Differentiable Phonon Simulations To Optimize Thermal Transport in Nanostructures

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Abstract

We introduce a methodology for large-scale optimization of non-Fourier thermal transport in nanostructures, based upon the forward and adjoint phonon Boltzmann transport equation (BTE) and density-based topology optimization. To this end, we also develop the transmission interpolation model (TIM), an interface-based method that allows for smooth interpolation between void and solid regions. We first use our approach to tailor the effective thermal conductivity tensor of a periodic nanomaterial; then, we maximize classical phonon size effects under constrained diffusive transport, obtaining more than a four-fold degradation in the thermal conductivity with respect to commonly-employed configurations. Our method enables systematic optimization of materials for heat management and conversion, and, more broadly, the design of devices where diffusive transport is not valid.

Keywords: Thermal transport, nanostructures, inverse design

1. Introduction

Tuning thermal transport at the nanoscale is crucial to many applications, such as thermal dissipation and thermoelectrics \cite{1,2}. However, heat-conduction optimization in nanostructures remains challenging: Fourier’s law breaks down \cite{3}, heat transport becomes nonlocal, and standard topology-optimization methods \cite{4} for diffusive theories \cite{5,6,7} are not readily appli-
cable. We fill this gap by solving the adjoint phonon Boltzmann transport equation (BTE) in the context of density-based topology optimization. A key component of our result is a new “transmission interpolation method” (TIM) (Sec. 3) to allow continuously varying the local material “density” by relating the density parameter to interfacial heat transport, in contrast to more straightforward approaches [8] that do not recover the correct boundary condition for the hard-wall case. The forward (Sec. 2) and adjoint BTE (Sec. 5) solvers are chained into a reverse-mode automatic differentiation pipeline [9], which also includes density filtering and projection [10] (Sec. 4). We apply our methodology to obtain new solutions to two exemplary problems: designing an anisotropic thermal-conductivity tensor in a periodic nanomaterial (Sec. 6) and, for thermoelectric applications [11], minimizing thermal transport while simultaneously maintaining high electrical conductivity (Sec. 7). (To the latter end, we assume charge transport to be diffusive and thus implement a differentiable Fourier solver.) Several technical aspects, including the preconditioned, matrix-free solution of the BTE solvers, are reported in the Appendices. The code developed for this work will be released in the OpenBTE package [12].

Nondiffusive thermal transport has been investigated from both theoretical [13, 14] and experimental [15, 16, 17] standpoints. The growth of nondiffusive phonons has opened up exciting engineering opportunities, but it has also made modeling heat transport computationally challenging. One key departure from familiar Fourier diffusion is that phonons must be tracked in momentum as well as position space, dramatically increasing the number of unknowns [13]. If forward modeling is challenging, inverse design is even more difficult. To date, there have only been a few studies aiming at optimizing nanoscale thermal transport [18, 19], and they have mostly been based on gradient-free approaches that cannot handle large parameter spaces [20].

In the simpler diffusive regime, large-scale topology optimization has been routinely applied to macroscopic heat-transport problems [5, 21, 7]. The basic idea of density-based topology optimization [10] is that each point in space, or each “pixel” in a discretized solver, is linked to a fictitious density \( \rho(\mathbf{r}) \) which is continuously varied between 0 and 1, representing two physical materials at the extremes, to optimize some figure of merit such as thermal conductivity. Filtering and projection regularization steps [10] ensure that the structure eventually converges to a physical material everywhere in the design domain, and a variety of methods are available to impose manufacturing constraints such as minimum lengthscales [22, 23]. Adjoint-based
sensitivity analysis allows such huge parameter spaces to be efficiently explored [20], enabling the computational discovery of surprising non-intuitive geometries. For instance, in Ref. 5, a heat-conducting material was designed to generate the least amount of heat under volume constraints. In that work, which mirrored the search for minimum-compliance materials for mechanical problems [24], the material density at each pixel could be directly related to the local bulk thermal conductivity. In contrast, such a local relationship does not hold for the BTE. However, the BTE supports the use of transmission coefficients associated with the interfaces between dissimilar materials [2]. In our work, therefore, we turn these coefficients into intermediate variables linking the material density to the phonon distributions using our TIM approach.

2. The 2D single-MFP BTE

The phonon BTE is an integro-differential equation that describes heat conduction beyond the diffusive regime [2, 25]. By taking into account the phonons’ mean-free-path (MFP) distribution, which is in general anisotropic, it captures the mode-resolved interaction between the geometry and the underlying material [26], a phenomenon commonly known as classical phonon size effects [2]. There are different flavors of the BTE, depending on the needed accuracy. In this work, we use the single-MFP version of the BTE, a textbook-case also known as the gray model [2]; within this approximation, a bulk material is simply parameterized by its thermal conductivity \( \kappa \) and MFP \( \Lambda \). Furthermore, we consider two-dimensional (2D) transport, i.e. phonon directions are parameterized by the polar angle \( \phi \). With these assumptions, the gray BTE reads as

\[
\Lambda \hat{s}(\phi) \cdot \nabla \Delta T(r, \phi) + \Delta T(r, \phi) = \frac{1}{2\pi} \int_{0}^{2\pi} \Delta T(r, \phi') d\phi',
\]

where \( \Delta T(r, \phi) \) is the pseudo phonon deviational temperature (in short, “phonon temperatures” throughout the text), the unknown of our problem, and \( \hat{s}(\phi) = \sin \phi \hat{x} + \cos \phi \hat{y} \) is the phonon direction. Note that the BTE is often formulated in terms of distribution functions or energy density [2, 27, 28]. The temperature formulation used here is simply obtained by a change of variables [29]. Lastly, the angular-resolved heat flux is given by

\[
J(r, \phi) = \frac{2 \kappa}{\Lambda} \Delta T(r, \phi) \hat{s}(\phi).
\]
Although here we employ a simplified version of the BTE, the developed methodology can be readily applied to more sophisticated versions (see sec. 6).

We are interested in computing the effective thermal conductivity tensor \( \kappa \) of a periodic nanostructure. To this end, we consider a simulation domain composed of a square with side \( L \), to which periodic boundary conditions are applied along both axes (see Fig. 1-a); furthermore, we apply a temperature jump, \( \Delta T_{\text{ext}} \), across, e.g., the \( x \)-axis. Then, once Eq. 1 is solved, we collect heat flux along the same axis and use Fourier’s law to estimate \( \kappa_{xx} \),

\[
\kappa_{xx} = -\frac{1}{\Delta T_{\text{ext}} L} \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^1 dl J(r(l), \phi) \cdot \hat{n},
\]

(3)

where \( r(l) = L/2\hat{x} + (l/L - L/2)\hat{y} \). Similarly, \( \kappa_{yy} \) is evaluated by applying a temperature gradient along the \( y \)-axis. In Sec. 6, we will describe the boundary conditions used to account for phonon transport in arbitrary material distribution. Throughout this work we use \( \Lambda = L \); furthermore, since we are interested in the normalized tensor \( \bar{\kappa} = \kappa/\kappa_{\text{bulk}} \), the bulk thermal conductivity (thanks to linearity) does not need to be specified.

3. Material Interpolation

Density-based topology optimization requires a differentiable transition between two or more materials [10], in our case between a hard wall and no interface at all. That is, one must be able to deal with arbitrary material distributions described by a fictitious density \( \rho \in [0, 1]^N \), where \( N \) is the number of “pixels” (design degrees of freedom) in the material [30]. An early study [8] investigated material interpolation in composite materials by defining the mean free path (MFP) \( \Lambda \) to be a smooth function, \( \Lambda^{-1}(\rho) \), that interpolates intermediate values from \( \Lambda_1^{-1} \) to \( \Lambda_2^{-2} \). While this approach successfully recovers the imaginary-interface limit, it may be problematic in our case for two reasons. First, in our systems, one phase is air (radiation is neglected), for which it is not possible to associate an MFP; secondly, MFP-based interpolation does not recover the diffuse boundary condition for the hard-wall case. To lift these limitations, we attack the problem from a different angle: we parameterize the material density via a transmission coefficient \( t \). In doing so, we borrow a methodology developed for thermal transport across dissimilar materials, where the transmission coefficient is used to impose the distributions leaving the interface [31]. Let us now adapt this concept to our scenario. Following the convention in Fig. 1-b, let us
assume we have an interface with normal \( \hat{n} \) pointing along \( \hat{x} \). Furthermore, let us define a generic point on the left (right) side of the interface with \( r^- \) (\( r^+ \)); similarly, we define the material density \( \rho(r^-) [\rho(r^+)] \) at the left (right) side of the interface; lastly, let us group phonons into those with polar angle \( \phi^+ : \hat{s}(\phi) \cdot \hat{n} \geq 0 \) and \( \phi^- : \hat{s}(\phi) \cdot \hat{n} < 0 \). Then, we define the boundary condition

\[
\Delta T(r^-, \phi^-) = t\Delta T(r^+, \phi^-) + (1 - t)\Delta T^B(r^-),
\]

where

\[
\Delta T^B(r^-) = \frac{\int_{\Omega^+} \Delta T(r^-, \phi)\hat{s}(\phi) \cdot \hat{n} d\phi}{\int_{\Omega^+} \hat{s}(\phi) \cdot \hat{n} d\phi}
\]

is the boundary temperature, computed assuming isotropic reflection [13, 32], and \( \Omega^+ \) spans \( \phi^+ \). At this point, we are left with the task of relating \( t \) to the material density. To this end, we define the following interpolation

\[
t = \frac{2\rho(r^-)\rho(r^+)}{\rho(r^-) + \rho(r^+)}.
\]

with \( \gamma \) a tuning parameter. It is straightforward to show that if either \( \rho(r^-) \) or \( \rho(r^+) \) is zero, then the RHS of Eq. 4 reduces to the hard-wall case. On the other side, if \( \rho(r^-) = \rho(r^+) = 1 \), there will be no interface. In light of this discussion, we note that a variation in the material density does not alter a bulk-like physical property, but rather the amount of incoming flux. To distinguish this approach from traditional material interpolation methods, we name it the “Transmission Interpolation Method” (TIM). The discretized version of TIM is described in Appendix B.
4. The three-field approach

Density-based topology optimization presents two major challenges: the emergence of rapidly oscillating “checkerboard” patterns that fail to converge with increasing spatial resolution; and gray ($0 < \rho < 1$) pixels, to which no physical material can be associated \[4\]. These two issues are commonly resolved using filtering and projection, respectively \[10\]. As shown in Fig. 2a, given a design density $\rho$ (for convenience, from now on, we will work with a discretized domain), we first filter it, $\tilde{\rho} = w * \rho$, where, in this case, $w$ is a conic filter with radius $R$,

$$w_i = \begin{cases} \frac{1}{a} \left( 1 - \frac{|\bar{c}_i|}{R} \right), & |\bar{r}| < R \\ 0, & \text{otherwise}; \end{cases}$$

(7)

In Eq. 7, $a$ is a normalization factor ($= \pi R^2 / 3$ in the continuum limit), $\bar{c}_i$ is the centroid of the grid point $i$, and $R$ is the radius of our filter. Then, projection, $\hat{\rho} = f_p(\tilde{\rho})$, is carried out using the following thresholding function \[33\]

$$\hat{\rho} = \frac{\tanh \beta \eta + \tanh(\beta(\tilde{\rho} - \eta))}{\tanh \beta \eta + \tanh(\beta(1 - \eta))},$$

(8)

where $\eta$ and $\beta$ are threshold parameters. The projected field is, therefore, used directly by the BTE solver; in this work, we use $\eta = 0.5$; the term $\beta$, on the other side, is increased during the optimization procedure \[34\], in order to guarantee a good degree of topology variability (especially early on in the optimization process) while ensuring a final binary structure.

5. Gradient of the BTE solver

In this work we are interested in minimizing cost functions that depend on the effective thermal conductivity, i.e. a scalar function of $\Delta T$ and $\rho$; its expression, derived in Appendix B, is compactly rewritten as

$$\bar{\kappa} = \sum_{\mu c} S_{\mu c}(\bar{\rho}) \Delta T_{\mu c}.$$  

(9)

For optimization purposes, we thus need the sensitivity of $\bar{\kappa}$ with respect to $\rho$. Using the chain rule, we have

$$\frac{\partial \bar{\kappa}}{\partial \rho_p} = \sum_{\mu c k} \frac{\partial \bar{\kappa}}{\partial \Delta T_{\mu c}} \frac{\partial \Delta T_{\mu c}}{\partial \bar{\rho}_k} \frac{\partial \bar{\rho}_k}{\partial \rho_p} + \sum_k \frac{\partial \bar{\kappa}}{\partial \bar{\rho}_k} \frac{\partial \bar{\rho}_k}{\partial \rho_p},$$

(10)
which is evaluated using reverse-mode automatic differentiation, implemented in JAX [9]; specifically, we use built-in primitives for all the operations except for the actual BTE solver, for which we explicitly develop the adjoint counterpart. As reported in Appendix B, solving the discretized version of Eq. 1 entails inverting the following matrix linear system

$$\sum_{\mu'c'} G_{\mu c}^{\mu'c'} \Delta T_{\mu'c'} = P_{\mu'c'}.$$  

Upon inverting and differentiating both sides of Eq. 11 with respect to $\rho_p$, and following the standard procedure for adjoint-based methods [35], we have

$$\frac{\partial \Delta T_{\mu c}}{\partial \rho_p} = \left( G^{-1} \right)_{\mu c} \sum_{\mu'c'} C_{\mu'c'p},$$  

where

$$C_{\mu'c'p} = \sum_{\mu''c''} \left( \frac{\partial P_{\mu''c''}}{\partial \rho_p} \delta_{\mu''c''} \Delta T_{\mu''c''} \frac{\partial G_{\mu'c'}^{\mu''c''}}{\partial \rho_p} \right).$$  

can also be computed using built-in primitives. In a reverse-mode AD context, evaluating Eq. 10 amounts to composing vector-Jacobian-products (vJps), thus the inversion of $G$ is never explicitly evaluated; rather, it is
possible to provide the vJp of the BTE solver, i.e.

\[
vJp(v) = \sum_{\mu \epsilon \mu' \epsilon'} v_{\mu c} \left[ G^{-1} \right]^\mu' \epsilon'_{\mu c} C_{\mu' \epsilon' p} = \sum_{\mu' \epsilon'} \Lambda_{\mu \epsilon'} C_{\mu' \epsilon' p}, \tag{14}
\]

where the matrix \( \Lambda_{\mu c} \) is the solution of the matrix linear system

\[
\sum_{\mu' \epsilon'} G^\mu' \epsilon'_{\mu c} \Lambda_{\mu' \epsilon'} = v_{\mu c}, \tag{15}
\]

that is, as expected, the adjoint of the original problem. In this case, the AD framework passes \( v_{\mu c} = \partial \kappa / \partial \Delta T_{\mu c} \) into the vJp defined in Eq. 14. To summarize, at each iteration of the optimizer, obtaining \( \bar{\kappa} \) and its sensitivity to \( \rho \) takes the following steps

1. Obtain \( \rho \) from the optimizer.
2. Apply filtering and projection, i.e. \( \rho \rightarrow \hat{\rho} \rightarrow \bar{\rho} \).
3. Solve the forward problem (Eq. 11), and obtain \( \Delta \bar{T}_{\mu c} \). During this step, the function vJp from Eq. 14 is also provided (but it is not computed since we are still in the forward pass and don’t have \( v \) yet).
4. Compute \( \bar{\kappa} \) using Eq. 9.
5. The reverse-mode AD library automatically invokes the backward pass to evaluate the vJp for a specific \( v \). In turn, this step entails solving Eq. 15.

A similar procedure applies to the Fourier solver used in Sec. 7. The procedure outlined above allows for the definition of generic cost functions that depend on \( \Delta T \) and \( \rho \), while relying on built-in primitives for reverse-mode AD. However, for the sake of computational efficiency, we also manually evaluate Eq. 13, \( \partial \kappa / \partial \Delta T_{\mu c} \), and \( \partial \bar{\kappa} / \partial \bar{\rho}_p \). The corresponding expressions are reported in Appendix D. In this case, we must provide vJp(\( a \)) = \( a \partial \kappa / \partial \bar{\rho}_p \), where the input vector is simply a scalar. In practice, however, we provide the Jacobian–vector product (Jvp) Jvp(\( v \)) = \( [\nabla \rho \kappa]^T \cdot v \), and JAX transposes it automatically.

6. Case I: Tailoring the Effective Thermal Conductivity Tensor

Thermal anisotropy may be induced by boundary engineering, even though the base material is isotropic. Symmetry-breaking boundaries are effective at all scales, although it has been shown numerically that nanostructuring may
enhance anisotropy with respect to the macroscopic counterpart [36]. In this section, we show an example of how topology optimization may be employed to design a material with a prescribed anisotropic effective thermal conductivity tensor, $\tilde{\kappa}$. In this example, we seek a configuration with $\tilde{\kappa}_{xx} = 0.3$ and $\tilde{\kappa}_{yy} = 0.1$, with associated anisotropy of $\tilde{\kappa}_{xx}/\tilde{\kappa}_{yy} = 3$. Furthermore, we constrained the solution to porosity $\tilde{\phi} > 0.25$. To this end, we define the objective function

$$g(\rho) = \|\tilde{\kappa}(\rho) - \tilde{\kappa}\|_{\text{Fro}} = \sqrt{\Delta\kappa_{xx}(\rho)^2 + \Delta\kappa_{yy}(\rho)^2},$$

where $\|\cdot\|_{\text{Fro}}$ is the Frobenius norm, and $\Delta\kappa_{ii}(\rho) = \tilde{\kappa}_{ii}(\rho) - \tilde{\kappa}_{ii}$. The effective thermal conductivity tensor,

$$\tilde{\kappa}(\rho) = \begin{pmatrix} \tilde{\kappa}_{xx}(\rho) & 0 \\ 0 & \tilde{\kappa}_{yy}(\rho) \end{pmatrix}$$

is evaluated by using Eq. 1, for each perturbation direction, after filtering and projecting. The sensitivity of the objective function is

$$\nabla_\rho g(\rho) = g(\rho)^{-1} [\Delta\kappa_{xx}(\rho) \nabla_\rho \tilde{\kappa}_{xx}(\rho) + \Delta\kappa_{yy}(\rho) \nabla_\rho \tilde{\kappa}_{yy}(\rho)],$$

where the terms $\nabla_\rho \tilde{\kappa}_{ii}(\rho)$ are computed using Eq. 10. The above discussion allows us to lay out the optimization algorithm

$$\min_\rho g(\rho) \quad 0 \leq \rho \leq 1$$

s.t. $\sum_n \tilde{\rho}_n \geq 0.25N^2,$

$$\sum_n \tilde{\rho}_n \geq 0.25N^2,$$
where $N^2 = 60 \times 60$ is the number of pixels. As the optimizer, we use an open-source implementation [37] of the method of moving asymptotes (MMA) [38], which converges globally (i.e., it guarantees to find a local minimum from every starting point). Following the approach outlined in [34], we increase $\beta$ during the optimization algorithm; in this case, we start with $\beta = 2$ and double it every 20 iterations, reaching a convergence within 100 iterations. The radius of the conic filter’s kernel is $R = L/10$. The first guess is simply a random structure with four-fold symmetry. The final structure, shown in Fig. 4-a, is made by two concatenated types of pores, which block heat along $y$ more effectively than along $x$. This effect is exemplified by the magnitude of thermal flux shown in Fig. 4-b and Fig. 4-c, for $\bar{\kappa}_{xx}$ and $\bar{\kappa}_{yy}$, respectively. Note that the final values obtained with Fourier’s law are $\bar{\kappa}_{xx}^F \approx 0.61$ and $\bar{\kappa}_{yy}^F \approx 0.46$, with anisotropy 1.33, well below the prescribed value.
7. Case II: Maximixing Phonon Scattering

In thermoelectric applications it is desirable to minimize thermal transport while not degrading the electrical conductivity \( \sigma \). In fact, the thermoelectric figure-of-merit is given by \( ZT = TS^2 \sigma / \kappa \), where \( S \) is the Seebeck coefficient. In highly-doped semiconducting nanostructures, these conditions can be met simultaneously due to the short phonon MFP compared to that of the electrons [14, 39]. If the MFPs of the electrons are much shorter than the material’s characteristic length, we may assume diffusive electronic transport. Consequently, minimizing the thermal conductivity while maintaining high diffusive transport is beneficial to \( ZT \). Furthermore, in order to understand phonon scattering, most studies focus on the value of the effective thermal conductivity compared to that obtained with Fourier’s law [40, 41]. In passing, we note that macroscopic geometrical effects, often referred to as “porosity factor” [42], in some cases have analytical solutions. For example, in aligned porous systems with circular pores and porosity \( \varphi \), it has the analytical solution \( \bar{\kappa}^F = (1 - \varphi) / (1 + \varphi) \) [43].

To assess the effectiveness of our method, we choose as baseline a porous material with staggered pores of circular shape, as shown in Fig. 5-a. This configuration has a smaller \( \bar{\kappa} \) than that of systems with a square lattice of pores (provided the porosity is the same) because of the vanishing “view factor” [44, 17, 45]. For this reason, such a configuration is often preferred. We choose a porosity of \( \varphi = 0.5 \), to which it corresponds the isotropic tensors \( \bar{\kappa}^F \approx 0.31 \) and \( \bar{\kappa} \approx 0.049 \). The goal of our optimization is, therefore, to achieve \( \bar{\kappa} < 0.049 \) under the constraint \( \bar{\kappa}^F \geq 0.31 \); furthermore, we require \( \bar{\kappa} \) to be isotropic. We use this baseline configuration as a first guess for our optimization algorithm, solving the problem:

\[
\min_{\rho} g(\rho) \quad \text{subject to} \quad 0 \leq \rho \leq 1
\]

\[
\text{s.t. } \bar{\kappa}_{xx}^F(\rho) \geq 0.31
\]

\[
\text{s.t. } \bar{\kappa}_{yy}^F(\rho) \geq 0.31,
\]

where

\[
g(\rho) = \frac{1}{\sqrt{2}} \sqrt{(\bar{\kappa}_{xx} - \bar{\kappa}_{yy})^2 + \bar{\kappa}_{xx}^2 + \bar{\kappa}_{yy}^2} = \sqrt{\bar{\kappa}_{xx}^2 + \bar{\kappa}_{yy}^2 - \bar{\kappa}_{xx}\bar{\kappa}_{yy}},
\]

is the cost function to be minimized. We run this optimization problem with conic filter radius \( R = L/10 \), and \( \beta \) doubling every 20 iterations starting...
from 2. Convergence is reached in 200 iterations, as shown in Fig. 5-e. Remarkably, the optimized structure, shown in Fig. 5-b, has an isotropic tensor of $\bar{\kappa} \approx 0.011$, roughly 4.25 times smaller than that of the baseline; yet, $\bar{\kappa}^F$ is right above the imposed constrain. The final porosity is 0.63. We point out the presence of small pores that are one or two pixels in size; to realize a structure that is more amenable from a manufacturing standpoint, we fill these small regions with solid phase, while making sure that the performance is not degraded (both $\bar{\kappa}$ and $\bar{\kappa}^F$ are within 1% of those of the unpolished structure). The polished configuration is shown in Fig. 5-d. In passing, we note that it is possible to impose minimum-linewidth and minimum-linespacing conditions by adding differentiable inequality constraints to the optimization algorithm [34, 22], and in the future we plan to optimize the design for specific manufacturing processes in this way.

The optimized structure can be analyzed either from the void or the solid regions’ point of view. In the former case, we have staggered pores with smaller void regions in between. More interestingly, from the solid regions’ perspective we note a regular pattern of islands interconnected via three thin bridges on four opposite sides. As shown in Fig. 5-c and as a consequence of energy conservation, heat flux peaks over these connections. The emergence of such a topology can be analyzed in terms of transport across a single orifice of width $a$. This problem was first investigated by Maxwell [46] in the diffusive regime, showing that the thermal resistance is proportional to $1/a$; on the other side, Sharvin [47] predicted that in the ballistic regime, i.e. for $\Lambda << a$ (such as in our case), the resistance goes as $\Lambda/a$. Thus, it is clear that thin channels are a promising platform for decoupling diffusive and nondiffusive transport. Both the abovementioned approximations assume infinite leads. A very recent study [48], however, investigates heat transport across a single Si-based orifice using the BTE within a Monte-Carlo framework, revealing a significant role of the geometry of the orifice and leads (i.e. the structures attached to the two ends of the channel) on the overall thermal resistance. Our optimization approach, therefore, automatically identifies a structure featuring orifices, while concurrently optimizing the geometries of the leads.

8. Conclusions

In this work, we develop a first-of-its-kind tool: a differentiable phonon transport simulator that is able to efficiently calculate the gradient of the
effective thermal conductivity tensor of a periodic nanomaterial with respect to every pixel of the material density. This tool is built on several key innovations, including an adjoint formulation and implementation of the phonon BTE and a novel material-interpolation method to be used in a density-based topology optimization setting. We first apply our methodology to tailoring the effective thermal conductivity tensor of a nanomaterial, with potential application in thermal management and routing. Then, we maximize classical size effects while keeping the diffusive transport above a certain threshold, achieving a four-fold improvement with respect to commonly studied staggered configurations. The latter result may have an impact on thermoelectric materials, as explained in the previous section.

While we have employed a single-MFP model, the developed methodology, along with the interpolation material models, can be readily applied to more sophisticated versions of the BTE. Possible future directions include employing the BTE in the relaxation-time-approximation (RTA) [13]. Specifically, using the recently-developed anisotropic MFP-BTE [26] would allow
one to model a real material using first-principles calculations while taking into account the interplay of phonon-focusing effects and, for example, the possible channels arising during optimization. Another possible extension includes optimizing thermal transport in 2D materials described by the full-scattering operator [49, 50].

9. Conflict of interest

The authors declare that they have no conflict of interest.

10. Replication of results

The code developed for this work will be made available as free/open-source software in the next release of OpenBTE [12].

11. Acknowledgement

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Appendix A. Discretization

For spatial discretization, we use a Cartesian grid with \( N = 60 \times 60 \) pixels and size \( L \). Conveniently, we define the following quantities:

\[
\hat{n}_{cc'} = \begin{cases} 
\text{normal pointing to } c', & \text{if } c \text{ and } c' \text{ are adjacent (including periodicity)} \\
0, & \text{otherwise},
\end{cases}
\]
\[
K_{cc'} = \begin{cases} 
1, & \text{if } c \in \text{ left and } c' \in \text{ right} \\
0, & \text{otherwise.}
\end{cases}
\] (A.1)

where \( \hat{n}_{cc'} \) and \( K \) describe volumes connectivity and external perturbation, respectively. We further define \( H = \Delta T_{\text{ext}} (K - K^T) \). Note that in this section, we assume that a temperature gradient is imposed along the \( x \)-axis. In the next two sections, we will describe the discretization of the BTE and Fourier solvers.
Appendix A.1. The BTE discretization

Equation 1 is first discretized in polar space, which we divide into \( M = 48 \) cells. To this end, we integrate both sides of Eq. 1 over the control angle \( \Delta \phi \) centered at \( \phi_\mu \). Assuming that the unknowns are constant within the single angular cell, we have

\[
S_\mu \cdot \nabla \Delta T_\mu(r) + \Delta T_\mu(r) = \frac{1}{M} \sum_{\mu'} \Delta T_{\mu'}(r), \tag{A.2}
\]

where

\[
S_\mu = \text{sinc} \left( \frac{\Delta \phi}{2} \right) \hat{s}(\phi_\mu). \tag{A.3}
\]

The spatial discretization is carried out using the upwind, finite-volume scheme [51, 52]. Accordingly, the distribution at the interface between the volumes \( c \) and \( c' \) along the direction \( \phi_\mu \) is given by

\[
\Delta T_\mu(r_{cc'}) S_\mu \cdot \hat{n}_{cc'} \approx \Delta T_{\mu c} \text{ReLu}(S_\mu \cdot \hat{n}_{cc'}) + \\
+ \text{ReLu}(-S_\mu \cdot \hat{n}_{cc'}) \left[ t_{cc'} (\Delta T_{\mu' c'} + H_{cc'}) \right] + (1 - t_{cc'}) \Delta T_{B_{cc'}} \tag{A.4}
\]

where \( \text{ReLu}(x) = \max(0, x) \), \( t_{cc'} \) is the discretized transmission coefficient, and

\[
\Delta T_{B_{cc'}} = \frac{\sum_{\mu} \Delta T_{c\mu} \text{ReLu}(S_\mu \cdot \hat{n}_{cc'})}{\sum_{\mu} \text{ReLu}(S_\mu \cdot \hat{n}_{cc'})}. \tag{A.5}
\]

With these definitions at hand, the linear system arising from space and angular discretization is obtained by integrating both sides of Eq. A.2 over the control area \( c \) and applying Gauss’ law,

\[
\sum_{c', \mu'} \left[ \delta_{cc'} \delta_{\mu \mu'} (1 + D_{\mu' c'}) + \delta_{\mu \mu'} A_{\mu' c c'} + \delta_{cc'} \left( B_{c\mu' \mu} - \frac{1}{M} \right) \right] \Delta T_{c' \mu'} = P_{\mu c}. \tag{A.7}
\]
where $\delta_{cc'}$ is the Kronecker delta. The terms in Eq. A.7 are

\begin{align*}
D_{\mu'c'} &= \sum_{c''} g^+_{\mu'c''c'}, \\
A_{\mu cc'} &= t_{cc'} g_{\mu cc'}, \\
P_{\mu c} &= \sum_{c'} H_{cc'} t_{cc'} g_{\mu cc'}, \\
B_{\mu'\mu c} &= \sum_{c''} h^+_{\mu'c''c} (1 - t_{cc''}).
\end{align*}

(A.8)

where

\begin{align*}
g^{- (+)}_{\mu cc'} &= \pm \text{KnReLu}(\pm S_\mu \cdot \hat{n}_{cc'}) \sqrt{N}, \\
h_{\mu'c''} &= g^+_{\mu c'} g^+_{\mu'c''} \left[ \sum_{\mu''} g_{\mu''cc''} \right]^{-1}.
\end{align*}

(A.9)

In Eq. A.9, we define $\text{Kn} = \Lambda/L$ as the Knudsen number. Lastly, the normalized thermal conductivity reads as

\begin{equation}
\bar{\kappa} = -\frac{1}{N\text{Kn}^2 \Delta T_{\text{ext}}} \sum_{\mu cc'} t_{cc'} K_{cc'} \left[ \Delta T_{\mu cc'} g^+_{\mu cc'} + (\Delta T_{\mu cc'} + \Delta T_{\text{ext}}) g^{- cc'} \right]
\end{equation}

(A.10)

Appendix A.2. The Fourier solver

In Sec. 7 we have used the normalized effective thermal conductivity computed by Fourier’s law; its expression is given by

\begin{equation}
\bar{\kappa}^F = -\frac{1}{\kappa_{\text{bulk}} \Delta T_{\text{ext}} L} \int_0^1 dl J(r(l)) \cdot \hat{n},
\end{equation}

(A.11)

where $l$ parameterizes the hot side, and $J(r) = -\kappa(r) \nabla \Delta T(r)$ is the diffusive heat flux. Finally, the temperature is evaluated using the standard steady-state heat conduction equation

\begin{equation}
\nabla \cdot [\kappa(r) \nabla \Delta T(r)] = 0.
\end{equation}

(A.12)

Similarly to the BTE, we use the finite-volume method. Upon integration of Eq. A.12 over the control volume $c$, we have

\begin{equation}
\sum_k \int_{\partial A_c} \kappa_c \frac{\partial \Delta T(r)}{\partial x_k} n_k dl = \frac{L}{\sqrt{N}} \sum_{c'} \kappa_{cc'} \left[ ||\hat{n}_{cc'}|| (\Delta T_{c'} - \Delta T_c) + H_{cc'} \right],
\end{equation}

(A.13)
where $\kappa_{cc'}$ is determined invoking energy conservation. To do so, we write the balance equation at the interface between volume $c$ and $c'$,

$$\frac{L}{\sqrt{N}} \mathbf{J}_{cc'} \cdot \mathbf{n}_{cc'} = -\frac{1}{2} \kappa_c (\Delta T_b - \Delta T_c) = -\frac{1}{2} \kappa_{c'} (\Delta T_{c'} - \Delta T_b),$$  

(A.14)

where $\Delta T_b$ is the temperature at the boundary, shared among both volumes (we assume no thermal boundary resistance), and $\mathbf{J}_{cc'}$ is the interfacial thermal flux. After solving for $\Delta T_b$ (and, for simplicity, assuming we at an internal volume), we have

$$\left(\frac{L}{\sqrt{N}}\right) \mathbf{J}_{cc'} \cdot \mathbf{n}_{cc'} = -\kappa_{cc'} (\Delta T_{c'} - \Delta T_c),$$

where

$$\kappa_{cc'} = \frac{2 \kappa_c \kappa_{c'}}{\kappa_c + \kappa_{c'}}.$$  

(A.15)

In passing, we note that Eq. A.15 is an harmonic average, an approach that has been compared favourably against the arithmetic average, in terms of ability of preventing checkerboard patterns [5]. Equation A.13 translates into the linear system

$$\sum_{cc'} A_{cc'} \Delta T_{c'} = b_c,$$  

(A.16)

where

$$A_{cc'} = \sum_{cc''} \kappa_{cc''} |\mathbf{n}_{cc''}| (\delta_{cc'} - \delta_{c'c''})$$

$$b_c = \sum_{cc''} \kappa_{cc''} H_{cc''}.$$  

(A.17)

Once Eq. A.17 is solved, the effective thermal conductivity is evaluated by

$$\bar{\kappa}^F = \frac{1}{\Delta T_{ext} \kappa_{bulk}} \sum_{cc'} \kappa_{cc'} K_{cc'} [\Delta T_{c'} + \Delta T_{ext} - \Delta T_c].$$  

(A.18)

Given the typically small size of $\mathbf{A}$, we solve this linear system using LU decomposition. Finally, the thermal conductivity is linked to the material density via $\kappa_c = \delta + (\kappa_{bulk} - \delta) \rho_c$, where $\delta$ is a small number introduced to avoid numerical instabilities. Since in density-based topology optimization, physical meaning is needed only for the final binary material distribution, we take the liberty of slightly altering the expression for $\kappa_{cc'}$ into

$$\kappa_{cc'} = \left[\frac{2 \kappa_c \kappa_{c'}}{\kappa_c + \kappa_{c'}}\right]^{\gamma},$$  

(A.19)
with \( \gamma \) being a tuning parameter. In Sec. 7, we use \( \gamma = 3 \), which has been heuristically set to ensure good quality structure and optimization convergence.

**Appendix B. The matrix-free solution of the BTE**

Equation A.7 can be compactly written as

\[
\sum_{\mu'c'} G_{\mu'c'}^{\mu'c} \Delta T_{\mu'c'} = P_{\mu c}, \quad c = 1, \ldots, N - 1, \mu = 1, \ldots, M - 1 \tag{B.1}
\]

and then cast into a standard linear system \( Ax = b \), with \( A \in \mathbb{R}^{NM,NM} \) and \( b \in \mathbb{R}^{NM} \). In practice, we use the matrix-free approach GMRES thus \( A \) is never evaluated. Specifically, we first implement the linear operator \( X \to L(X) \),

\[
L : \mathbb{R}^{NM,NM} \to \mathbb{R}^{NM,NM},
\]

and then we solve the linear system

\[
\bar{L}(x) = b, \tag{B.3}
\]

where

\[
\bar{L} = F \circ L \circ F^{-1} : \mathbb{R}^{NM} \to \mathbb{R}^{NM}
\]

\[
b = F(P). \tag{B.4}
\]

The terms \( F : \mathbb{R}^{N,M} \to \mathbb{R}^{NM} \) and \( F^{-1} : \mathbb{R}^{NM} \to \mathbb{R}^{N,M} \) are the flattening and reshaping operator, respectively. In this work, we use the Jacobi preconditioner, represented by the linear operator

\[
M(X) = \left[ 1 + D_{\mu c} - \frac{1}{M} \right]^{-1} X_{\mu c}, \tag{B.5}
\]

where we used the fact that in Eq. A.7 \( g_{\mu c k}^- g_{\mu' c k}^+ = 0 \) for \( \mu = \mu' \). Similarly to Eq. B.4, we use the flattened version, i.e.

\[
\bar{M} = F \circ M \circ F^{-1} : \mathbb{R}^{NM} \to \mathbb{R}^{NM}. \tag{B.6}
\]

Since \( M \) is related to the diagonal of \( G \) is used for both the forward and backward solver. Lastly, as a first guess to the GMRES solver, we use the solution from the previous optimization iteration.
Appendix C. Gradient of the Fourier solver

Computing the gradient of \( \tilde{\kappa}^F \) with respect to the design field translates into the following chained calculations

\[
\frac{d\tilde{\kappa}^F}{d\rho_p} = \sum_{ij} \left( \frac{\partial \tilde{\kappa}^F}{\partial \Delta T_i} \frac{\partial \Delta T_j}{\partial \rho_i} \right) + \sum_i \tilde{\kappa}^F \frac{\partial \rho_i}{\partial \rho_p}.
\]

(C.1)

Similarly to the BTE case, we employ the “adjoint method”[35], i.e. we differentiate analytically Eq. A.16 and then invert it, obtaining

\[
\frac{\partial \Delta T_c}{\partial \rho_p} = \sum_j \left[ A^{-1} \right]_{cj} C_{jp},
\]

(C.2)

where

\[
C_{jp} = \sum_{c'} \left[ \frac{\partial b_{c'}\delta_{j c'}}{\partial \rho_p} - \Delta T_c' \frac{\partial A_{j c'}}{\partial \rho_p} \right].
\]

(C.3)

Since in our case we are interested in the gradient of a scalar function of \( \Delta T \), the inversion of the matrix \( A \) is never evaluated. In fact, it is possible to provide the custom “vector-Jacobian-product” (or vJp) associated to our linear solver, i.e.

\[
vJp(v) = \sum_{cc'} v_c [A^{-1}]_{cc'} C_{cp} = \sum_c \Lambda_c C_{cp},
\]

(C.4)

where

\[
v_c = \frac{\partial \tilde{\kappa}^F}{\partial \Delta T_c},
\]

(C.5)

and \( \Lambda \) is the solution of the equation

\[
\sum_c A_{cc'} \Lambda_c = v_{c'}. \]

(C.6)

Equation C.6 is the adjoint of the original problem. Once Eq. C.6 is evaluated, reverse-mode AD will then use the result of the vJp in Eq. C.4 to evaluate Eq C.1 using JAX’s built-in primitives. Similarly to the BTE, however, we provide the custom-Jvp \( Jvp(v) = (\nabla_p \tilde{\kappa}^F)^T \cdot v \), which will then be transposed by JAX. To evaluate it, we first note that

\[
\frac{\partial \tilde{\kappa}^{c'}}{\partial \rho_p} = r_{cc'} \delta_{cp} + r_{c'c} \delta_{cp},
\]

(C.7)
where
\[ r_{cc'} = \frac{2\gamma}{\bar{\rho}_c} \left[ \frac{\bar{\rho}_{cc'} + \bar{\rho}_{c'}}{\bar{\rho}_c + \bar{\rho}_{c'}} \right]^{\gamma+1}. \] (C.8)

Note that for simplicity we haven’t included the small \( \delta \) introduced for numerical stability. Then, after some algebra, we have
\[ \sum_c \Lambda_c \frac{\partial b_c}{\partial \bar{\rho}_p} = \sum_{c'} r_{pc'} \left( \Delta T_{pc'} \Lambda_{p} + \Delta T_{cp} \Lambda_{c} \right) \] (C.9)

\[ \sum_{cc'} \Lambda_c \frac{\partial A_{cc'}}{\partial \bar{\rho}_p} \Delta T_{c'}, = \sum_{c'} r_{pc'} |n_{pc'}| \left[ \Delta T_{p} \Lambda_{p} + \Delta T_{c'} \Lambda_{c'} - \Delta T_{c} \Lambda_{p} - \Delta T_{p} \Lambda_{c'} \right], \]

\[ \frac{\partial \bar{\kappa}^F}{\partial \Delta T_c} = g \sum_{c} (\kappa_{cc'} K_{c'} - \kappa_{cc} K_{c}), \]

\[ \frac{\partial \bar{\kappa}^F}{\partial \bar{\rho}_p} = g \sum_{c} r_{pc} (K_{pc} + K_{cp}) \left( \Delta T_{c} + \Delta T_{ext} - T_{p} \right), \] (C.10)

with \( g = (\kappa_{bulk} \Delta T_{ext})^{-1} \).

**Appendix D. The Jacobian-vector-product for the BTE solver**

The adjoint BTE solver can be integrated into an AD-framework via a custom-vJp rule. This approach allows for a seamless differentiation of user-defined functions of phonon distributions and material density. However, as shown in Sec. 5, for computational efficiency we manually derive the expression for \( \nabla \bar{\rho} \bar{\kappa} \),
\[ \frac{\partial \bar{\kappa}}{\partial \bar{\rho}_p} = \sum_{\mu c} \frac{\partial \bar{\kappa}}{\partial \Delta T_{\mu c}} \frac{\partial \Delta T_{\mu c}}{\partial \bar{\rho}_p} + \frac{\partial \bar{\kappa}}{\partial \bar{\rho}_p} = \sum_{\mu c} \Lambda_{\mu c} C_{\mu cp} + \frac{\partial \bar{\kappa}}{\partial \bar{\rho}_p}, \] (D.1)

and then provide the custom-Jvp rule, Jvp(\( \mathbf{v} \)) = \( (\nabla \bar{\rho} \bar{\kappa})^T \cdot \mathbf{v} \). In Eq. D.1, \( \Lambda_{\mu c} \) and \( C_{\mu cp} \) are defined in 5. JAX will then transpose this rule. The starting point in evaluating Eq. D.1 is the derivative of the transmission coefficients,
\[ \frac{\partial t_{cc'}}{\partial \bar{\rho}_\alpha} = \alpha_{cc'} \delta_{\alpha \alpha} + \alpha_{c'c} \delta_{\alpha} \alpha, \] (D.2)
where \( \alpha_{cc'} = 1/2 \left( t_{cc'}/\bar{\rho}_c \right)^2 \). The derivative of the effective thermal conductivity with respect to the material density is

\[
\frac{\partial \tilde{\kappa}}{\partial \bar{\rho}_p} = \frac{1}{\Delta T_{\text{ext}} N \text{Kn}^2} \sum_{\mu_c} \alpha_{pc} \left[ K_{pc} g_{\mu_p c}^c \Delta T_{\mu c} + K_{cp} \Delta T_{\mu p} g_{\mu_c p}^c + K_{pc} \Delta T_{\mu p} g_{\mu_p c}^c + \Delta T_{\text{ext}} \left( K_{pc} g_{\mu_p c}^c + K_{cp} g_{\mu_c p}^c \right) \right]. \tag{D.3}
\]

The derivative of the perturbation with respect to the material density reads

\[
\frac{\partial P_{\mu c}}{\partial \bar{\rho}_p} = H_{cp} g_{\mu_c p}^c \alpha_{pc} + \delta_{cp} \left( \sum_{c'} H_{pc'} g_{\mu_p c}^c \alpha_{pc'} \right) \tag{D.4}
\]

Meanwhile, we have

\[
\frac{\partial G_{\mu c'}}{\partial \bar{\rho}_p} = \delta_{\mu c'} (\alpha_{cc'} \delta_{cp} + \alpha_{cc'} g_{\mu_c c}) + \delta_{cp} \delta_{cc'} \sum_{c''} \left( \alpha_{cc'} h_{\mu_c c}^{c''} \right) + \delta_{cc'} \alpha_{pc} h_{\mu_c p}. \tag{D.5}
\]

Combining Eqs. D.4-D.5, we have

\[
C_{\mu c p} = \sum_{\mu c'} \left[ \frac{\partial P_{\mu c'}}{\partial \bar{\rho}_p} \delta_{cc'} \delta_{\mu c'} - \Delta T_{\mu c'} \frac{\partial G_{\mu c'}}{\partial \bar{\rho}_p} \right] = \delta_{cp} \sum_{c'} \left( H_{cc'} g_{\mu_c c}^c \alpha_{cc'} \right) + H_{cp} g_{\mu_c p}^c \alpha_{pc} - \delta_{cp} \sum_{c'} \left( \Delta T_{\mu c'} \alpha_{cc'} g_{\mu_c c}^c \right) - \Delta T_{\mu p} \alpha_{pc} g_{\mu_c p}^c + \delta_{cp} \sum_{c'} \left( \Delta T_{\mu c'} \alpha_{cc'} h_{\mu_c c}^{c'} \right) - \alpha_{pc} \sum_{\mu'} \Delta T_{\mu c'} h_{\mu_c c}^{\mu'}. \tag{D.6}
\]

Lastly, we have

\[
\sum_{\mu_c} \Lambda_{\mu c} C_{\mu c p} = \sum_{\mu_c} \alpha_{pc} \left[ \Lambda_{\mu p} H_{pc} g_{\mu p c} - \Lambda_{\mu c} H_{cp} g_{\mu c p} - \Lambda_{\mu p} g_{\mu p c} \Delta T_{\mu c} - \Lambda_{\mu c} g_{\mu c p} \Delta T_{\mu p} \right] - \sum_{\mu c'} \alpha_{pc} \left[ \Lambda_{\mu p} \Delta T_{\mu c'} h_{\mu c}^{\mu c'} + \Lambda_{\mu c} \Delta T_{\mu c'} h_{\mu c}^{\mu c'} \right]. \tag{D.7}
\]
We remind that $\Lambda_{\mu c}$ is the solution of

$$
\sum_{\mu'c'} G_{\mu c}^{\mu'c'} \Lambda_{\mu'c'} = \frac{\partial \bar{\kappa}}{\partial \Delta T_{\mu c}},
$$

where

$$
\frac{\partial \bar{\kappa}}{\partial \Delta T_{\mu c}} = \frac{1}{\Delta T_{\text{ext}} N \text{Kn}^2} \sum_{c'} \left[ t_{cc'} K_{cc'} g_{\mu c c'}^+ + t_{c'c} K_{c'c} g_{\mu c c'}^- \right].
$$

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