

Supplementary Information: Free-form thermal cloaks in three dimensions

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1 Definition of 3D domains used in this study

The 3D domains of thermal cloaks are defined by two closed surfaces, which are mathematically defined through the distance functions $R_1(\theta, \psi)$ and $R_2(\theta, \psi)$ where $\theta \in [0, \pi]$ is the polar angle and $\psi \in [0, 2\pi)$ is the azimuthal angle. In the following, we show the specific forms and parameter values of R_i used in this study.

1.1 Surfaces of revolution

For the shapes defined by surfaces of revolution, we use the form of $R_j(\bar{\theta})$ ($j = 1, 2$) below.

$$R_j(\bar{\theta}) = R_{0,j} + \sum_{m=1}^M A_{jm} \cos(T_{jm}\bar{\theta}) \quad (1)$$

where $R_{0,j} > 0$ and A_{jm} are user-defined coefficients, and T_{jm} are non-negative integers to ensure $\cos(T_{jm}\pi) = 0$. Below are the parameter values for the cloaks presented in the main text.

For the pear-apple cloak, the apple shape R_1 uses $R_{0,1} = 15$, $A_{11} = -9$, $A_{12} = -3$, $T_{11} = 1$; $T_{12} = 2$, and the pear shape R_2 uses $R_{0,2} = 33$, $A_{21} = -5$, $A_{22} = 5$, $T_{21} = 1$; $T_{22} = 2$.

For Dsg.1 cloak, the inner surface R_1 uses $R_{0,1} = 17$, $A_{11} = 3$, $A_{12} = 3$, $T_{11} = 1$; $T_{12} = 5$, and the outer surface R_2 uses $R_{0,2} = 32$, $A_{21} = 7$, $T_{21} = 4$.

For Dsg.2 cloak, the inner surface R_1 uses $R_{0,1} = 20$, $A_{11} = 3$, $T_{12} = 6$, and the outer surface R_2 uses $R_{0,2} = 36$, $A_{21} = 5$, $T_{21} = 2$.

For Dsg.3 cloak, the inner shape R_1 uses $R_{0,1} = 18$, $A_{11} = A_{12} = -3$, $T_{11} = 1$; $T_{12} = 2$, and the outer shape $R_2 = 1.5R_1$.

1.2 General analytical surfaces

For analytical general surfaces defined as $R_j(\bar{\theta}, \bar{\psi})$, we use the following form:

$$R_j(\bar{\theta}, \bar{\psi}) = R_{0,j} + \left[\sum_{m=1}^M A_{jm} \cos(T_{jm}\bar{\theta}) - \sum_{m=1}^M A_{jm} \right] \cdot \left[\sum_{n=1}^N B_{jn} \cos(S_{jn}\bar{\psi}) \right] \quad (2)$$

where $R_{0,j} > 0$, A_{jm} , and B_{jn} are user-defined coefficients, T_{jm} and S_{jn} are non-negative integers. The parameter values for the shapes presented in Figure 3 of the main text are as follows.

For Dsg. 4, the inner shape R_1 uses $R_{0,1} = 18$, $A_{11} = 1$, $T_{11} = 2$, $B_{11} = 5$, $S_{11} = 2$, and the outer shape $R_2 = 1.4R_1$.

For Dsg. 5, the inner shape R_1 uses $R_{0,1} = 24$, $A_{11} = 1$, $T_{11} = 0$, $B_{11} = 2$, $S_{11} = 2$, and the outer shape R_2 uses $R_{0,2} = 36$, $A_{21} = 1$, $T_{21} = 2$, $B_{21} = 4$, $S_{21} = 4$.

1.3 General complex surfaces defined by spherical harmonics

To generate more complex surfaces of any given object, we adopt spherical harmonics to represent and fit more complex surfaces of any given object (such as the characters' faces). Here, we lay out the process of performing the surface fitting provided the STL file of a closed surface. Spherical harmonics are a generalization of the two-dimensional Fourier transform to the surface of a sphere. They are particularly well-suited for handling the boundary conditions associated with spherical domains, specifically the periodicity in the azimuthal angle $\phi \in [0, 2\pi]$ and the singularities that arise as the polar angle θ approaches 0 or π .

Any real-valued scalar function (in our case, the distant function of the surface) $R : \mathbb{S}^2 \rightarrow \mathbb{R}$ defined on the surface of a sphere can be represented as a linear combination of spherical harmonic base functions, i.e.,

$$R(\theta, \psi) = \sum_{\ell=0}^{\infty} \sum_{m=0}^{\ell} c_{\ell}^m Y_{\ell}^m(\theta, \psi), \quad (3)$$

where ℓ and m are integers with $\ell \geq 0$ and $0 \leq m \leq \ell$, c_{ℓ}^m are the expansion coefficients corresponding to each spherical harmonic basis function indexed by degree ℓ and order m , and $Y_{\ell}^m(\theta, \psi)$ are the angular basis function (also known as spherical harmonics), which can be expressed in terms of the associated Legendre functions $P_{\ell}^m(x)$ as:

$$Y_{\ell}^m(\theta, \psi) = \sqrt{\frac{2\ell+1}{4\pi} \cdot \frac{(\ell-m)!}{(\ell+m)!}} P_{\ell}^m(\cos \theta) e^{im\psi} \quad (4)$$

The associated Legendre function $P_{\ell}^m(x)$ is defined by

$$P_{\ell}^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_{\ell}(x), \quad (5)$$

where $P_{\ell}(x)$ is the Legendre polynomial of degree ℓ , given explicitly by:

$$P_{\ell}(x) = 2^{-\ell} \sum_{r=0}^{\lfloor \ell/2 \rfloor} (-1)^r \frac{(2\ell-2r)!}{r!(\ell-r)!(\ell-2r)!} x^{\ell-2r}. \quad (6)$$

To simplify the computation, we alternatively utilize the real and imaginary components of the complex spherical harmonics $Y_{\ell}^m(\theta, \psi)$, known as "Tesseral Harmonics", to serve as real-valued basis functions. These are defined as:

$$U_{\ell}^m(\theta, \psi) \triangleq \Re\{Y_{\ell}^m(\theta, \psi)\}, \quad (7)$$

$$V_{\ell}^m(\theta, \psi) \triangleq \Im\{Y_{\ell}^m(\theta, \psi)\}, \quad (8)$$

Based on the above setup, the reconstructed shape's distant function can be expressed using these real-valued harmonics as:

$$R(\theta, \psi) = \sum_{\ell=0}^K \sum_{m=0}^{\ell} A_{\ell}^m U_{\ell}^m(\theta, \psi) + B_{\ell}^m V_{\ell}^m(\theta, \psi), \quad (9)$$

where K denotes the highest degree of expansion, and A_{ℓ}^m and B_{ℓ}^m are the corresponding real-valued coefficients.

To determine these coefficients, we construct a system of linear equations by evaluating the radial distance function at N sampling positions across the target surface. Let

$$\mathbf{r} = (r(\theta_1, \psi_1), \dots, r(\theta_i, \psi_i), \dots, r(\theta_N, \psi_N))^T, \quad (10)$$

represent the vector of sampled radial distances, where i denotes the i -th sampling point, and N is the total number of samples. The basis functions evaluated at these sample points form the coefficient matrix $\mathbf{X}$, defined as:

$$\mathbf{X} = (\mathbf{U}, \mathbf{V}), \quad (11)$$

where $\mathbf{U}$ is the matrix of real spherical harmonics evaluated at all sampling points:

$$\mathbf{U} = \begin{pmatrix} U_0^0(\theta_1, \psi_1) & U_1^0(\theta_1, \psi_1) & U_1^1(\theta_1, \psi_1) & \cdots & U_K^K(\theta_1, \psi_1) \\ U_0^0(\theta_2, \psi_2) & U_1^0(\theta_2, \psi_2) & U_1^1(\theta_2, \psi_2) & \cdots & U_K^K(\theta_2, \psi_2) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ U_0^0(\theta_N, \psi_N) & U_1^0(\theta_N, \psi_N) & U_1^1(\theta_N, \psi_N) & \cdots & U_K^K(\theta_N, \psi_N) \end{pmatrix}, \quad (12)$$

and $\mathbf{V}$ is constructed similarly using V_ℓ^m . The unknown coefficients are collected into a vector $\mathbf{c}$ as follows.

$$\mathbf{c} = (\mathbf{a}, \mathbf{b})^T, \quad (13)$$

where $\mathbf{a}$ is the vector of coefficients A_ℓ^m , arranged by harmonic order:

$$\mathbf{a} = (A_0^0, A_1^0, A_1^1, A_2^0, A_2^1, A_2^2, \dots, A_K^K)^T, \quad (14)$$

and $\mathbf{b}$ is formed similarly from B_ℓ^m .

Thus, the overall system of equations is compactly written as:

$$\mathbf{r} = \mathbf{X}\mathbf{c}, \quad (15)$$

which can then be solved using standard linear least squares methods to obtain the optimal coefficients A_ℓ^m and B_ℓ^m for reconstructing the target surface. It is important to note, however, that in our case, the number of equations—corresponding to the number of sampling locations—typically exceeds the number of unknown coefficients, leading to an over-determined system. To solve it, we employ Singular Value Decomposition (SVD), which provides a stable solution that minimizes the residual error in the least-square sense. The resulting coefficients represent the best approximation of the true surface within the constraints of the chosen harmonic basis and the available sampling data.

After solving for the coefficients of the full system, the radial function of the target surface, $R(\theta, \psi)$, can be explicitly expressed as a linear combination of trigonometric functions in terms of the angular variables θ and ψ , as shown in Equation 9. This analytical representation ensures that the reconstructed target surface is fully compatible with the required functional form for designing cloaking structures based on the principles of transformation thermotics.

2 Transformation thermotics for 3D cloak

This section introduces the basic process of transformation thermotics for 3D cloaks. This is carried out using spherical coordinate, with the physical space coordinate r, θ, ψ such that $r > 0$ is the radius, $\theta \in [0, \pi]$ is the polar angle, and $\psi \in [0, 2\pi)$ is the azimuthal angle. Correspondingly, we denote $\bar{r}, \bar{\theta}, \bar{\psi}$ as the virtual spherical coordinates. Additionally, the inner and outer boundaries of the cloak are two surfaces defined by their distance to the origin $R_1(\bar{\theta}, \bar{\psi})$ and $R_2(\bar{\theta}, \bar{\psi})$, respectively. Also, we assume a homogeneous and isotropic background with thermal conductivity denoted by κ_0 .

Based on the above setup, the coordinate transformation for 3D cloak is [1]:

$$\begin{aligned} r(\bar{r}, \bar{\theta}, \bar{\psi}) &= R_1(\bar{\theta}, \bar{\psi}) + \frac{R_2(\bar{\theta}, \bar{\psi}) - R_1(\bar{\theta}, \bar{\psi})}{R_2(\bar{\theta}, \bar{\psi})} \bar{r} =: R_1(\bar{\theta}, \bar{\psi}) + C(\bar{\theta}, \bar{\psi}) \bar{r} \\ \theta(\bar{r}, \bar{\theta}, \bar{\psi}) &= \bar{\theta} \\ \psi(\bar{r}, \bar{\theta}, \bar{\psi}) &= \bar{\psi} \end{aligned} \quad (16)$$

where the inner and outer boundaries (surfaces) in the physical coordinate are defined by $R_1(\theta, \psi)$ and $R_2(\theta, \psi)$, respectively, and we have defined $C := (R_2 - R_1)/R_1$ with $C \in (0, 1)$. For convenience, we denote $\bar{\mathbf{s}} := [\bar{r}, \bar{\theta}, \bar{\psi}]$ and $\mathbf{s} := [r, \theta, \psi]$, $\bar{\mathbf{x}} := [\bar{x}_1, \bar{x}_2, \bar{x}_3]$, and $\mathbf{x} := [x_1, x_2, x_3]$. The Jacobian linking the

physical and virtual space Cartesian coordinates are computed by chain rule $\mathbf{J} = \frac{\partial \mathbf{x}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \bar{\mathbf{s}}} \frac{\partial \bar{\mathbf{s}}}{\partial \bar{\mathbf{x}}}$. The key is to get the expression of $\frac{\partial \mathbf{s}}{\partial \bar{\mathbf{s}}}$ based on (16). The expression of $\frac{\partial \mathbf{s}}{\partial \bar{\mathbf{s}}}$ is

$$\frac{\partial \mathbf{s}}{\partial \bar{\mathbf{s}}} = \begin{bmatrix} C & \frac{\partial R_1}{\partial \bar{\theta}} + \bar{r} \frac{\partial C}{\partial \bar{\theta}} & \frac{\partial R_1}{\partial \bar{\psi}} + \bar{r} \frac{\partial C}{\partial \bar{\psi}} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (17)$$

where $\bar{r} = (r - R_1)/C$. The Cartesian-spherical coordinate relations $\frac{\partial \mathbf{x}}{\partial \mathbf{s}}$ and $\frac{\partial \bar{\mathbf{s}}}{\partial \bar{\mathbf{x}}}$ are general and independent of the specific transformation. They are given as:

$$\frac{\partial \mathbf{x}}{\partial \mathbf{s}} = \begin{bmatrix} s_\theta c_\psi & c_\theta c_\psi & -s_\theta s_\psi \\ s_\theta s_\psi & c_\theta s_\psi & s_\theta c_\psi \\ c_\theta & -s_\theta & 0 \end{bmatrix} \begin{bmatrix} 1 \\ r \\ r \end{bmatrix} \quad (18)$$

and

$$\frac{\partial \bar{\mathbf{s}}}{\partial \bar{\mathbf{x}}} = \begin{bmatrix} 1 & & \\ & \frac{1}{\bar{r}} & \\ & & \frac{1}{\bar{r}} \end{bmatrix} \begin{bmatrix} s_{\bar{\theta}} c_{\bar{\psi}} & s_{\bar{\theta}} s_{\bar{\psi}} & c_{\bar{\theta}} \\ c_{\bar{\theta}} c_{\bar{\psi}} & c_{\bar{\theta}} s_{\bar{\psi}} & -s_{\bar{\theta}} \\ -\frac{s_{\bar{\psi}}}{s_{\bar{\theta}}} & \frac{c_{\bar{\psi}}}{s_{\bar{\theta}}} & 0 \end{bmatrix} \quad (19)$$

where c and s denote cosine and sine functions, respectively. Based on the above computation, the transformed conductivity is obtained as $\boldsymbol{\kappa} = \frac{\kappa_0}{\det(\mathbf{J})} \mathbf{J} \mathbf{J}^T$ with an isotropic κ_0 .

In the special case of surface of revolution where R_1 and R_2 depend only on $\bar{\theta}$, i.e., $R_1(\bar{\theta})$ and $R_2(\bar{\theta})$, the expression of $\frac{\partial \mathbf{s}}{\partial \bar{\mathbf{s}}}$ simplifies to:

$$\frac{\partial \mathbf{s}}{\partial \bar{\mathbf{s}}} = \begin{bmatrix} C & R'_1 + \bar{r} C' & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (20)$$

where the prime denotes the derivative w.r.t. $\bar{\theta}$ (or equivalently θ).

By construction, the $\boldsymbol{\kappa}$ is symmetric positive semi-definite, and hence it has three real, positive eigenvalues and an orthonormal eigenbasis. As shown in the following section, the eigenvalues and eigenvectors of $\boldsymbol{\kappa}$ have special properties that can be exploited for the subsequent de-homogenization.

3 Special spectral properties of $\boldsymbol{\kappa}$

The transformed thermal conductivity obtained as $\boldsymbol{\kappa} = \frac{\kappa_0}{\det(\mathbf{J})} \mathbf{J} \mathbf{J}^T$ has special properties in its eigenvalues (and eigenvectors for the case of surface of revolution). Here, we reveal and analyze these properties, some of which have significant implications for the generation of microstructures at later stages.

3.1 General surfaces $R_1(\bar{\theta}, \bar{\psi})$ and $R_2(\bar{\theta}, \bar{\psi})$

The $\boldsymbol{\kappa}$ of general-shape 3D cloaks has two important properties. Denoting κ_1 , κ_2 , and κ_3 the three eigenvalues of $\boldsymbol{\kappa}$ in ascending-magnitude order, we have:

Property 1: $\kappa_2 = \frac{\kappa_0}{C}$.

Property 2: $\kappa_1 \leq C \kappa_0 \leq \kappa_2 \leq \kappa_3$.

Property 1 says the second eigenvalue κ_2 in terms of magnitude is equal to $\frac{\kappa_0}{C}$, and hence its spatial variation depends solely on θ and ψ (and not on r) through the geometric parameter $C(\theta, \psi)$. In the special case that the outer and inner surfaces have the same shape (but different sizes), C becomes a constant and leads to a constant eigenvalue κ_2 .

Property 1 can be shown by verifying $\det(\boldsymbol{\kappa} - \frac{\kappa_0}{C} \mathbf{I}) = 0$ identically, where $\boldsymbol{\kappa}$'s expression comes from the transformation thermotics formula, and $\mathbf{I}$ is the identity matrix. The verification is carried out using Matlab symbolic computation, and the result is an identical zero with no dependence on the entries of the involved matrices. We note that the property holds for any $\frac{\partial \mathbf{s}}{\partial \bar{\mathbf{s}}}$ featuring the pattern

in (17), i.e., the entries in the first line can have any values, and the second line and third line have only one unit entry in the second and third columns, respectively. This corresponds to a coordinate transformation where the angular coordinates' relations between the reference and physical frames are identity, which is the case for the cloak.

Property 2 says $\kappa_2 = \frac{\kappa_0}{C}$ is always the second in magnitude among the three eigenvalues, and the smallest κ_1 is bounded from above by $C\kappa_0$. The three ordered eigenvalues are used to classify the corresponding three families of eigenvector fields for the 3D de-homogenization.

Property 2 is shown through the following. For conciseness, denote $\tilde{\kappa}_1 := \kappa_1/\kappa_2$ and $\tilde{\kappa}_3 := \kappa_3/\kappa_2$. First, taking the determinant of $\boldsymbol{\kappa}$ and knowing $\kappa_2 = \frac{C}{\kappa_0}$, we can obtain

$$\tilde{\kappa}_1 \tilde{\kappa}_3 = C^2 \leq 1 \quad (21)$$

This implies that $\tilde{\kappa}_1 \leq 1$.

Next, taking the trace of $\boldsymbol{\kappa}$, and knowing $\kappa_2 = \frac{C}{\kappa_0}$, we can get

$$\tilde{\kappa}_1 + \tilde{\kappa}_3 = 1 + a^2 + e^2 \quad (22)$$

where the expressions of a and e depend on r, θ, ψ whose exact form is irrelevant to the analysis here. Combining the two equations above leads to a quadratic equation of $\tilde{\kappa}_3$:

$$\tilde{\kappa}_3^2 - (1 + a^2 + e^2)\tilde{\kappa}_3 + a^2 = 0 \quad (23)$$

Using the root formula and taking the larger root (by definition $\tilde{\kappa}_3$ is the larger root), we obtain

$$\begin{aligned} \tilde{\kappa}_3 &= \frac{1}{2}(1 + a^2 + e^2) + \frac{1}{2}\sqrt{[(1 + a)^2 + e^2][(1 - a)^2 + e^2]} \\ &\geq \frac{1}{2}(1 + a^2 + e^2) + \frac{1}{2}\sqrt{(1 + a)^2(1 - a)^2} \\ &= \frac{1}{2}(1 + a^2 + e^2) + \frac{1}{2}(1 - a^2) \\ &= 1 + \frac{1}{2}e^2 \\ &\geq 1 \end{aligned} \quad (24)$$

and hence $\tilde{\kappa}_3 \geq 1$. Together with the previous $\tilde{\kappa}_1 \leq 1$ and (21), we can conclude $\kappa_1 \leq C\kappa_0 \leq \kappa_0 \leq \kappa_2 = \frac{\kappa_0}{C} \leq \kappa_3$, and hence Property 2 holds. The inequality also implies $\kappa_1/\kappa_2 \leq C^2$, and for most domains, $C \leq 0.5$, which means κ_1 is usually much smaller than κ_2 . This is observed in Figure 2 A and also in all the studied cases.

The eigenvectors of the general-shape surfaces, unlike the eigenvalues, appear to lack desirable properties for design simplification. However, for the special case of surface of revolution, as shown in the following subsection, there are additional special properties about the eigenvectors that have significant implications for the subsequent de-homogenization.

3.2 Special case of surface of revolution $R_1(\bar{\theta})$ and $R_2(\bar{\theta})$

The special case of surface of revolution (R_1 and R_2 depend solely on θ) has additional special properties about its eigenvalues and eigenvectors. Denote $\mathbf{v}_\psi = [-\sin(\psi), \cos(\psi), 0]$ as the unit vector field circulating the axis of rotation, we have:

Property 3 (surface of revolution): $\mathbf{v}_\psi$ is the eigenvector of $\boldsymbol{\kappa}$ associated with $\kappa_2 = \frac{\kappa_0}{C}$.

Property 4 (surface of revolution): The other two eigenvalues of $\boldsymbol{\kappa}$, i.e., κ_1 and κ_3 , depend solely on r and θ (and not on ψ).

Property 3 says the circulating vector field $\mathbf{v}_\psi$ is the eigenvector field corresponding to the second eigenvalue κ_2 . This implies the other two eigenvectors, denoted as $\mathbf{v}_1$ and $\mathbf{v}_3$ and corresponding to κ_1 and κ_3 , respectively, lie in the meridian plane of the cloaking region. Property 3 is proved by symbolically verifying $\boldsymbol{\kappa}\mathbf{v}_\psi = \frac{\kappa_0}{C}\mathbf{v}_\psi$.

Property 4 says that all three eigenvalues vary in the meridian plane and not along the circulating direction $\mathbf{v}_\psi$. This is proved by showing all three principal invariants of $\boldsymbol{\kappa}$ depend only on r and θ , and not on ψ .

Properties 3 and 4 have significant implications for the de-homogenization and generation of global cloaking structures for domains defined by surface or revolution. They allow us to solve for the mapping ϕ_i and parameter identification of microstructures on a reduced 2D domain instead of the physical 3D domain, which greatly reduces the design cost. We will elaborate on this in later sections of the parameter identification and the solution for the mapping.

4 3D lattice microstructure

Throughout this study, we adopt the 3D lattice structure made of three perpendicular and square-sectioned Material A bars embedded in the Material B matrix, as shown in Figure 1 A. The lattice is parameterized by the widths of the three cross-sectional widths b_1 , b_2 , and b_3 . The microstructure has four advantages: 1) its three-variable parameterization is simple, hence the parameter identification based on surrogate model can be accomplished efficiently; 2) it is compatible with the subsequent de-homogenization technique for the global structure; 3) it is highly robust in that it achieves the great majority of anisotropic conductivities within the physical bounds (shown in a later subsection); and 4) it is free of closed spaces and hence fabricable by powder-bed metal 3D printing. These advantages are not all available from some other simple microstructures, such as the rank-3 laminates, as its achievable range of homogenized properties is considerably smaller, and its closed-wall structures cannot be fabricated by powder-bed printing (discussed in detail later).

4.1 Numerical homogenization and surrogate model of parameter-homogenized conductivity relation

The 3D lattice does not have a closed-form formula for its homogenized conductivity, and we adopt a surrogate model constructed based on off-line numerical homogenization. Here, we provide the relevant details. For the off-line numerical homogenization, we focus on one unit cell with parameters b_i and follow the standard procedure as described below. For a unit cell with local coordinate denoted as $\mathbf{y}$, the effective/homogenized conductivity $\boldsymbol{\kappa}$ is evaluated through

$$\boldsymbol{\kappa} = \int_Y \hat{\boldsymbol{\kappa}} (\boldsymbol{\delta} - \nabla \boldsymbol{\xi}) dV \quad (25)$$

where $\hat{\boldsymbol{\kappa}}$ is the local constituent's conductivity tensor, $\boldsymbol{\delta}$ is Kronecker's delta (identity matrix), Y denotes the unit cell domain, ∇ denotes the gradient, and vector $\boldsymbol{\xi}$ is obtained as follows. Let scalar field $\gamma = \mathbf{E} \cdot (\mathbf{y} - \boldsymbol{\xi})$ where $\mathbf{E} := [1, 0, 0]$ or $[0, 1, 0]$ or $[0, 0, 1]$ is the probing vector in the principal frame of the unit cell. The γ is obtained by solving the following PDE (source-free heat equation)

$$\nabla \cdot (\hat{\boldsymbol{\kappa}} \nabla \gamma) = 0 \quad (26)$$

subjected to periodic boundary conditions $\gamma^{(q)} - \gamma^{(p)} = \mathbf{E} \cdot (\mathbf{y}^{(q)} - \mathbf{y}^{(p)})$, where $\nabla \cdot$ denotes the divergence, and p and q denote periodic pairs of the unit cell's boundary.

Equation (26) is solved using FEM with a $64 \times 64 \times 64$ structured mesh. The problem is solved for the three probing vectors, resulting in the corresponding three γ fields, with which we can compute $\boldsymbol{\xi}$ and then evaluate the homogenized $\boldsymbol{\kappa}$ using (25). As the FE coordinate frame aligns with the microstructure's principal frame, the obtained $\boldsymbol{\kappa}$ is in diagonal form with three principal values κ_i .

Based on the above numerical homogenization, we construct the surrogate model of $\mathbf{b} \rightarrow \boldsymbol{\kappa}$ off-line via parameter sweep of $b_i \in [0, 1]$. The corresponding homogenized κ_i are collected. Additionally, we also compute the gradient information of $\partial \kappa_i / \partial b_j$ using finite difference (3-point central difference) on the $\mathbf{b} \rightarrow \boldsymbol{\kappa}$ database and store them for later parameter identification. For our implementation, we used a discretization of 32 intervals (33 points) for the parameter sweep of b_i . Our investigation on discretization resolution shows that the chosen one is a good balance between accuracy and efficiency for the proposed 3D microstructure. The parameter sweep is performed in four parallel groups on a desktop workstation and takes approximately 32 hours. The surrogate model needs to be constructed only once and is reused for creating any new 3D thermal cloak.

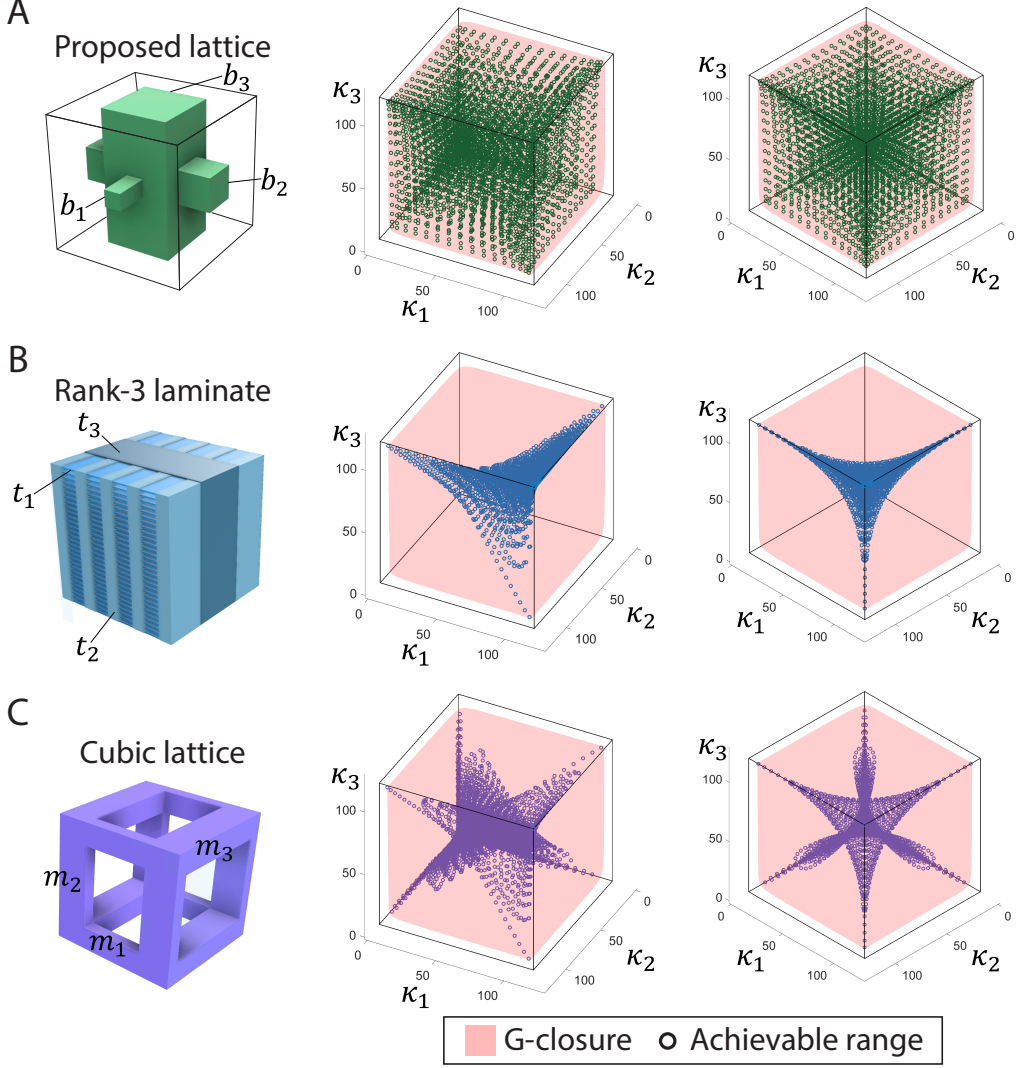


Figure 1: Microstructures and their achievable range of anisotropic thermal conductivity relative to the theoretical bound. A) Proposed lattice; B) rank-3 laminates; C) cubic lattice [2].

4.2 The lattice's achievable conductivities relative to theoretical bounds and some other microstructures

We demonstrate the large range of achievable anisotropic conductivity of the proposed 3D lattice relative to theoretical bounds and two other popular microstructures that are also compatible with the 3D de-homogenization. Given two base materials and regardless of their relative usage and microstructure, the physically achievable (anisotropic) κ is bounded in the principal space (i.e., κ_i space) by a closed surface known as the “G-closure” [3, 4, 5]. The G-closure can be constructed via assembly of six patches $\mathbb{R}^2 \rightarrow \mathbb{R}^3$. Here, we use one patch for illustration, the others can be obtained by cyclic permutation of κ_i . The patch is defined as $(\kappa_1, f_A) \rightarrow (\kappa_1, \kappa_2(\kappa_1, f_A), \kappa_3(f_A))$ where $\kappa_2(\kappa_1, f_A)$ is such that [5]

$$\frac{1}{\kappa_2 - \kappa_B} = \frac{1}{f_A} \left(\frac{3}{\kappa_A - \kappa_B} + \frac{1 - f_A}{\kappa_B} \right) - \frac{1}{\kappa_3(f_A) - \kappa_B} - \frac{1}{\kappa_1 - \kappa_B} \quad (27)$$

and $\kappa_3(f_A) = w_U(f_A)$ attains the Wiener upper bound $w_U(f_A) = f_A \kappa_A + (1 - f_A) \kappa_B$. The domain for (κ_1, f_A) is $f_A \in (0, 1)$ and $\kappa_1 \in [w_L(f_A), w_U(f_A)]$ with $w_L(f_A) = 1/(f_A/\kappa_A + (1 - f_A)/\kappa_B)$ being the Wiener lower bound. The complete G-closure consisting of six patches can be obtained by cyclic permutation of κ_i . The G-closure have diagonal vertices $(\kappa_A, \kappa_A, \kappa_A)$ and $(\kappa_B, \kappa_B, \kappa_B)$, the two base materials' isotropic conductivity.

The G-closure corresponding to the two base materials used in this study is plotted in Figure 1 A together with the achievable conductivity range of the 3D lattice (two viewing perspectives) and the cubic box (a loose bound) defined by the diagonal vertices $(\kappa_A, \kappa_A, \kappa_A)$ and $(\kappa_B, \kappa_B, \kappa_B)$. The 3D lattice achieves the great majority (but not all) of the G-closure, demonstrating high robustness and design freedom. The non-achievable zones are small and concentrate mainly on the three sharp edges of the G-closure, which correspond to rank-1 laminates. Indeed, the metal parts of the lattice have square cross-sections that cannot represent the 3D rank-1 laminate.

The proposed 3D lattice's achievable range is significantly larger than the 3D rank-3 laminates and another type of 3D cubic lattice used in [2], as shown in Figures 1 B and C. The three-scale rank-3 laminates' homogenized properties are obtained analytically through the iterative lamination formula, and they are known to reach extreme values of the bounds. For the cubic lattice, the homogenized properties are obtained numerically. We note that the rank- N laminate can attain the complete G-closure in the two-dimensional setup [6, 7, 8, 9, 5, 10], but its robustness considerably deteriorates in 3D. All three microstructures are defined through three parameters and are compatible with the de-homogenization, with rank-3 laminates characterized by the relative thickness of the plates t_i (Figure 1 B) and cubic lattice defined by the size of the openings m_i (Figure 1 C). As shown in Figure 1, the achievable conductivity ranges of the rank-3 laminates and the cubic lattice are only a fraction of the G-closure. Also, the three different scales and the closed plate-like features of the rank-3 laminates are difficult, if not impossible, to realize in practice.

4.3 Parameter identification based on the surrogate model

To realize thermal meta-devices, we need to perform parameter identification to obtain the microstructure triplets b_i producing the required conductivity from transformation thermotics. With the database set up, the parameter identification $\boldsymbol{\kappa} \rightarrow \mathbf{b}$ at a given location is realized by solving the following three-variable least-square problem

$$\begin{aligned} \min_{\mathbf{b}} \quad & \sum_{i=1}^3 (\kappa_i(\mathbf{b}) - \kappa_i^*)^2 \\ \text{s.t.} \quad & b_i \in [b_{\min}, 1], \quad i = 1, 2, 3 \end{aligned} \quad (28)$$

where $\kappa_i(\mathbf{b})$ is evaluated by interpolating the database, the target κ_i^* is obtained from transformation thermotics, and $b_{\min} > 0$ is the minimal relative size. The problem is solved efficiently using the projected gradient descent algorithm, where the gradient is also directly interpolated based on the database of gradients obtained with finite difference as described in 4.1.

For a general domain (not defined by surfaces of revolution), the problem (28) is solved at each discretized location of the 3D meta-device domain in a fully parallel fashion. With a discretization of $64 \times 64 \times 128$ or $48 \times 96 \times 96$ used in this study, the solution takes about 12 - 20 minutes on a desktop workstation (AMD Ryzen Threadripper 3970X 32-Core Processor 3.69 GHz, 256 GB RAM).

For domains defined by surfaces of revolution, as discussed in 3.2, the resulting κ_i depends solely on r and θ (and not on ψ). Hence, we can choose any meridian plane and solve the problem (28) on locations within that plane instead of the full 3D space. After obtaining the 2D distribution of b_i , we can revolve them around the axis of revolution and get the corresponding 3D distributions. The reduction of the 3D domain to 2D significantly reduces the computational cost.

For illustration, Figures 2A and B show the eigenvalues κ_i and resulting b_i obtained by solving (28) for Dsg. 4. The $\kappa_2 = \kappa_0/C$ is constant because the inner and outer surfaces of Dsg.4 have the same shape as analyzed in Sec. 3.1, but b_2 is not a constant as it also depends on κ_1 and κ_3 . Also, larger κ_i generally leads to larger b_i as expected. Another observation is that κ_1 is significantly smaller than κ_2 as predicted by the $\kappa_1/\kappa_2 \leq C^2$ in Sec. 3.1. For Dsg. 4, $C = 0.286$ and $\kappa_1/\kappa_2 \leq 0.082$.

5 Solution for global mapping ϕ_i

To generate the global structure for the 3D thermal meta-device, we adopt the 3D de-homogenization approach, which requires solving for the mappings ϕ_i in the 3D domain such that $\nabla \phi_i = \alpha_i \mathbf{v}_i$ with some scalar field α_i [10]. This is attained by solving the following least-square problem (take ϕ_1 as an example):

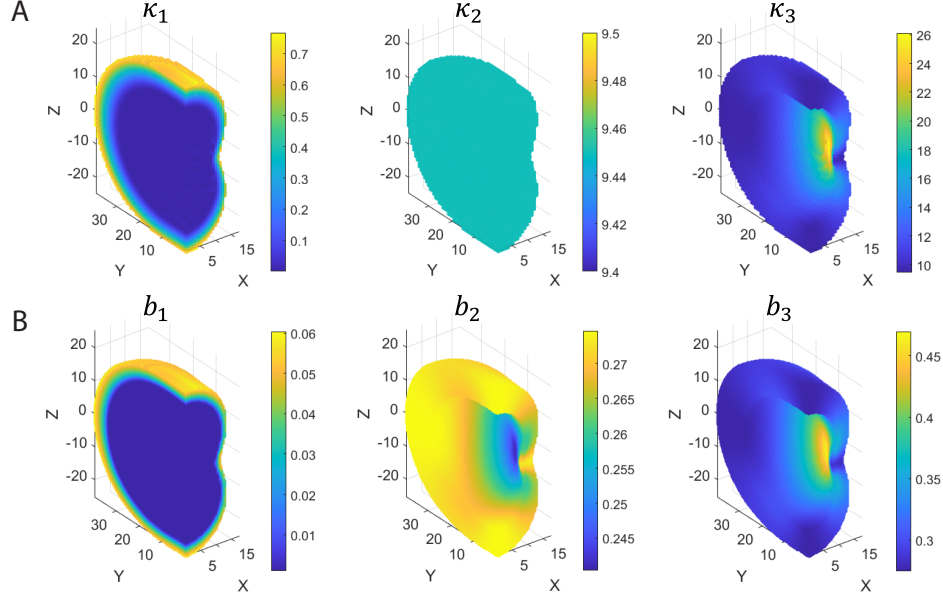


Figure 2: Distributions of A) eigenvalues of κ ; B) lattice microstructure parameters.

$$\begin{aligned} \min_{\phi_1} \int_{\Omega} \|\nabla \phi_1 - \mathbf{v}_1\|^2 d\Omega \\ \text{s.t.} \quad \nabla \phi_1 \cdot \mathbf{v}_2 = 0, \quad \nabla \phi_1 \cdot \mathbf{v}_3 = 0 \end{aligned} \quad (29)$$

In general, we solve the problem in the 3D domain using FEA with the penalty approach for the equality constraints. Symmetry is exploited to reduce the problem's domain to a half or a quarter of the full domain. The resulting nonlinear algebraic system is solved through the Newton-Raphson method. Details of the FEA procedure are introduced in [10] with a simpler 2D setup. For general 3D domains, the problem is solved on an FE structured mesh of $64 \times 64 \times 128$ or $48 \times 96 \times 96$, depending on whether the domain can be reduced to a quarter or half. The elements in the core and background regions are removed, leaving only those in the cloaking region between R_1 and R_2 .

Unless with simple geometries, general 3D analytical domains can produce complex and rapidly varying $\mathbf{v}_i$ distributions, which can lead to convergence issues for the Newton-Raphson iteration. To alleviate this issue, we smooth the $\mathbf{v}_i$ fields by applying a linear filter as follows.

$$\tilde{\mathbf{v}}_i = \frac{\sum_{j \in S_i} w_j \mathbf{v}_j}{\sum_{j \in S_i} w_j}, \quad \tilde{\tilde{\mathbf{v}}}_i = \frac{1}{|\tilde{\mathbf{v}}_i|} \tilde{\mathbf{v}}_i \quad (30)$$

where $S_i = \{j | |\mathbf{x}_j - \mathbf{x}_i| \leq d\}$, and the weights are $w_j = 1 - |\mathbf{x}_j - \mathbf{x}_i|/d$. The filtered unit vector $\tilde{\tilde{\mathbf{v}}}_i$ is used in solving (29).

For illustration, Figure 3 A shows the three eigenvectors of Dsg. 4 (on a reduced quarter domain due to symmetry), and Figure 3 B shows the three corresponding ϕ_i obtained by solving (29). It is visually apparent that $\nabla \phi_i$ follows $\mathbf{v}_i$.

5.1 Simplification for surfaces of revolution

For domains defined by surfaces of revolution, such as the pear-apple cloak, the solution to ϕ_i can be significantly simplified, with analytical solution for ϕ_2 and numerical FEM solution for ϕ_1 and ϕ_3 on a reduced 2D meridian domain.

Analytical solution for ϕ_2 As revealed in Sec. 3.2, for surfaces of revolution, the second eigenvector $\mathbf{v}_2 = \mathbf{v}_\psi$ circulates the axis of revolution. The corresponding ϕ_2 can be obtained analytically: $\phi_2 =$

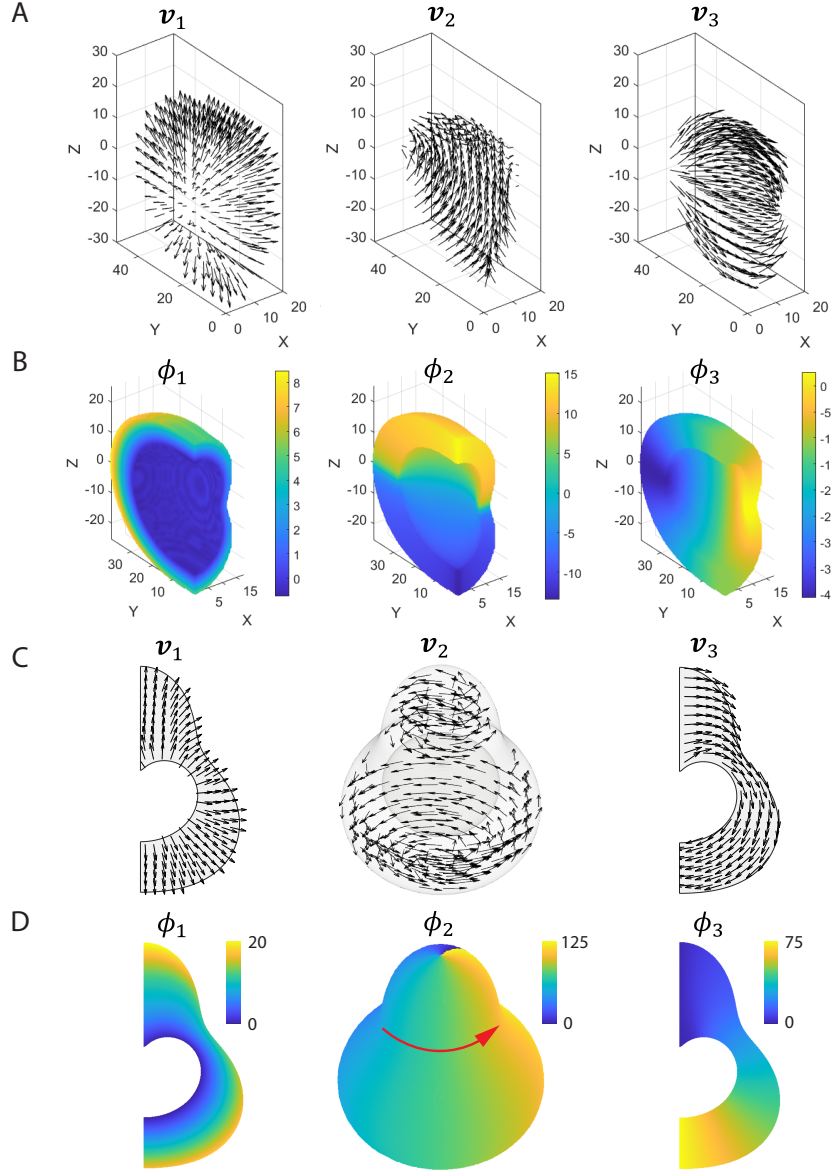


Figure 3: Distributions of A) eigenvectors of κ and resulting mappings for Dsg. 4; C) - D) eigenvectors of κ and resulting mappings for pear-apple cloak.

$D_1\psi + D_2$ where $D_1 \neq 0$ and D_2 are arbitrary constants. One small issue with such a ϕ_2 is that it has singularity at the axis of revolution with $|\nabla\phi_2| \rightarrow \infty$, which would produce infinitely small members. Resolution of this issue is discussed in Sec. 6.1.

Numerical solution for ϕ_1 and ϕ_3 The ϕ_1 and ϕ_3 depend only on r and θ (and not on ψ), and hence they are numerically solved on the 2D meridian plane instead of the general 3D domain, which significantly reduces the computational cost. The 3D solution can be obtained by simply popping the 2D into 3D space based on r and θ .

For illustration, the three eigenvectors of the pear-apple cloak (surface of revolution) are shown in Figure 3 C, with $\mathbf{v}_2$ circulating the axis of revolution. The corresponding three ϕ_i are shown in Figure 3 D, where their gradients are aligned with the eigenvectors.

5.2 Special pre-processing for human-face surfaces

For highly complex surfaces such as the face-shaped cloak in the main text, the $\mathbf{v}_i$ distributions can be highly irregular and disordered, which could cause failures for the numerical solution of ϕ_i . As shown in Figure 4 A, the distributions of $\mathbf{v}_2$ and $\mathbf{v}_3$ are highly complicated and close to discontinuous, although the $\mathbf{v}_1$ distribution remains largely radial.

To resolve this issue, we propose a pre-processing of the disordered eigenvectors based on the special characteristics of the eigenvalues. Specifically, for the face-shaped cloak, we observe that κ at most locations is close to transversely isotropic within the $\mathbf{v}_2 - \mathbf{v}_3$ plane. As shown in Figure 4 B shows the distributions of the three eigenvalues in the principal space with κ_2 and κ_3 showing similar magnitudes while both are significantly larger than κ_1 as analyzed. To quantitatively show κ_2 and κ_3 is close at most locations, we define a proportion parameter $p(\eta)$ which equals the ratio of the total number of discrete locations satisfying $(\kappa_3 - \kappa_2)/\kappa_3 \leq \eta$ over the total number of all discrete locations. This shows the proportion of locations with close κ_2 and κ_3 under tolerance of η . The $p(\eta)$ curve is shown in Figure 4 C, which shows approximately 60% of all locations satisfy $(\kappa_3 - \kappa_2)/\kappa_3 \leq 0.05$, and roughly 85% shows $(\kappa_3 - \kappa_2)/\kappa_3 \leq 0.15$.

The observation that κ at most locations are close to transverse isotropy inspires us to approximate κ_2 and κ_3 with an “averaged” value and produce transverse isotropy, which in turn allows us to modify $\mathbf{v}_2$ and $\mathbf{v}_3$ within their subspace (as any vector in the isotropic subspace is an eigenvector) to obtain more regular and numerically friendly distributions usable for solving ϕ_i . Denote $\tilde{\kappa}_i$ the approximated and modified eigenvalues. We take $\tilde{\kappa}_1 = \kappa_1$ (no modification) and $\tilde{\kappa}_2 = \tilde{\kappa}_3 = \sqrt{\kappa_2\kappa_3}$, the latter is the homogenized isotropic conductivity of checkerboard microstructure made of base materials κ_2 and κ_3 . The specific form of $\tilde{\kappa}_2$ and $\tilde{\kappa}_3$ should not make a huge difference as long as it is some averaging of $\tilde{\kappa}_2$ and $\tilde{\kappa}_3$.

The transversely isotropic $\bar{\kappa}$ allows us to freely modify the mutually orthogonal eigenvector pairs $\bar{\mathbf{v}}_2$ and $\bar{\mathbf{v}}_3$ as long as $\bar{\mathbf{v}}_2, \bar{\mathbf{v}}_3 \in \text{span}\{\mathbf{v}_2, \mathbf{v}_3\}$. In this study, $\bar{\mathbf{v}}_2$ and $\bar{\mathbf{v}}_3$ are constructed as follows. First, we generate a smooth vector field $\mathbf{u}$ and project it onto $\text{span}\{\mathbf{v}_2, \mathbf{v}_3\}$ with normalization to obtain $\bar{\mathbf{v}}_2$, i.e., $\bar{\mathbf{v}}_2 = \mathbf{P}\mathbf{u}/|\mathbf{P}\mathbf{u}|$, where $\mathbf{P} := \mathbf{I} - \mathbf{v}_1 \otimes \mathbf{v}_1$ is the projector and $\otimes$ is the outer product. Then, we obtain $\bar{\mathbf{v}}_3 = \mathbf{v}_1 \wedge \bar{\mathbf{v}}_2$ where $\wedge$ is the cross product. By construction, the resulting $\bar{\mathbf{v}}_2$ and $\bar{\mathbf{v}}_3$ are mutually orthogonal and belong to $\text{span}\{\mathbf{v}_2, \mathbf{v}_3\}$ (hence orthogonal to $\mathbf{v}_1$). The smoothness of $\bar{\mathbf{v}}_2$ and $\bar{\mathbf{v}}_3$ depend mainly on $\mathbf{u}$ which is chosen by the user.

For the face-shaped cloak in this study, specifically, we use $\mathbf{u} = \mathbf{v}_\psi$, the vector circulating the z -axis. The resulting $\bar{\mathbf{v}}_2$ and $\bar{\mathbf{v}}_3$ are shown in Figure 4 D, showing a much more regular distribution. These $\bar{\mathbf{v}}_i$ are used for the solution for ϕ_i , and the obtained results are shown in Figure 4 E, also displaying an overall smooth distribution.

5.3 Interpolation of general surface ϕ_i to finer mesh

To obtain high-resolution structures, we interpolate the ϕ_i of the general surface obtained on a medium mesh of $64 \times 64 \times 128$ or $48 \times 96 \times 96$ to a finer mesh of $288 \times 288 \times 576$ or $240 \times 480 \times 480$. The interpolation is linear and based on the fine mesh’s location. The interpolated ϕ_i are used for the generation of structures with the same resolution, which is then also used in the FEA. For the surface of revolution, thanks to the reduced computational cost, we directly use the fine mesh of 288×576 in the 2D solution for ϕ_1 and ϕ_3 .

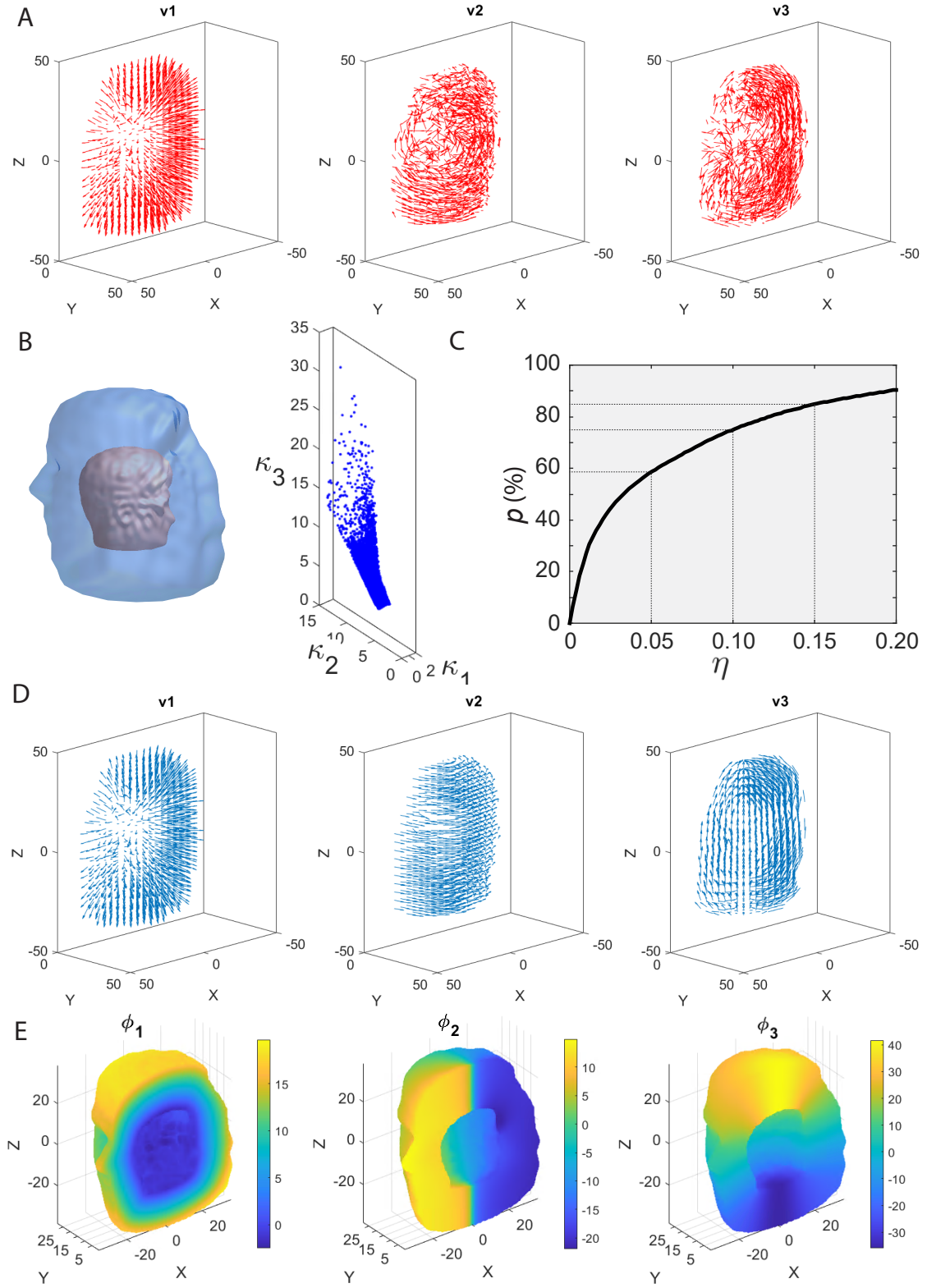


Figure 4: Pre-processing of eigenvectors for face-shaped cloak. A) Eigenvectors of human face-shaped cloak before pre-processing; B) Distribution of the three eigenvalues; C) $p - \eta$ curve; D) eigenvectors after pre-processing; E) obtained mappings.

6 Global representation of the graded 3D lattice structures

Based on the obtained microstructure member size b_i and mappings ϕ_i , we generate the global lattice structure through a wave level set function. Similar strategies are used for generating 2D rank-2 laminates structures [11, 12, 13, 14, 10], 3D rank-3 laminates structures [15], and 3D cubic lattices [2]. The method used here is developed based on [2] and generalized to the current 3D lattice microstructure.

First, we define the 3D wave function as follows.

$$\rho_{ij}(r, \theta, \psi) = -\cos\left(\frac{2\pi}{\varepsilon_i}\phi_i(r, \theta, \psi)\right) + \cos(\pi b_j(r, \theta, \psi)), \quad i, j = 1, 2, 3 \quad (31)$$

where ε_i is a user-defined feature size parameter that controls the feature size of the generated structures. It is set to 2π in this study. Based on the wave function, we defined the level set $\chi_{ij} = \{r, \theta, \psi | \rho_{ij}(r, \theta, \psi) \geq 0\}$, which represents a family of spatial shells with the normal of the surfaces (isosurface of ϕ_i) pointing to $\nabla\phi_i$ (or $\mathbf{v}_i$) and relative thickness of b_j . This is illustrated in the first column of Figure 5 using Dsg. 4.

We then use the Boolean intersection operation of different families of shells to represent the orientations and relative widths of the three groups of lattices. Specifically, the first group is defined by $\chi_{21} \cap \chi_{31}$ (Boolean AND) as it is aligned in $\mathbf{v}_1 = \mathbf{v}_2 \times \mathbf{v}_3$ and with relative width b_1 . As illustrated in the top part of the second column of Figure 5, taking the intersection leads to small and largely radially aligned members, which reflect the small sizes of b_1 (shown in Figure 2B) and orientation of $\mathbf{v}_1$ (shown in Figure 3A). A similar procedure applies to obtain the second and third groups of lattices, which are represented by the set $\chi_{12} \cap \chi_{32}$ and $\chi_{13} \cap \chi_{23}$, respectively, as illustrated in the second column of Figure 5. The global structure is then obtained by taking the union (Boolean OR) of the three lattice groups as shown in the right column of Figure 5.

As a final step, we need to add a thin layer of lattice shells at the outer boundary of the cloaking region to achieve a smooth transition from the lattice structure to the continuum background. This is needed because the eigenvectors $\mathbf{v}_2$ and $\mathbf{v}_3$ do not align with the domain's boundary in general, leading to lattices non-conformal to the boundary and non-smooth heat paths. The thin shell can also be added through the level-set approach. Specifically, we use the following three sets: $\chi_{shell} = \{\mathbf{x} | R_2 - t_{shell} \leq r(\mathbf{x}) \leq R_2\}$ where t_{shell} is the thickness of the shell and assigned with a small value, and χ_{24} and χ_{34} defined through (31) with a small b_4 . The lattice thin shell is obtained as $(\chi_{shell} \cap \chi_{24}) \cup (\chi_{shell} \cap \chi_{34})$. The final structure with the added thin shell is shown in the bottom right of Figure 5.

6.1 Treatments for the singularity points of surfaces of revolution

As discussed in Sec. 5.1, for surfaces of revolution, $\phi_2 = D_1\psi + D_2$ with $\nabla\phi_2$ circulating the axis of rotation. One small issue with this solution is that $\nabla\phi_2$ is singular (approaches infinity) at the axis of revolution, i.e., locations with $\theta = 0$ or π . This would result in infinitely small members at those locations that cannot be represented with a finite resolution and cannot be fabricated.

To tackle this issue, we propose a theory-based post-processing of the structures near the axis of revolution. Specifically, we can show analytically that the κ at $\theta = 0$ or π are transversely isotropic with $\kappa_2 = \kappa_3 = \kappa_0/C$ independent of r . The transversely isotropic κ can be realized by the 3D rank-1 laminate, where the thickness of Material A is computed by

$$t = \frac{\frac{\kappa_0}{C} - \kappa_B}{\kappa_A - \kappa_B} \quad (32)$$

Along the axis of revolution (perpendicular to the laminate), however, the computed t would not exactly produce the κ_1 value, but as κ_1 is always significantly smaller than κ_2 and κ_3 (see Sec. 3.1), which is qualitatively same as rank-1 laminate's small conductivity in the cross-laminate direction, the error should not produce significant perturbation to global cloaking performance. The local use of rank-1 laminate is also compatible with the de-homogenization based on wave level-set functions. They are represented by χ_{1t} with ϕ_1 and size t .

Take the pear-apple cloak for illustration, the structures before and after the proposed post-processing are shown in Figure 6. The theory-based post-processing resolves the singularity issue while retaining the theoretical planar conductivity.

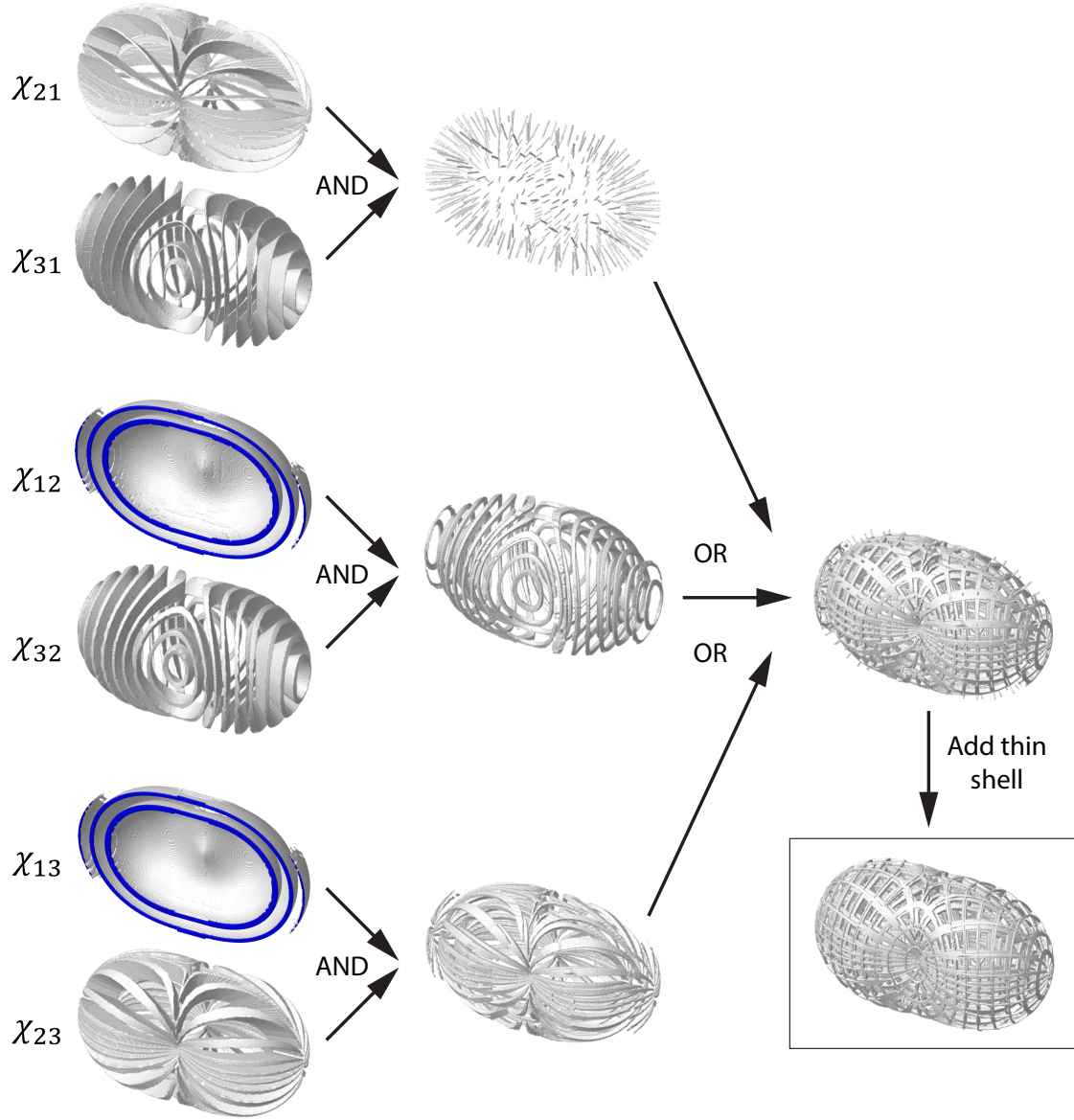


Figure 5: Generation of global 3D structures based on the wave-function level set and Boolean operations.

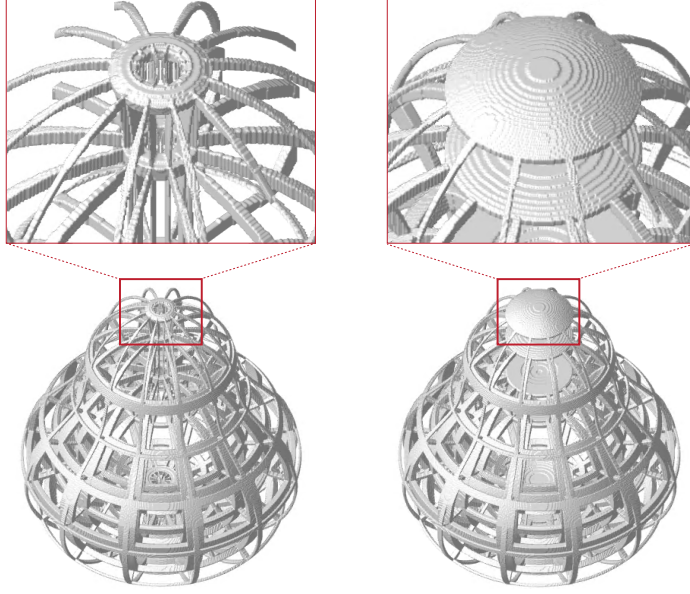


Figure 6: Post-processing of singularity along the axis of revolution: structures before and after post-processing.

7 Computational cost of the design process

The computational cost for generating a global cloaking structure consists of three parts: 1) the nonlinear FE solution of the pseudo-conformal mapping, 2) the parameter identification based on the surrogate model, and 3) global structure generation. The cost of building the off-line surrogate model of the 3D lattice is not included in the design cost because it is design-independent and needs to be computed only once and then stored for the design of any other thermal meta-devices.

Here, we report the computational cost of a representative Dsg.4 in the main text Figure 3, which has a general 3D shape. We use a $64 \times 64 \times 64$ base structured mesh with those in the background and core regions removed. Using a workstation with AMD EPYC 7K62 96-Core Processor 2.60 GHz (actual use of 16 cores) and 256 GB RAM, the computational costs are: 1) 235.1 s for nonlinear FE solution of pseudo-conformal mapping, 2) 1333.8 s for the parameter identification of 27864 microstructures (0.05 s for each microstructure), and 3) 51.8 s for structure generation with $576 \times 576 \times 576$ pixels. We note that for 3D domains defined by surfaces of revolution, the computational cost can be significantly reduced for the pseudo-conformal mapping solution and parameter identification by harnessing the special spectral properties of κ . Also, further cost reduction can be achieved by special programming techniques such as mixed-language programming with the C language.

8 Qualitative comparison of different methods for designing omnidirectional thermal meta-device

We provide a qualitative comparison and assessment of some of the latest methods for designing free-form omnidirectional thermal meta-devices with transformation thermotics. Methods for non-omnidirectional performance or non-free-form geometries are beyond the scope of our discussion. The main strategies other than the current method for designing 2D free-form thermal meta-device adopt a “divide-and-conquer” strategy, where the domain is partitioned into many square-shaped unit cells, and their microstructures are designed with topology optimization (TO) [16, 17, 18] or artificial intelligence (AI) [19], and the microstructures are later assembled back to the meta-device. These methods have produced fabricable thermal meta-devices in the 2D setup, but have not been used in the design of free-form 3D meta-devices. Here, we provide a speculative analysis of these methods in the 3D design setup and compare them to this study’s method. Table 1 summarizes the key features of these methods,

Table 1: Summary of three strategies for the design of free-form omnidirectional thermal metamaterials in 2D and 3D spaces

Metamaterial design strategy	Divide and conquer + TO microstructure (e.g., Nat. Commun., 12(1):7228, 2021)	Divide and conquer + AI microstructure (e.g., Advanced Materials, 35(33):2302387, 2023)	3D de-homogenization + simple 3D microstructure (This study)
Dimension realized	2D	2D	3D
Direction dependence	Omnidirectional	Omnidirectional	Omnidirectional
Microstructure inverse design cost in 3D case	Not demonstrated in 3D, but expectedly very high cost as each unit cell requires a 3D TO process with numerical homogenization (quantitative computational cost not reported)	Not demonstrated in 3D, but presumably low-cost after potentially expensive ML training (quantitative computational cost not reported)	Low cost, thanks to geometric simplicity and surrogate model (1 sec. per microstructure)
Global structure generation method	Unit cell assembly + post-processing	ML-based unit cell assembly	3D de-homogenization
Global 3D connectivity	Not demonstrated in 3D, but based on the 2D version, heavy post-processing should be required	Not demonstrated in 3D, connectivity guaranteed in 2D	Naturally guaranteed without post-processing
Global structure fabricability	Not demonstrated in 3D, but the high complexity of 3D TO-microstructure would be challenging to fabricate	Not demonstrated in 3D, but the high complexity of 3D AI-microstructure would be challenging to fabricate	Practically fabricable as demonstrated
Cloaking performance in RTD	Not demonstrated in 3D nor reported in 2D	Not demonstrated in 3D, the 2D reported values of free-form geometries are 0.13 - 0.39	RTD in 3D with similar geometric complexity is 0.03 - 0.15

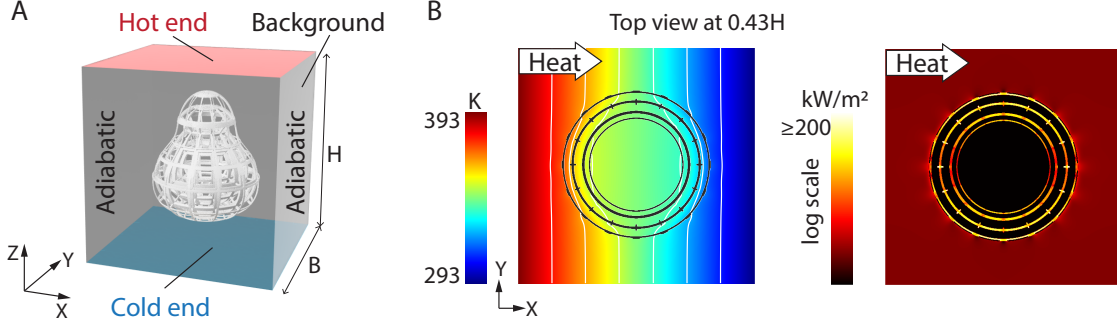


Figure 7: FE post-evaluation of thermal performance. A) Basic FE setup; B) top view of FE result for pear-apple cloak under X-direction applied heat.

which are also discussed in more detail as follows.

For the design of 3D (and 2D) microstructures, free-form microstructures designed by TO or AI generally have no guarantee to attain the global optimum due to non-convexity of the design problem. By contrast, the proposed 3D lattice has only three design variables, and the parameter-property mapping is one-to-one as demonstrated by the property space plot in Figure 1A except for the extrema boundaries of any $b_i = 1$, which corresponds to the isotropic maximum $\kappa_1 = \kappa_2 = \kappa_3 = \kappa_A$. The global optimum corresponding to a feasible κ is likely to be attainable by the proposed method.

In terms of computational cost, the TO-based method would be expensive as each 3D unit cell needs a 3D topology optimization consisting of at least hundreds of thousands of design variables and typically hundreds of optimization steps, each of which requires solving three FEA in the numerical homogenization process. The AI-based method should significantly accelerate the microstructural design process after the neural network is trained albeit through a potentially expensive process. The method proposed here is highly efficient thanks to the three-parameter microstructure and surrogate model. As shown in the previous section, the parameter identification for one unit cell is about 0.05 seconds via 16-core parallel computation (or 0.8 s per computer core).

Regarding 3D global connectivity, the TO-based method would require heavy post-processing as evidenced in its 2D application [16, 17, 18]. The challenges of post-processing 3D connectivity would be significantly greater than 2D and degrade the performance. The AI-based method trained with selected TO-generated 2D microstructures should exhibit improved connectivity [19], although whether such an advantage can be generalized to 3D microstructures remains unclear. Our proposed method naturally guarantees global connectivity thanks to the continuous and smooth pseudo-conformal mapping and 3D de-homogenization.

For fabricability, both the TO- and AI-based methods tend to generate highly complex microstructures that can be challenging to fabricate in a general 3D setup. In particular, the microstructures need to be free of closed spaces for powder-bed metal 3D printing, and the overall structure needs to be simple enough for workability, such as support removal. It is unknown how these requirements can be efficiently and systematically met by the TO- and AI-based methods. The proposed 3D lattice is simple in geometry and free of closed spaces, and the global structure is practically fabricable as demonstrated.

9 3D FE post-evaluation of 3D cloak's performance

9.1 Basic FEA setup

We use FEA for the numerical post-evaluation of the cloaks' performance. The PDE is the 3D steady-state heat conduction equation, i.e., $\nabla \cdot (\kappa \nabla T) = 0$, where $\nabla \cdot$ denotes the divergence operator and κ is one of the following depending on the location: 1) $\kappa_0 \mathbf{I}$ if at the background; 2) $\kappa_A \mathbf{I}$ if at the aluminum lattice; 3) $\kappa_B \mathbf{I}$ if at the PDMS parts; and 4) $\kappa_C \mathbf{I}$ if at the core region.

The boundary conditions for post-evaluation is illustrated in Figure 7 A. In the applied heat direction (e.g., Z direction), the upstream plane is set to a high temperature, and the downstream surface is set to a low temperature. The four side surfaces are set to adiabatic. We make use of

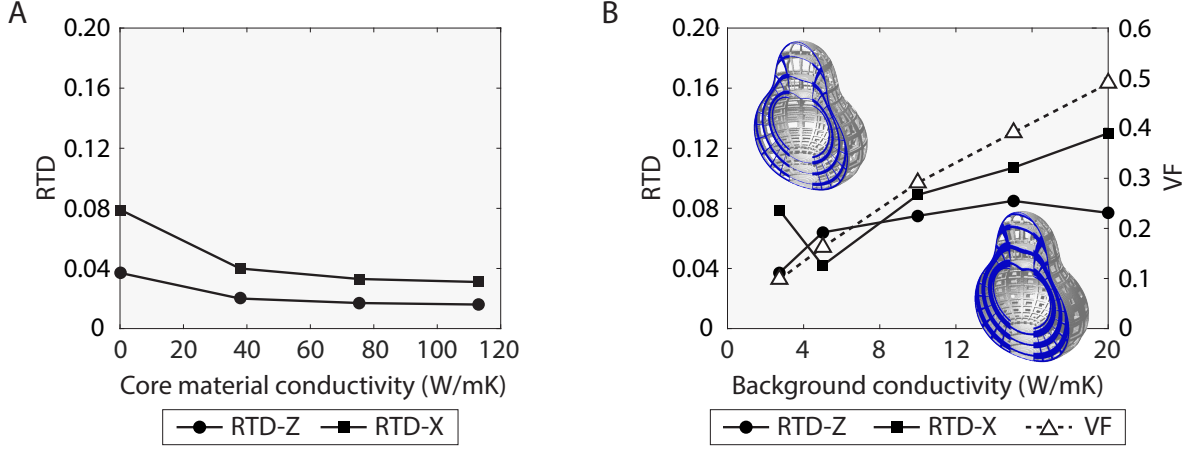


Figure 8: Parametric study of the pear-apple cloak. A) RTD values v.s. core material's conductivity; B) RTD and Material A's volume fraction v.s. background material's conductivity.

symmetry to reduce computational cost. For the surfaces of revolution, we use a quarter of the full domain, discretized with a $288 \times 288 \times 576$ structured FE mesh, and for surfaces with plane symmetry, we use half of the full domain meshed with $240 \times 480 \times 480$ elements. The symmetric planes are adiabatic. The element type is the 8-node first-order trilinear brick element. The resulting linear system is solved using a multigrid-preconditioned conjugate gradient solver [20, 21, 22] with five or six grid levels. The tolerance for the relative residual is 10^{-8} . The computational time of solving the linear system on a desktop workstation (AMD Ryzen Threadripper 3970X 32-Core Processor 3.69 GHz, 256 GB RAM) is about 4 - 6 minutes.

As a complementary analysis of the FE result in the main text Figure 1, Figure 7 B shows the temperature and heat flux distribution from a top plane view at $0.43H$ under the X-direction applied heat. The main features of cloaking remain: the isotherms in the background are uniform and straight, and the temperature gradient and heat flux at the core are diminished.

9.2 Performance measures: relative temperature difference (RTD)

We adopt the RTD to evaluate the cloaks' performance quantitatively. The RTD measures the relative difference between the background temperature and the reference (linear) temperature and is adopted in other studies on 2D thermal meta-devices [19, 10]. Its definition is

$$RTD = \sqrt{\frac{\sum_{j \in \Omega_{bg}} (T_j - T_{ref,j})^2}{\sum_{j \in \Omega_{bg}} (T_{bare,j} - T_{ref,j})^2}} \quad (33)$$

where T_j denotes the nodal temperature of the j th node, $T_{ref,j}$ is reference temperature at the same location, which is known explicitly, $T_{bare,j}$ the background temperature of the bare case, with only the core object and the background material, and Ω_{bg} denotes the background region. The $RTD = 0$ for an ideal cloak, and $RTD = 1$ for the bare case.

10 Complementary parametric study

We perform several parametric studies of the pear-apple cloak using FEA.

10.1 Change of core material

The cloaks' performance is insensitive to the change of core materials. As shown in Figure 8A, the RTD values of the pear-apple cloak under Z- and X-direction applied heat decrease as the core material's thermal conductivity increases from $0.16 \text{ Wm}^{-1}\text{K}^{-1}$ (PDMS) to $113 \text{ Wm}^{-1}\text{K}^{-1}$ (AlSi10Mg), hence demonstrating a high degree of robustness.

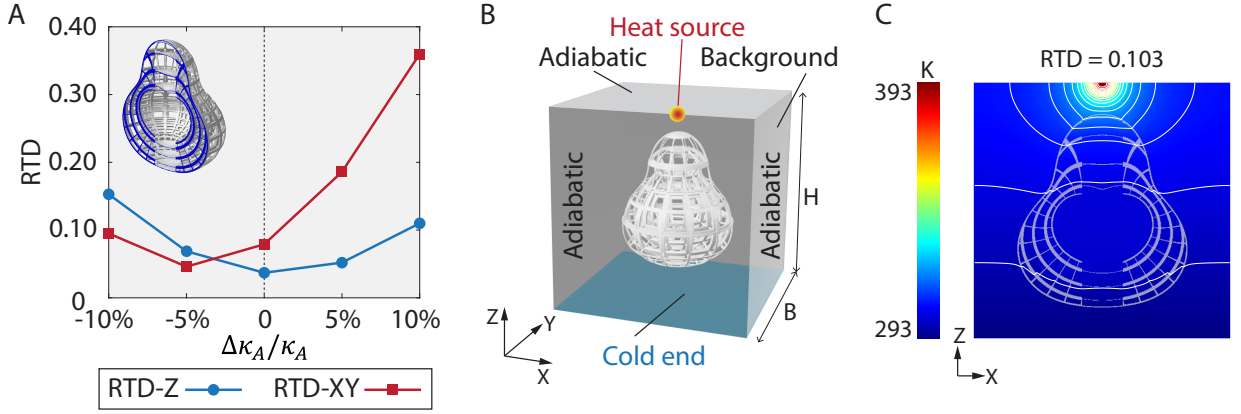


Figure 9: Sensitivity of cloaking performance to material property fluctuation and non-uniform background temperature. A) RTD values in Z and X-Y directions corresponding to various κ_A perturbations; B) FEA setup with heat source; C) temperature distribution of mid-X-Z plane under applied heat source.

10.2 Change of background material

The proposed method can generate good cloaking performance for different backgrounds. As shown in Figure 8B, the cloaks obtained with different background κ_0 ranging from $2.72 \text{ Wm}^{-1}\text{K}^{-1}$ (encapsulant) to $20 \text{ Wm}^{-1}\text{K}^{-1}$ consistently show small RTD values. The increase in κ_0 leads to a larger required κ , which in turn results in an increase in Material A's volume fraction (VF). The relation between κ_0 and VF appears to be largely linear as shown in Figure 8B.

10.3 Performance with heat source in the background

The 3D cloak also performs well with the presence of a point heat source in the background. We demonstrate this by FEA with a concentrated heat source placed near the top of the pear-apple cloak, as shown in Figure 9B. For boundary conditions, the bottom face of the domain is set to a constant temperature, while the other five faces are adiabatic. The heat generated at the top will travel through the domain and reach the cold end at the bottom. The resulting temperature distribution of the X-Z mid-plane is shown in Figure 9C, overlaid with the 3D cloak. The RTD value measuring the relative difference between the temperature and that of the homogeneous background is 0.103, an overall satisfactory performance. This demonstrates the consistent cloaking performance under a non-uniform background temperature caused by a heat source.

10.4 Sensitivity to material property fluctuations

In practice, material properties can deviate from their designed values due to, for example, manufacturing inconsistencies or aging. In the current context of thermal cloak, the conductivities of AlSi10Mg and PDMS can differ from their nominal values. Here, we investigate the influence of such fluctuation on the cloaking performance (RTD values) under $\pm 5\%$ and $\pm 10\%$ variation in κ_A . For Material B (PDMS), as its κ_B is three orders of magnitude smaller than κ_A , its limited variation should not cause a huge change in RTD values.

The RTD values of the pear-apple cloak under the perturbation of κ_A are shown in Figure 9A. The RTD-Z is relatively insensitive to material's fluctuation, and all values within 10% of property change are below 0.16. In contrast, the RTD-XY values are more sensitive when κ_A increases, reaching a value of 0.36 at 10% increase. The sensitivity to material property variation, however, is generally case- and design-dependent.

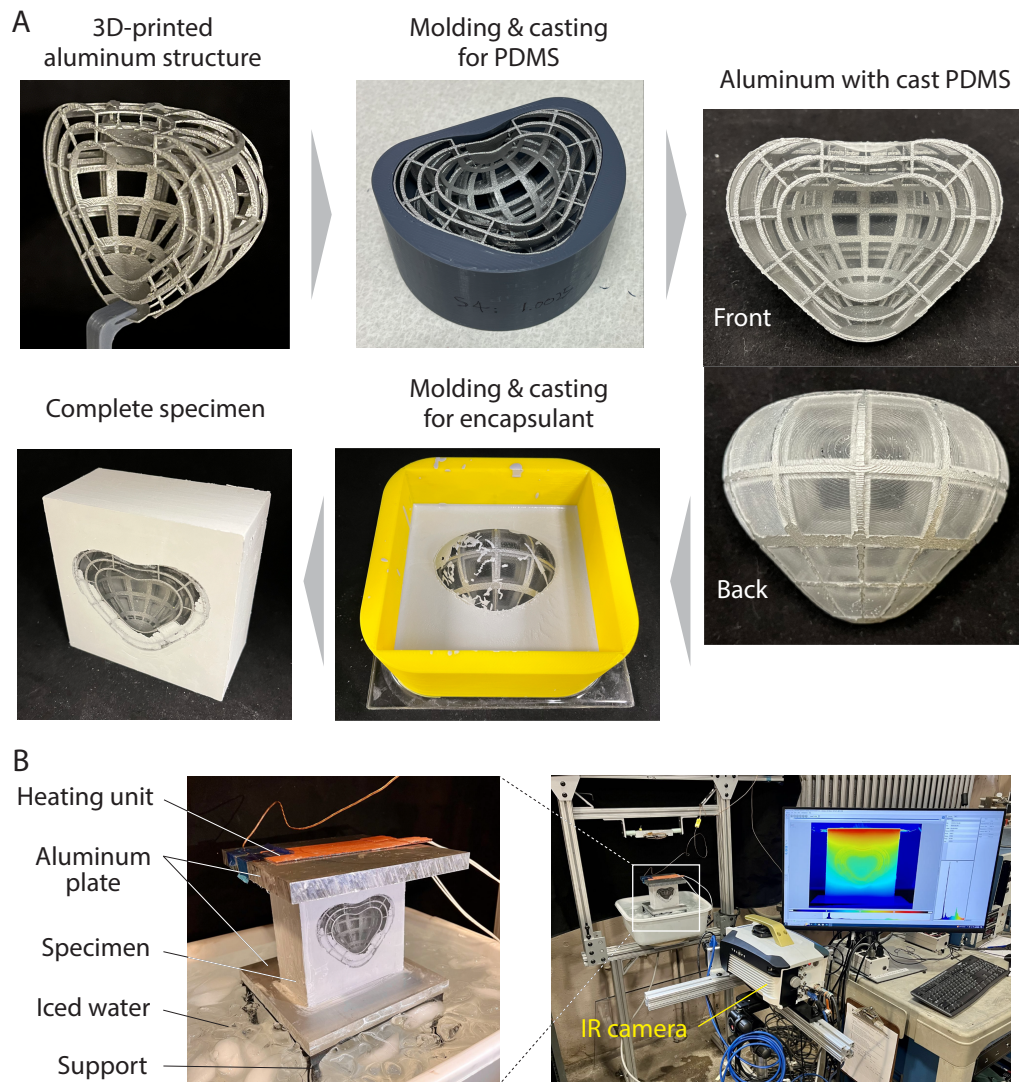


Figure 10: Fabrication and experimental setup of 3D thermal cloak. A) Molding and casting for the fabrication of the specimen; B) experimental setup for thermal conduction.

11 Fabrication and experimental setup

Thanks to the plane symmetry of the cloaks, we fabricate half of the cloak structure and the background following the procedure shown in Figure 10 A. The aluminum lattice of the cloak is 3D-printed using Direct Metal Laser Sintering (Protolab Inc.). It is then placed into a 3D-printed polylactide (PLA) mold and cast with the PDMS. After casting, the setup is degassed for 2 hours under a -0.8 atmosphere pressure to remove the bubbles, and then it is cured in the oven for 12 hours at 40 C°. The lattice-PDMS composite is then placed into a second PLA mold to cast the background material (thermal encapsulant). After casting, the specimen is cured for another 12 hours at 40 C°. As the last step, we cast a 2 mm-thick layer of PDMS on the specimen’s four side surfaces (not on the hot and cold ends) to better represent the adiabatic boundary condition.

For testing, we use the setup shown in Figure 10 B, which is similar to that in [23]. The hot end of the specimen is realized by electric heating with a specified temperature of 40 degrees Celsius, and the cold end is realized by a tank of iced water at the bottom. Both ends have aluminum plates to ensure smooth heat paths and good thermal contact with the relatively soft background encapsulant. An infrared camera (Telops FAST M100hd) is used to capture the temperature distribution. The reported temperature in the main text is recorded after 60 minutes when the heat conduction reaches the steady state.

12 Discussions on practical application aspects

Here, we provide some perspectives on the practical application aspects of the cloak, including the range of operational temperature, influence of interfacial thermal resistance, and transient performance.

12.1 Range of operational temperature

In general, materials’ properties (such as thermal conductivity, mechanical stiffness, and chemical stability) are temperature-dependent, which may impact the cloak’s performance under different operational temperatures. For our realization with AlSi10Mg and PDMS, the thermal conductivity of AlSi10Mg remains relatively stable when the temperature is below 150 C° [24]. For PDMS, as its conductivity is about 0.1% of the conductivity of AlSi10Mg, the variation should not greatly impact the overall cloaking performance. The chemically stable temperature for PDMS is below 200 C°. Hence, the operational temperature for the current realization of 3D cloak shall be lower than 150 C°. An operational temperature higher than this value may require a change of the base materials, to which the proposed design method is also directly applicable.

12.2 Potential influence of interfacial thermal resistance

Interfacial thermal resistance between the aluminum and PDMS parts may arise, but its impact on the overall cloaking performance appears to be limited, as the experimental temperature distribution across the two materials is, by and large, smooth and gradual (Figure 11 A), without the sharp changes that typically signify strong interfacial resistance. This observation, however, may not be generalizable to other materials and setups. Numerical and experimental investigations into the influence of interfacial resistance on the performance of thermal meta-devices would be a valuable future investigation.

12.3 Transient performance and estimate of characteristic time scale

In principle, a steady-state thermal cloak cannot conceal an object perfectly from transient thermal detection because transient heat manipulation requires the accurate realization of material density and specific heat capacity, in addition to conductivity [25]. This would pose a greater challenge for engineering compared to the steady-state cloaking.

Another important aspect of the transient behavior is the estimate of the characteristic time to reach steady state. Here, we use the pear-apple cloak to provide an approximate analysis based on the composite’s material properties and show that it qualitatively matches our experimental observation. The specific heat (per unit volume) for AlSi10Mg and PDMS are $\rho_{AcA} = 2.46 \text{ Jcm}^{-3}\text{K}^{-1}$ and $\rho_{BcB} = 1.46 \text{ Jcm}^{-3}\text{K}^{-1}$, respectively. The volume fraction of AlSi10Mg for the pear-apple cloak averaged over the shell domain is 0.004. Using the rule of mixture, the volume-averaged specific heat per unit volume

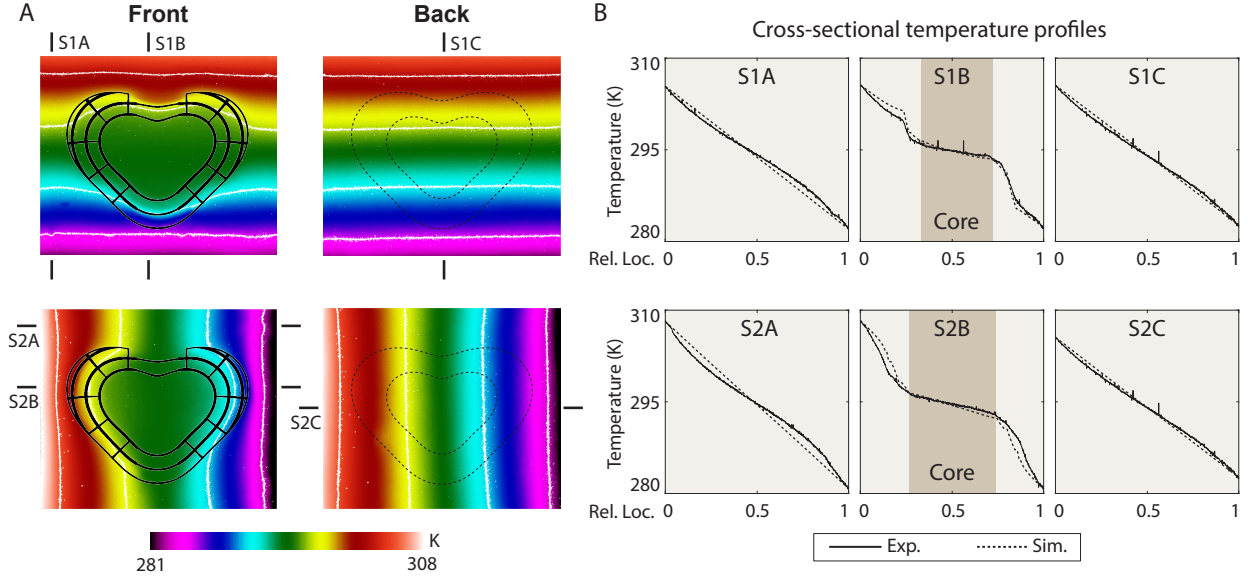


Figure 11: Experimental result of heart-shaped cloak. A) Experimental temperature distribution under Z- and X-direction applied heat on the front and back surfaces; B) experimental cross-sectional temperature profiles and their simulation counterparts.

is $\bar{\rho c} = 1.46 \text{ Jcm}^{-3}\text{K}^{-1}$. For thermal conductivity of the pear-apple cloak, we take the mean of the three eigenvalues and average it over the shell domain, leading to $\bar{\kappa} = 3.92 \text{ Wm}^{-1}\text{K}^{-1}$. The resulting averaged thermal diffusivity is $\bar{\beta} = 2.68 \text{ mm}^2\text{s}^{-1}$. For the pear-apple cloak, the characteristic length (height of the cloaking structure) is $L = 78 \text{ mm}$, and hence the characteristic time is $\tau = L^2/\bar{\beta} = 38 \text{ mins}$, which qualitatively matches well with our experimental observation of 50-60 mins for entering the steady state. Additionally, the formula of the characteristic time shows a quadratic scaling with characteristic length and inverse scaling with diffusivity.

13 Experimental result of heart-shaped cloak

This section provides a more detailed discussion of the experimental results of the heart-shaped cloak. The 3D omnidirectional thermal cloaking is experimentally reproduced. As shown in Figure 11 A, the isotherms in the background of the front face remain largely uniform under both Z- and X-direction applied heat, and the temperature gradient at the core is close to zero. On the back face, the isotherms are also uniform and straight as in the homogeneous medium case, which is a direct display of 3D thermal cloaking. The cross-sectional temperature profiles at S1A, S1B, S1C, S2A, S2B, and S2C are shown in Figure 11 B. The front face's background profiles (S1A and S2A) are close to a straight line, indicating a constant thermal gradient and heat flux. The profiles crossing the cloak and core (S1B and S2B) show a clear plateau at the core with diminished gradient. The profiles on the back face are also close to a straight line that represents a constant heat flux. All six experimental temperature profiles match well with the simulation result, thereby validating the proposed 3D de-homogenization approach.

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