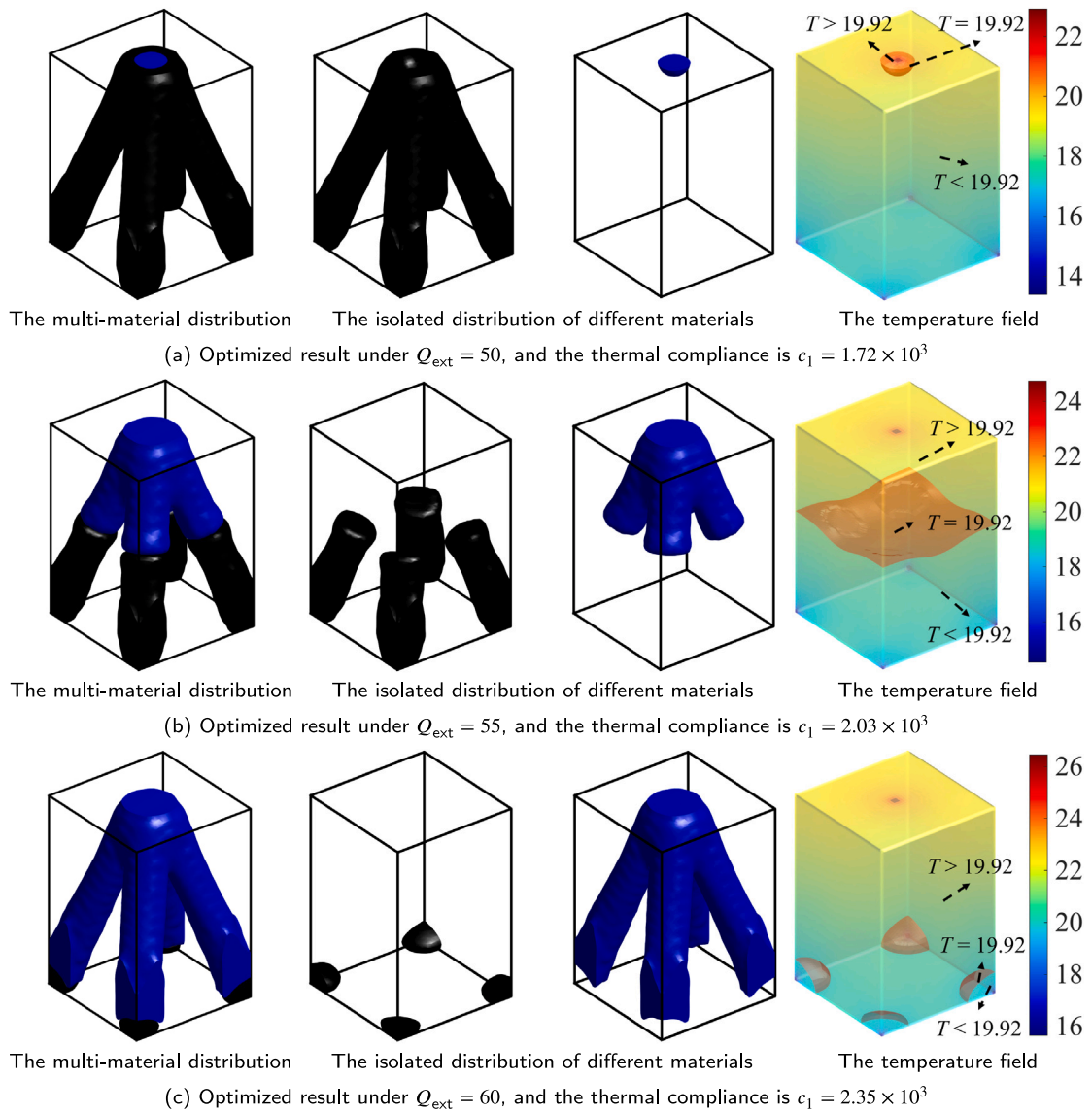


Fig. 15. Problem setup for Example 3.

Fig. 16. Optimized 3D material distributions and corresponding temperature fields under varying external thermal loads ($Q_{\text{ext}} = 50, 55$, and 60), respectively.

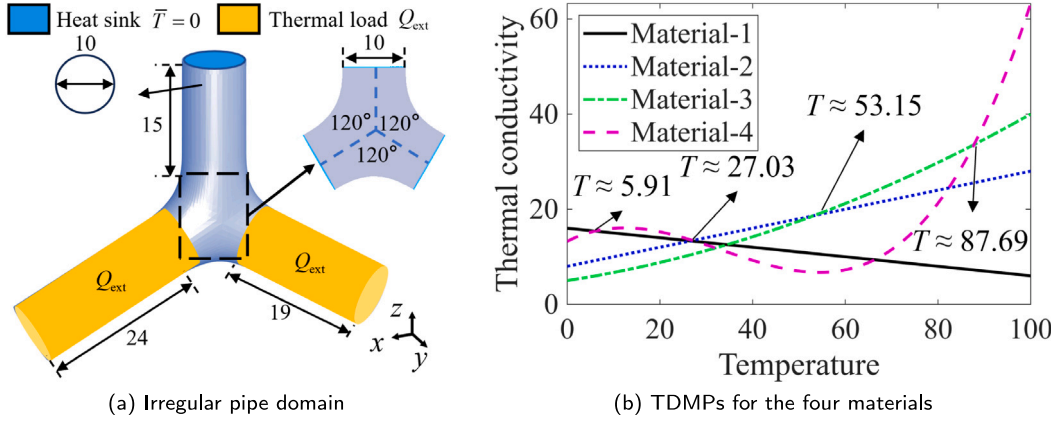


Fig. 17. Problem setup for Example 4.

the structure is predominantly composed of Material 1 (black), with Material 2 (blue) activated only near the heat source, where the local temperature exceeds the transition threshold ($T > 19.92$). As the external thermal load increases to $Q_{\text{ext}} = 55$ and $Q_{\text{ext}} = 60$, a progressive material substitution is observed. The high-temperature region propagates downward from the external heat source, prompting the optimizer to replace Material 1 with the higher-conductivity Material 2 along the primary heat transfer paths.

This material-switching behavior is further illustrated in the rightmost column of Fig. 16, where the isothermal surface corresponding to the transition temperature ($T = 19.92$) is plotted. A clear spatial correspondence is observed between this isothermal surface and the material interface, as the region occupied by Material 2 coincides with $T > 19.92$. Consequently, at $Q_{\text{ext}} = 60$, the upper branches of the structure are primarily composed of Material 2, while Material 1 is confined to cooler regions near the thermal outlets.

The optimized thermal compliance values for the three cases in Figs. 16(a)–(c) are 1.72×10^3 , 2.03×10^3 , and 2.35×10^3 , respectively. These results demonstrate that the proposed framework effectively captures the material-switching mechanism in 3D, enabling spatial allocation of materials to maximize global heat conduction performance without requiring additional heuristic operations.

3.4. Example 4: Irregular pipe domain

In the final 3D example, an irregular pipe design domain (Sun et al., 2024a), shown in Fig. 17(a), is considered to verify the engineering applicability of the proposed method. The top boundary of the pipe is prescribed as a heat sink ($\bar{T} = 0$), while the two lower branches are subjected to a uniform external volumetric thermal load Q_{ext} . To accurately capture the geometric features, this irregular domain is discretized into 264,650 voxel elements with 287,487 degrees of freedom, using the voxelization strategy developed in our previous work (Sun et al., 2025). In this example, the temperature-dependent properties of the four candidate materials are defined in Eq. (18) and are redrawn in Fig. 17(b) for clarity.

3.4.1. 3D irregular pipe designs considering two materials

The optimization is first conducted for a two-material scenario (Material 1 and Material 2, as shown in Fig. 17(b)) under a 25% volume fraction constraint. The external thermal loads are set to $Q_{\text{ext}} = 150$, 200, and 250. The optimized results for both thermal compliance minimization and peak temperature minimization are presented in Fig. 18. Consistent with the 2D cases, a clear material-switching mechanism is observed: as the thermal load Q_{ext} increases, the high-conductivity Material 2 (blue) progressively extends from the high-temperature branches toward the thermal outlet. Meanwhile, the comparison reveals that the choice of objective function significantly influences the optimized material layout.

From an engineering perspective, minimizing thermal compliance focuses on reducing the global average thermal resistance. As a result, the optimizer tends to generate evenly distributed structures with relatively uniform branches, facilitating global heat dissipation, as shown in Figs. 18(a)–(c). Conversely, minimizing the peak temperature aims to suppress local hot spots. To achieve this, the optimizer concentrates high-conductivity materials in the hottest regions of the branches, as shown in Figs. 18(d)–(f), thereby creating efficient pathways to rapidly dissipate localized heat, even at the expense of reduced temperature uniformity in other regions.

3.4.2. 3D irregular pipe designs considering four materials

To further evaluate the effectiveness of the proposed method in complex design scenarios, the problem is extended to a four-material case (defined in Fig. 17(b)) under a high external thermal load of $Q_{\text{ext}} = 350$. The objective function is set to peak temperature minimization, and the maximum allowable volume fraction f_{vol} is progressively reduced from 20% to 15% and 10%. The optimized results, showing distinct material distributions and topological configurations, are presented in Figs. 19(a)–(c). The corresponding p_{norm} -based aggregation peak temperatures c_2 are 144.13, 177.02, and 210.11, respectively.

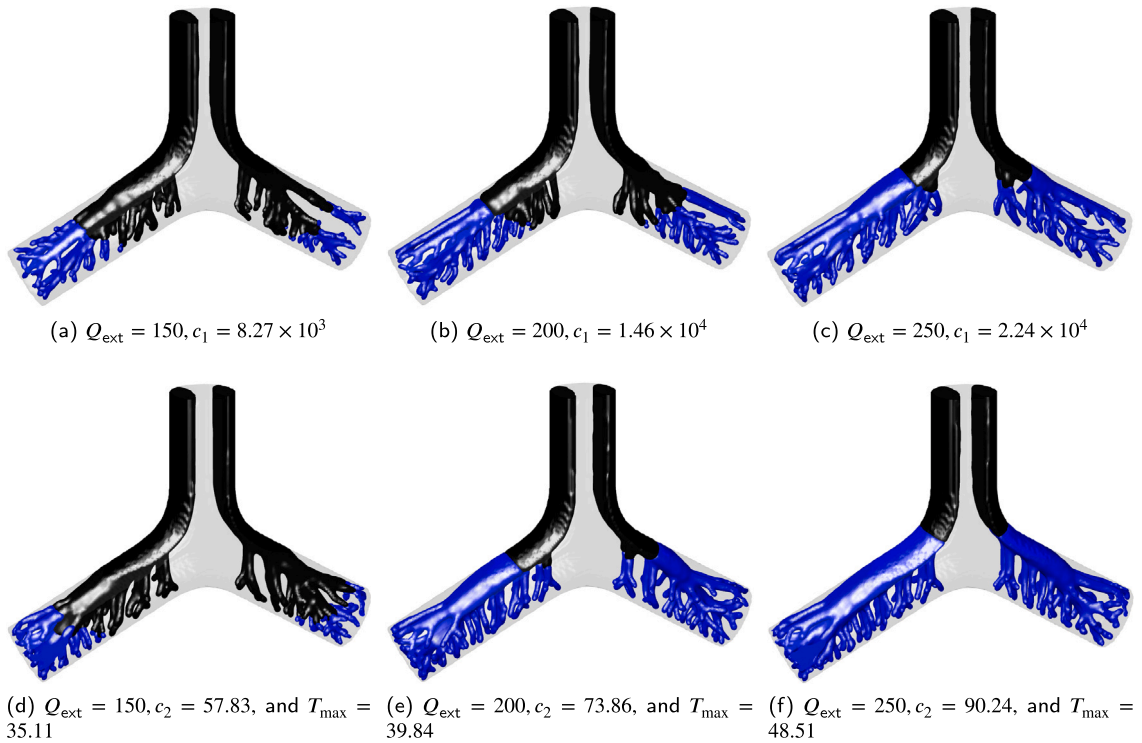


Fig. 18. Optimized 3D irregular pipe heat conduction structure for Example 4: Under different objective functions and volumetric thermal loads based on the two-material assumption. ((a–c) thermal compliance minimization; (d–f) peak temperature minimization.)

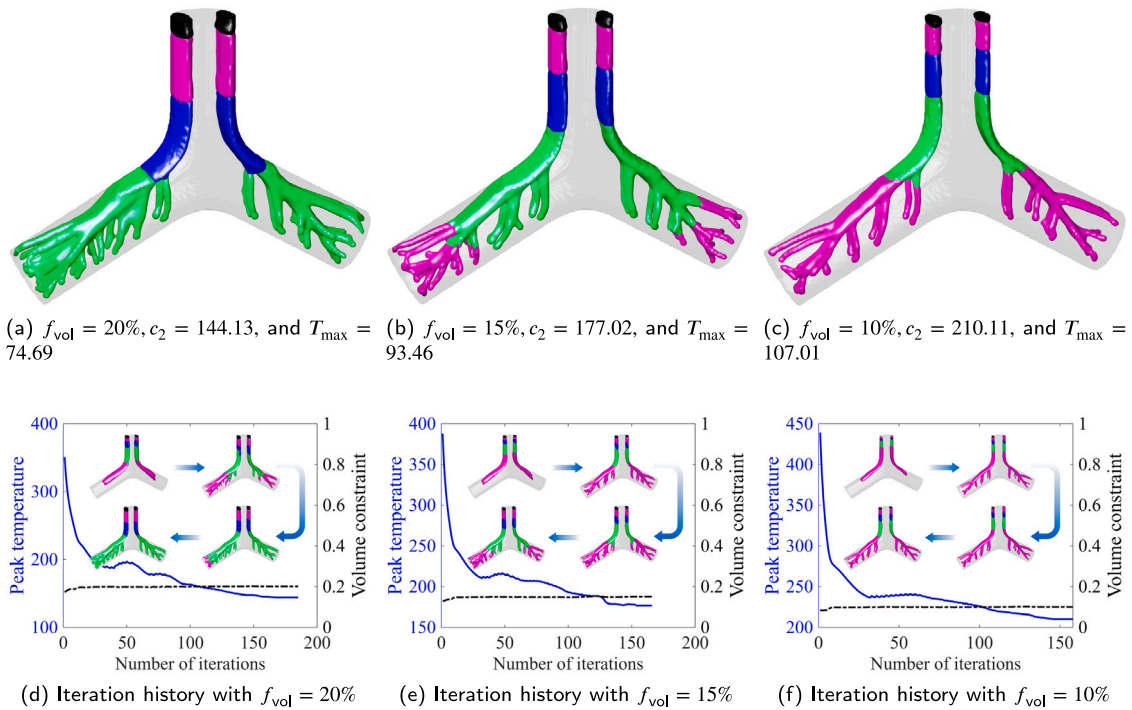


Fig. 19. Optimized 3D irregular pipe heat conduction structure for Example 4: Under peak temperature minimization and volumetric thermal load $Q_{\text{ext}} = 350$ based on the four-material assumption. ((a–c) material distributions under maximum volume fraction constraints f_{vol} of 20%, 15%, and 10%, respectively; (d–f) the corresponding iteration histories and the intermediate structural configurations per 30 iterations).

As the available material volume decreases, the peak temperature $T_{\max}$ increases. To compensate for the reduced material usage, the proposed method generates more complex material distributions to maintain efficient heat transfer pathways. The corresponding iteration histories and intermediate structural configurations at intervals of 30 iterations, shown in Figs. 19(d)–(f), demonstrate smooth convergence behavior. This confirms the numerical stability of the proposed method when applied to complex 3D engineering problems.

4. Conclusions

In this work, a multi-material topology optimization framework for heat conduction with temperature-dependent material properties (TDMPs) has been developed, considering two objective functions, namely, thermal compliance and peak temperature. By integrating nonlinear finite element analysis with the discrete material optimization (DMO) scheme, the proposed method enables the simultaneous optimization of multiple TDMP materials within a design domain. The effectiveness of the method is demonstrated through a series of 2D and 3D numerical examples, ranging from regular domains to complex irregular engineering structures.

The main findings of this study are summarized as follows. First, the introduction of multiple temperature-dependent materials significantly expands the design space compared to the single-material assumption. By overcoming the limitations of conventional CMP-based DMO thermal design methods, the proposed method accommodates temperature-dependent constitutive behavior within the optimization model. Hence, the proposed method captures the material-switching mechanism in nonlinear multi-material heat conduction, where materials are allocated to regions that match their thermally optimal performance based on the local temperature distribution. Second, the choice of objective function leads to distinct material distributions; minimizing thermal compliance promotes more uniform material layouts and temperature fields, whereas minimizing peak temperature concentrates material in localized high-temperature regions.

In addition, both visual and quantitative verification strategies are proposed to assess the physical correctness of the optimized results. As detailed in Section 3.2.4 and visually compared in Fig. 13, a quantitative comparison shows that the proposed method significantly outperforms the classical experience-based sequential design approach, whose thermal compliance is up to 31.5% higher in the tested case. Based on these results, the proposed framework provides an effective tool for thermal management design in environments with large temperature variations. For instance, in applications such as aerospace structures or electronic devices, the material-switching mechanism enables the selective placement of high-temperature-resistant materials only in critical hot regions, while utilizing lightweight and highly conductive materials elsewhere, thereby achieving a balance between thermal performance and cost.

Nevertheless, the current framework represents a fundamental step focused on steady-state heat conduction, and several challenges remain for practical applications. From a computational perspective, the number of design variables in the DMO scheme scales linearly with the number of candidate materials, which may lead to memory and non-convexity issues for large material sets. In addition, the physical realization of optimized multi-material structures via additive manufacturing requires the incorporation of manufacturing constraints, such as minimum and maximum length scales, overhang constraints, and casting limitations. Future developments should also consider multi-physics compatibility issues, including mismatches in thermal expansion and interfacial bonding strength.

Furthermore, real-world thermal systems often involve transient conditions. Extending the present framework to transient heat conduction, where both thermal conductivity and heat capacity are temperature-dependent, is an important direction for future work. In such cases, computational cost will increase significantly due to nonlinear evaluations over multiple time steps. At the same time, the interaction between temperature-dependent properties may further intensify the material-switching mechanism, necessitating new quantitative criteria for evaluating the physical correctness of the optimized result. Incorporating design-dependent Robin boundary conditions is another promising direction, as it enables the automatic generation of fin-like structures that enhance heat dissipation through increased surface area.

CRedit authorship contribution statement

Zhaoyou Sun: Writing – original draft, Visualization, Software, Methodology, Funding acquisition. **Jike Han:** Writing – review & editing, Resources, Project administration, Conceptualization. **Shinji Nishiwaki:** Writing – review & editing, Supervision. **Yangjun Luo:** Writing – review & editing, Project administration, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Sensitivity analysis

A.1. Sensitivity analysis of the objective function and volume constraints

To employ the Method of Moving Asymptotes (MMA), the optimization problem defined in Eq. (15) requires the sensitivities of both the objective function and the volume constraint with respect to the design variables $x_{e,i}$ ($i = 1, 2, \dots, m$). The detailed derivation based on the adjoint method is presented below.

According to the chain rule, the sensitivity of the objective function c with respect to the design variable $x_{e,i}$ (corresponding to element e and material i) can be expressed as follows:

$$\begin{cases} \frac{dc}{dx_{e,i}} = \sum_{j \in \mathbb{N}_e} \left(\sum_{k=1}^m \frac{dc}{dw_{j,k}} \frac{\partial w_{j,k}}{\partial \hat{x}_{j,i}} \right) \frac{\partial \hat{x}_{j,i}}{\partial \tilde{x}_{j,i}} \frac{\partial \tilde{x}_{j,i}}{\partial x_{e,i}}, \\ \frac{dV}{dx_{e,i}} = \sum_{j \in \mathbb{N}_e} v_j \frac{d\hat{x}_{j,i}}{d\tilde{x}_{j,i}} \frac{\partial \tilde{x}_{j,i}}{\partial x_{e,i}} \end{cases}, \quad (\text{A.1})$$

where $\mathbb{N}_e$ denotes the set of neighboring elements j whose center-to-center distance $\Delta(e, j)$ from element e is smaller than the filter radius $r_{\min}$. The derivative of the physical density $\hat{x}_{j,i}$ with respect to the design variable $x_{e,i}$ is obtained through the application of the filtering and projection operations, expressed as follows:

$$\frac{\partial \hat{x}_{j,i}}{\partial x_{e,i}} = \frac{d\hat{x}_{j,i}}{d\tilde{x}_{j,i}} \frac{\partial \tilde{x}_{j,i}}{\partial x_{e,i}} = \frac{\beta \text{sech}^2(\beta(\tilde{x}_{j,i} - \eta))}{\tanh(\beta\eta) + \tanh(\beta(1 - \eta))} \frac{H_{je} v_e}{\sum_{k \in \mathbb{N}_j} H_{jk} v_k}. \quad (\text{A.2})$$

The total volume is defined as $V = \sum_{e=1}^{n_e} \sum_{i=1}^m v_e \hat{x}_{e,i}$. Since it is independent of the temperature field, its sensitivity with respect to the design variables can be directly obtained. Comparing the sensitivities of the objective function and the volume constraint, the main difference arises from the interpolation scheme and the governing state equation. The term $\frac{\partial \hat{x}_{j,i}}{\partial x_{e,i}} w_{j,k}$ captures the multi-material coupling effect in the DMO scheme and can be analytically derived as follows:

$$\frac{\partial w_{j,k}}{\partial \hat{x}_{j,i}} = \begin{cases} (1 - \epsilon) p(\hat{x}_{j,i})^{p-1} \prod_{r=1, r \neq i}^m (1 - \gamma_r(\hat{x}_{j,r})^p), & \text{if } k = i \\ -(1 - \epsilon) \gamma_i p(\hat{x}_{j,i})^{p-1} (\hat{x}_{j,k})^p \prod_{r=1, r \neq i, k}^m (1 - \gamma_r(\hat{x}_{j,r})^p), & \text{if } k \neq i. \end{cases} \quad (\text{A.3})$$

Thus, the remaining task is to derive the term $\frac{dc}{dw_{e,i}}$. The objective function $c = f(T(\mathbf{x}), \mathbf{x})$ depends on the design variables both explicitly, through the material weights, and implicitly, through the temperature field. Considering the steady-state nonlinear governing equation $\mathbf{R}(\mathbf{x}, T) = \mathbf{K}(\mathbf{w}(\mathbf{x}), T) \mathbf{T} - \mathbf{Q}_{\text{ext}} = \mathbf{0}$, the augmented Lagrangian (AL) functional is defined as follows:

$$\hat{c} \equiv c = f(T(\mathbf{x}), \mathbf{x}) + \lambda^T [\mathbf{K}(\mathbf{w}(\mathbf{x}), T) \mathbf{T} - \mathbf{Q}_{\text{ext}}], \quad (\text{A.4})$$

where λ is the arbitrary adjoint vector. Since the external thermal load $\mathbf{Q}_{\text{ext}}$ is design-independent, differentiating $\hat{c}$ with respect to $w_{e,i}$ yields

$$\begin{aligned} \frac{\partial \hat{c}}{\partial w_{e,i}} &= \frac{\partial f}{\partial T} \frac{\partial T}{\partial w_{e,i}} + \frac{\partial f}{\partial w_{e,i}} + \lambda^T \left[\frac{\partial \mathbf{K}}{\partial w_{e,i}} \mathbf{T} + \frac{\partial (\mathbf{K} \mathbf{T})}{\partial T} \frac{\partial T}{\partial w_{e,i}} \right] \\ &= \left(\frac{\partial f}{\partial T} + \lambda^T \mathbf{J} \right) \frac{\partial T}{\partial w_{e,i}} + \frac{\partial f}{\partial w_{e,i}} + \lambda^T \frac{\partial \mathbf{K}}{\partial w_{e,i}} \mathbf{T}, \end{aligned} \quad (\text{A.5})$$

where $\mathbf{J}$ denotes the tangent conductivity matrix of the nonlinear system defined in Eq. (14). Since the FE equilibrium equation is satisfied at each optimization iteration by the Newton-Raphson procedure ($\mathbf{R}(\mathbf{x}, T) = \mathbf{0}$), the implicit derivative $\frac{\partial w_{e,i}}{\partial w_{e,i}} \mathbf{T}$ can be eliminated by introducing the following adjoint equation:

$$\mathbf{J}^T \lambda = - \left(\frac{\partial f}{\partial T} \right)^T. \quad (\text{A.6})$$

Hence, the final sensitivity $\frac{\partial c}{\partial w_{e,i}}$ is given by

$$\frac{\partial c}{\partial w_{e,i}} \equiv \frac{\partial \hat{c}}{\partial w_{e,i}} = \frac{\partial f}{\partial w_{e,i}} + \lambda^T \frac{\partial \mathbf{K}}{\partial w_{e,i}} \mathbf{T}, \quad (\text{A.7})$$

where the remaining term can be determined from the definition of the objective function. Recalling that the effective global temperature-dependent thermal conductivity matrix is defined as $\mathbf{K}(\mathbf{w}, T) = \bigcup_{e=1}^{n_e} \mathbf{K}_e(\mathbf{w}_e, T_e)$, its sensitivity with respect to the weight $w_{e,i}$ is given by

$$\frac{\partial \mathbf{K}}{\partial w_{e,i}} = \frac{\partial \mathbf{K}_e}{\partial w_{e,i}} = k_i(T_e) \int_{\Omega_e} \mathbf{B}^T \mathbf{B} dV. \quad (\text{A.8})$$

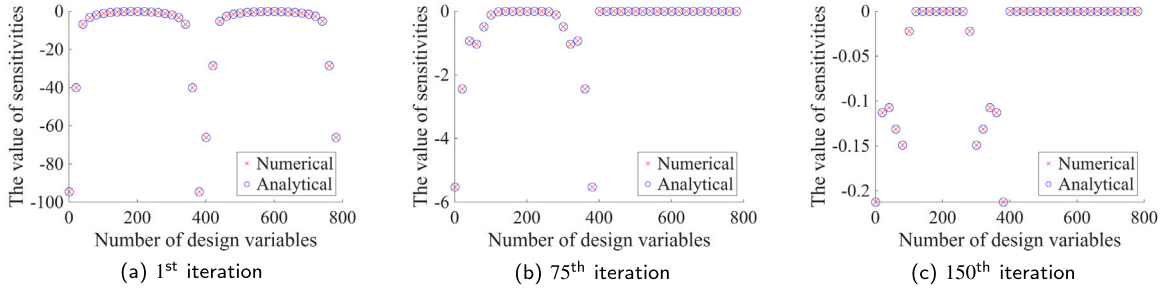


Fig. 20. Verification results for the derived design sensitivity.

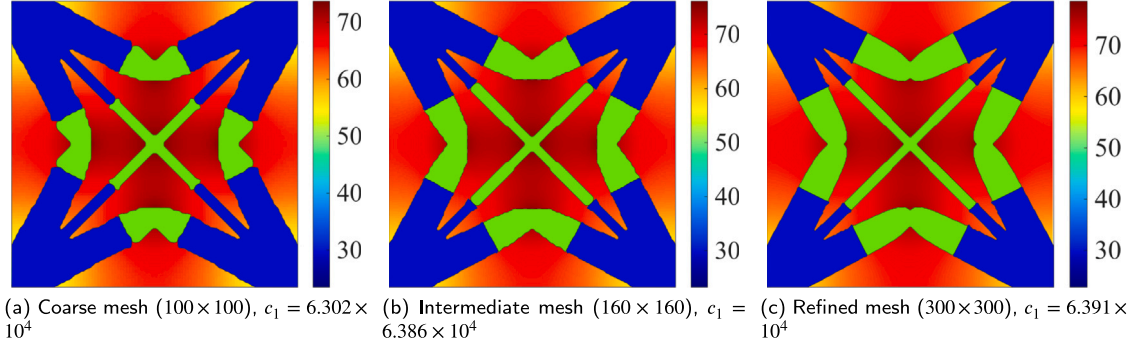


Fig. 21. Mesh convergence study under three mesh resolutions for $Q_{\text{ext}} = 180$.

For the two objective functions defined in Eq. (16), the sensitivity $\partial_{w_{e,i}} f$ vanishes, and the derivative of c_1 with respect to the temperature field is given by $\partial_T c_1 = \mathbf{Q}_{\text{ext}}^T$. For the p_{norm} -based aggregation peak temperature objective function $c_2 = (\sum_{J=1}^{n_{\text{dof}}} T_J^{p_{\text{norm}}})^{1/p_{\text{norm}}}$, the derivative with respect to the nodal temperature T_J is expressed as

$$\frac{\partial c_2}{\partial T_J} = \frac{1}{p_{\text{norm}}} \left(\sum_{J=1}^{n_{\text{dof}}} T_J^{p_{\text{norm}}} \right)^{1/p_{\text{norm}}-1} p_{\text{norm}} T_J^{p_{\text{norm}}-1} = \left(\frac{T_J}{c_2} \right)^{p_{\text{norm}}-1}. \quad (\text{A.9})$$

A.2. Verification of sensitivity analysis for the objective function

To verify the correctness of the derived analytical sensitivities and their numerical implementation, a numerical verification is conducted using the finite difference method. Without loss of generality, the two-material design scenario described in Section 3.1.2 is considered with a 20×20 mesh, while all other parameters are kept consistent. The finite difference approximation is used as a numerical reference to evaluate the analytical sensitivities, formulated as

$$\frac{\partial c}{\partial x_{e,i}} \approx \frac{\Delta c}{\Delta x} = \frac{c(x_{e,i} + \Delta x) - c(x_{e,i})}{\Delta x}, \quad (\text{A.10})$$

where $\Delta x = 10^{-6}$ is used to perturb the design variable, thereby obtaining the corresponding variation in the objective function. To ensure a comprehensive verification, the comparison is performed at three representative stages of the optimization process: the initial stage (1st iteration), an intermediate stage (75th iteration), and a near-converged stage (150th iteration). To facilitate clear visualization and avoid overlap, the results are plotted for every 20th design variable.

The comparison results are shown in Fig. 20. It can be observed that the analytical sensitivities (marked in circles) are in high agreement with the numerical sensitivities (marked in dots) across all stages. Notably, at the 150th iteration, the sensitivity values approach zero, indicating that the optimization process has converged to a local optimum.

Appendix B. Mesh convergence analysis

In the present nonlinear finite element formulation, the temperature-dependent thermal conductivity $k(T_e)$ is evaluated based on the element-averaged temperature T_e following previous works (Tang et al., 2019; Ha et al., 2004), which improves computational efficiency. From a numerical integration perspective, this treatment represents a zero-order approximation of the spatially varying conductivity field within each element. Since the design variables are defined as element-wise constants in the employed density-based TO framework, the adoption of T_e ensures consistency between the spatial discretization of the material interpolation and that of the conductivity evaluation at the element level.

Table B.1

Comparison of the thermal compliances evaluated using the element-averaged temperature (T_e) and the four-point Gauss quadrature scheme.

Mesh resolution	Thermal compliance ($\times 10^4$)		Relative difference
	Average temperature (T_e)	Gauss point quadrature	
100 $\times$ 100	6.302	6.359	0.91%
160 $\times$ 160	6.386	6.439	0.83%
200 $\times$ 200 (Baseline)	6.390	6.441	0.80%
300 $\times$ 300	6.391	6.440	0.77%

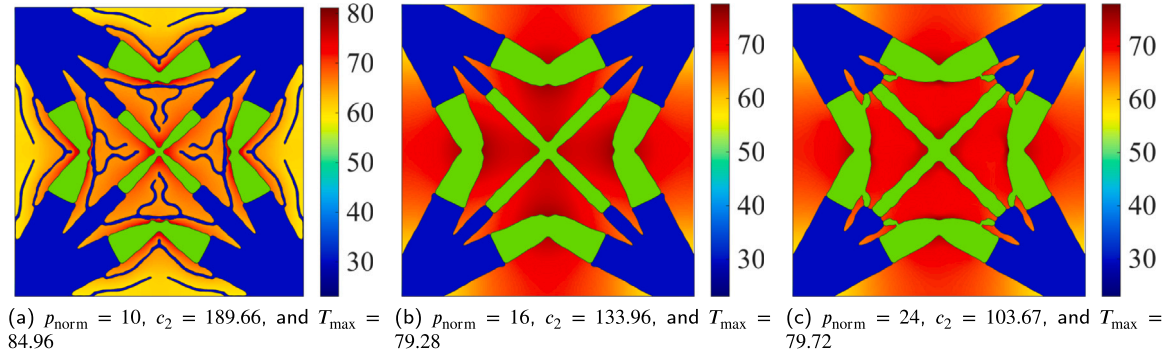


Fig. 22. Influence of the p_{norm} parameter on the optimization result aimed at peak temperature minimization.

To assess the discretization quality under the conditions of high thermal gradient and material nonlinearity, the three-material design configuration from Example 1 (Section 3.1.2) is evaluated under the maximum external thermal load ($Q_{\text{ext}} = 180$). Three mesh resolutions are considered: a coarse mesh (100 $\times$ 100), an intermediate mesh (160 $\times$ 160), and a refined mesh (300 $\times$ 300). The structural configurations and the corresponding thermal compliances are presented in Fig. 21.

The results in Fig. 21 indicate that the values of the objective function gradually converge as the element size decreases. The relative deviation in thermal compliance between the baseline (200 $\times$ 200 in Fig. 5(b)) and the refined (300 $\times$ 300) meshes is less than 0.5% (i.e., $c_1 = 6.390 \times 10^4$ and $c_1 = 6.391 \times 10^4$), while the optimized topological configurations remain almost the same. Hence, the discretization error associated with the element-averaged temperature evaluation is negligible at the adopted mesh resolution.

To quantify the numerical discrepancy induced by the element-averaged temperature formulation, a comparative analysis is performed for these optimized results using a four-point Gauss quadrature integration. In the adopted element-averaged formulation, the thermal conductivity is evaluated as a constant based on the centroidal temperature T_e , yielding the element conductivity matrix $\mathbf{K}_e = k(T_e) \int_{\Omega_e} \mathbf{B}^T \mathbf{B} dV$. In comparison, an evaluation accounting for the intra-element spatial variation of the temperature field $T(\mathbf{r})$ is expressed as $\mathbf{K}'_e = \int_{\Omega_e} k(T(\mathbf{r})) \mathbf{B}^T \mathbf{B} dV$, where $\mathbf{r}$ denotes the spatial coordinate vector of integration points. The thermal compliances calculated via these two methods are compared in Table B.1, showing a consistent relative deviation of less than 1% across all mesh resolutions. This deviation confirms that, within the context of element-wise constant density variables, the element-averaged approximation can capture the thermal compliance without introducing significant integration errors.

Appendix C. Selection of the p_{norm} parameter in the aggregation function

In TO problems involving min-max objective functions, such as peak-temperature minimization, the p_{norm} -based aggregation function is commonly employed as a smooth and differentiable approximation of the non-differentiable maximum operator. The effectiveness of this formulation relies on the monotonic correlation between the aggregation function $c_2 = (\sum_{j=1}^{n_{\text{dof}}} T_j^{p_{\text{norm}}})^{1/p_{\text{norm}}}$ and the true peak temperature T_{max} . From the definition of c_2 , it follows that $\lim_{p_{\text{norm}} \rightarrow \infty} c_2 = T_{\text{max}}$, indicating that increasing p_{norm} improves the approximation accuracy by reducing the gap ($c_2 - T_{\text{max}}$). However, this simultaneously strengthens the numerical non-convexity of the optimization problem. In particular, for problems involving localized heat sources, the choice of p_{norm} can significantly influence the optimized topological configurations. A relatively small value of p_{norm} tends to overestimate the spatial extent of the hotspot, distributing sensitivity contributions over a broad region and potentially inducing excessive or artificial structural branching. In contrast, a large value of p_{norm} causes severe gradient localization, where sensitivities become concentrated almost exclusively around the maximum-temperature region. This increases the likelihood of oscillatory convergence behavior and premature trapping in poor local minima. Therefore, the parameter p_{norm} must be carefully selected to balance approximation accuracy and optimization stability.

To confirm the effectiveness of the selected parameter $p_{\text{norm}} = 16$, the peak temperature minimization case from Section 3.1.3 is re-optimized using two additional aggregation parameters, namely, $p_{\text{norm}} = 10$, and 24. The optimized results are summarized in Fig. 22, reporting their corresponding objective function c_2 and true peak temperature T_{max} . As visually and quantitatively indicated in

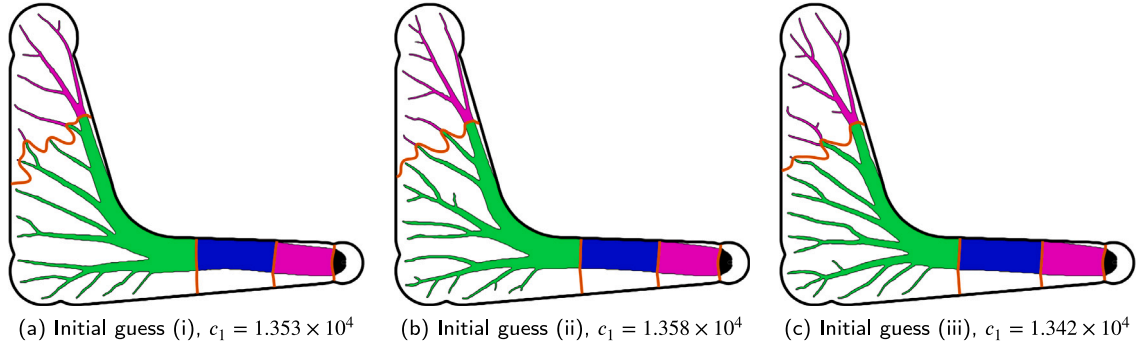


Fig. 23. Influence of the initial material distribution on the optimized topological configurations.

Fig. 22, the choice of p_{norm} influences the optimized results and thermal performance. For a relatively small parameter ($p_{\text{norm}} = 10$), the substantial approximation gap ($c_2 = 189.66$ and $T_{\text{max}} = 84.96$) drives the optimizer to cool down a broad region, generating several artificial branches that yield a higher true peak temperature. When a large parameter is adopted ($p_{\text{norm}} = 24$), the approximation gap is minimized ($c_2 = 103.67$ and $T_{\text{max}} = 79.72$). Nevertheless, the resulting gradient localization traps the optimizer in a sub-optimal local minimum, characterized by the configuration oscillations near the center. Thus, its true peak temperature ($T_{\text{max}} = 79.72$) is inferior to the baseline design with parameter $p_{\text{norm}} = 16$ ($T_{\text{max}} = 79.28$). Therefore, the parameter $p_{\text{norm}} = 16$ represents a numerical compromise, which can suppress the localized hotspot while precluding the emergence of aggregation artifacts.

Meanwhile, it is acknowledged that the parameter selection is problem-dependent. For instance, design domains subjected to distributed thermal loads exhibit reduced sensitivity to variations in p_{norm} . Furthermore, numerical strategies, such as condensation techniques (Le et al., 2010) or active-set methods for the degrees of freedom corresponding to the external thermal load (Luo et al., 2013), could be employed to reduce the number of aggregated degrees of freedom and enhance the convexity of the design space. However, the exploration of such strategies falls outside the scope of the present study. To maintain methodological consistency across all numerical examples, a uniform parameter of $p_{\text{norm}} = 16$ is adopted.

Appendix D. Dependency of the initial guess

The multi-material TO problem involving TDMPs is characterized by pronounced non-convexity, which arises from the nonlinear coupling in the state equations and the multi-material interpolation scheme. In this work, the initial guess for all numerical examples is a uniform distribution where each element is assigned an equal volume fraction of all candidate materials ($x_{e,i}^{(0)} = f_{\text{vol}}/m$). Here, the influence of the initial material distribution is evaluated using the suspension triangle domain and four-material assumption described in Section 3.2.2, and the objective function is thermal compliance minimization.

To evaluate the dependency of the initial guess, a generalized formulation for the initial material distribution is defined as

$$x_{e,i}^{(0)} = w_i f_{\text{vol}}, \quad \text{subject to} \quad \sum_{i=1}^m w_i = 1, \quad i = 1, 2, \dots, m, \quad (\text{D.1})$$

where $x_{e,i}^{(0)}$ denotes the initial design variable of the i th candidate material in element e , w_i is the prescribed weight factor, f_{vol} is the maximum global volume fraction, and $m = 4$ is the total number of candidate materials in this specific case. The external thermal load is maintained at $Q_{\text{ext}} = 160$ across all cases to ensure consistent boundary conditions for the comparative evaluation.

Based on this formulation, three initial guesses are considered to examine the initial dependence of the proposed method, namely,

- (i) a biased distribution favoring Material-1 ($w_1 = 1/2$, and $w_j = 1/6$ for $j \neq 1$);
- (ii) a biased distribution favoring Material-2 ($w_2 = 1/2$, and $w_j = 1/6$ for $j \neq 2$);
- (iii) a biased distribution favoring Material-3 ($w_3 = 1/2$, and $w_j = 1/6$ for $j \neq 3$).

The optimized configurations of the above three initial guesses, superimposed with theoretical transition isotherms, are presented in Fig. 23, yielding thermal compliances of $c_1 = 1.353 \times 10^4$, 1.358×10^4 , and 1.342×10^4 , respectively. Numerical observations indicate that variations in the initial guess introduce variations in the final topological layouts. Although the heat-conduction pathways remain consistent across the configurations, the local branching and material interfaces exhibit discernible differences, confirming the existence of multiple stationary points in the design space. Quantitatively, the relative variation in the converged thermal compliance among the three cases is recorded at approximately 1.19%. This demonstrates that while the optimization process exhibits a certain degree of sensitivity to the initial guess, the proposed framework consistently identifies qualitatively similar high-performance structural layouts facilitated by the parameter continuation scheme (γ in Eq. (10), and β in Eq. (11)).

Data availability

Data will be made available on request.

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