Inverse design in nanoscale heat transport via interpolating interfacial phonon transmission

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Received: 12 February 2022 / Revised: 30 August 2022 / Accepted: 1 September 2022 / Published online: 6 October 2022 © The Author(s) 2022

Abstract
We introduce a methodology for density-based topology optimization of non-Fourier thermal transport in nanostructures, based upon adjoint-based sensitivity analysis of the phonon Boltzmann transport equation (BTE) and a novel material interpolation technique, the “transmission interpolation model” (TIM). The key challenge in BTE optimization is handling the interplay between real- and momentum-resolved material properties. By parameterizing the material density with an interfacial transmission coefficient, TIM is able to recover the hard-wall and no-interface limits, while guaranteeing a smooth transition 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, identifying a promising new thermoelectric material design. Our method enables the 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
Designing a nanomaterial with prescribed thermal properties is critical to many applications, such as heat management and thermoelectrics (Vineis et al. 2010; Cahill et al. 2003). However, heat-conduction optimization in nanostructures remains challenging: Fourier’s law breaks down (Chen 2021), heat transport becomes nonlocal, and standard topology-optimization methods (Sigmund and Maute 2013) for diffusive theories (Dede 2009; Haertel et al. 2015) are not readily applicable. An early study (Evgrafov et al. 2009) developed the adjoint phonon Boltzmann transport equation (BTE) to design a material with a prescribed difference of temperature between two given points; in Ref. Evgrafov et al. (2009), the local material density was related to the bulk phonon mean-free-path (MFP), a method that was proven successful for boundary conditions applied to influx phonon flux. However, such an approach is not suitable when shape optimization includes arbitrary adiabatic boundaries, a scenario that presents a challenge on its own: How to interpolate a material so that phonons are scattered back isotropically at adiabatic walls (assuming diffuse boundaries), while also recovering the no-interface limit for uniform densities? We tackle this challenge by introducing the “transmission interpolation method” (TIM). The key concept behind TIM is that instead of relating the local density to volume-based parameters, such as the MFP, TIM parametrized the material density in terms of phonon interfacial transmission.

In our implementation, we combine a BTE solver (Sec. 1) with TIM (Sec. 2), and chained them into a reverse-mode automatic differentiation pipeline (Bradbury et al. 2018), which also includes density filtering and projection (Sigmund and Maute 2013) (Sec. 3). We apply our methodology to obtain new solutions to two exemplary problems: designing an anisotropic thermal-conductivity tensor in a periodic nanomaterial (Sec. 4) and, for thermoelectric applications (Vineis et al. 2010), minimizing thermal transport while simultaneously maintaining high electrical conductivity (Sec. 5). (To the latter end, we assume charge transport...
to be diffusive and thus implement an differentiable Fourier solver.) Several technical aspects, including the matrix-free solution of the BTE solver and the relationship between its forward and adjoint counterparts, are reported in the Appendices. The code developed for this work will be released in the OpenBTE package (Romano 2021a).

Nondiffusive thermal transport, investigated from both theoretical (Ziman 2001) and experimental (Lee et al. 2015; Hochbaum et al. 2008; Song and Chen 2004) standpoints, has opened up exciting engineering opportunities; however, 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 (Ziman 2001). If forward modeling is challenging, inverse design is even more difficult. In addition to Ref. Evgrafov et al. (2009), mentioned above, there have only been a few studies aiming at gradient-based optimization of nanoscale thermal transport. For example, in a recent preprint (Chen et al. 2022), the adjoint BTE was used in conjunction with experiments to estimate phonon-related material properties. However, none of these works focus on systems with arbitrary adiabatic boundaries. In the simpler diffusive regime, density-based topology optimization has been routinely applied to macroscopic heat-transport problems (Gersborg-Hansen et al. 2006; Zhang and Liu 2008; Haertel et al. 2015; Imediegwu et al. 2022; Song and Youn 2006). The basic idea of density-based topology optimization (Sigmund and Maute 2013) 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 (Sigmund and Maute 2013) 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 (Zhou et al. 2015; Lazarov et al. 2016). Adjoint-based sensitivity analysis allows such huge parameter spaces to be efficiently explored (Sigmund 2011), enabling the computational discovery of surprising non-intuitive geometries. For instance, in Ref. Gersborg-Hansen et al. (2006), 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 (Sigmund 2001), 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 (Chen 2005). 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

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. 1a). To calculate, for example, \( \kappa_{xx} \), we apply a temperature jump of \( \Delta T_{\text{ext}} = 1 \) K across the \( x \)-axis, and average the \( x \)-component of heat flux,

\[
\kappa_{xx} = -\frac{1}{\Delta T_{\text{ext}}} \int_{-L/2}^{L/2} \mathbf{J}(L/2, y) \cdot \hat{x} dy. \tag{1}
\]

To calculate the heat flux, we note that, at the nanoscales, heat conduction deviates from the standard Fourier law because the mean-free-path (MFP) of heat carriers, i.e. phonons, becomes comparable with the material’s feature size. This phenomenon, commonly known as classical phonon size effects (Chen 2005), can be captured by the phonon Boltzmann transport equation (BTE) (Chen 2005; Peierls...
and \( \Lambda \) (in real- and angular-space. The resulting linear system reads

\[
\sum_{\mu \nu} G_{\mu \nu} c^* \hat{T}_{\mu c} = P_{\mu c},
\]

where \( \mu \) and \( c \) label angular and real-space, respectively. Equation 5 is solved using a matrix-free Krylov subspace method. The expressions for the terms \( G_{\mu c} \) and \( P_{\mu c} \), as well as details on the iterative solution of Eq. 5, are provided in Sec. B.

Lastly, we note that in this work a Fourier solver is also used, where the temperature is only described in real-space. We will refer to the corresponding normalized effective thermal conductivity as \( k^{F} \). In this case, the linear system to solve is \( \sum_{\mu} A_{\mu} \hat{T}_{\mu} = b \). The expressions for \( A_{\mu} \) and \( b \), as well as details on gradient calculations of the Fourier solver are reported in Sec. A.

3 The transmission interpolation method

Density-based topology optimization requires a differentiable transition between material properties (Sigmund and Maute 2013); 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 (Bendsoe and Sigmund 1999). Following Fig. 1b, we begin by considering an interface between two pixels, with different densities, \( \rho_1 \) and \( \rho_2 \). The interface between them has normal \( \hat{n} \) pointing toward pixel 2. Furthermore, we define the phonon temperatures in those two pixels as \( T_{1}(\phi) \) and \( T_{2}(\phi) \). Note that while we have discretized the real space, in this section we use a continuous representation for \( \phi \). In our case, a material interpolation model must satisfy two limit cases: When \( \rho_1 = \rho_2 \), there should be no extra phonon scattering across their interface; on the other side, when \( \rho_1 = 0 \) and \( \rho_2 = 1 \), phonons must scattered back isotropically toward region 1.

A possible material interpolation model is given in Ref. Evgrafov et al. (2009), where the MFP depends on the material density through \( \Lambda^{-1}(\rho) = \Lambda_a^{-1}(1-\rho)+\Lambda_b^{-1}(\rho) \), with \( \Lambda_a \) and \( \Lambda_b \) associated to two different phases. This approach was successfully applied for boundary conditions on incoming phonon flux. However, it may be problematic for the adiabatic hard-wall limit, as explained in the following. Adopting the approach from Evgrafov et al. (2009), the heat flux at the interface between the two pixels is

\[
\mathbf{J}(\mathbf{r}) \cdot \hat{n} = \frac{2k}{\pi} \left[ \frac{\rho_1}{\Lambda_a} + \frac{(1-\rho_1)}{\Lambda_b} \right] \int_{\hat{T}(\phi,\hat{n} > 0)} \hat{T}_{1}(\phi)\hat{s}(\phi) \cdot \hat{n} d\phi + \frac{2k}{\pi} \left[ \frac{\rho_2}{\Lambda_a} + \frac{(1-\rho_2)}{\Lambda_b} \right] \int_{\hat{T}(\phi,\hat{n} < 0)} \hat{T}_{2}(\phi)\hat{s}(\phi) \cdot \hat{n} d\phi.
\]

\( \text{Equation 5:} \)
For adiabatic boundaries, we may assign $\Lambda_t$ to the solid phase and a fictitious $\Lambda_t = \infty$ to the void one; in this case, the second part of Eq. 6 will be zero because $p_2 = 0$ but the first part (which has $p_1 = 1$) will be different than zero. Consequently, such an approach would lead to a nonzero net thermal current, while we wish to have an adiabatic surface. Note that this conclusion applies to generic adiabatic surfaces within the context of the BTE and is not tied to our choice of diffuse scattering.

To lift these limitations, we attack the problem from a different angle: We parameterize the material density via a phonon 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 (Singh et al. 2011). Specifically, we introduce the boundary conditions

\[
\begin{align*}
\tilde{T}_1(\phi) &= t \tilde{T}_2(\phi) + (1 - t) \tilde{T}_{12}^B, \quad \text{for } \phi : \hat{s}(\phi) \cdot \hat{n} < 0 \\
\tilde{T}_2(\phi) &= t \tilde{T}_1(\phi) + (1 - t) \tilde{T}_{21}^B, \quad \text{for } \phi : \hat{s}(\phi) \cdot \hat{n} \geq 0
\end{align*}
\]

(7)

where $\tilde{T}_{ij}^B$ is the boundary temperature at the interface between pixels $i$ and $j$, thermalizing phonons traveling into pixel $i$. Its expression is given by

\[
\begin{align*}
\tilde{T}_{12}^B &= \frac{1}{2} \int_{\hat{s}(\phi) \cdot \hat{n} \geq 0} \tilde{T}_1(\phi) \hat{s}(\phi) \cdot \hat{n} d\phi \\
\tilde{T}_{21}^B &= -\frac{1}{2} \int_{\hat{s}(\phi) \cdot \hat{n} < 0} \tilde{T}_2(\phi) \hat{s}(\phi) \cdot \hat{n} d\phi,
\end{align*}
\]

(8)

where we used $\int_{\hat{s}(\phi) \cdot \hat{n} \geq 0} \hat{s}(\phi) \cdot \hat{n} d\phi = -\int_{\hat{s}(\phi) \cdot \hat{n} < 0} \hat{s}(\phi) \cdot \hat{n} d\phi = 2$. The term $t$ in Eq. 7 is a transmission coefficient, which we define as

\[
t = 2 - \frac{p_1 p_2}{p_1 + p_2}.
\]

(9)

It is straightforward to show that if either $p_1$ or $p_2$ is zero, then the RHS of Eq. 7 reduces to the hard-wall case. On the other side, if $p_1 = p_2$, there will be no interface. To summarize, our parameterization does not relate the material density to a bulk-like property (such as the MFP from Ref. Evgrafov et al. 2009), but rather to the amount of incoming flux. To distinguish this approach from traditional material interpolation methods, we name it the “Transmission Interpolation Method” (TIM). In passing, we note that transmission coefficients of the form $t'$, with $\gamma > 1$ would also be a suitable interpolation approach. However, investigating this more general case is outside the scope of our work. Details on the angular discretization of TIM is reported in Sec. B.

4 The optimization pipeline

In this section, we outline the method for computing $V_{\rho} \tilde{\kappa}$, which will be used in our optimization algorithm. We begin by noting that 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 (Bendsoe and Sigmund 2003). These two issues are commonly resolved using filtering and thresholding, respectively (Sigmund and Maute 2013). As shown in Fig. 2, given a design density $\rho$ (for convenience, from now on, we will work with a discretized domain), we first filter it, $\check{\rho} = w * \rho$, where in this case, $w$ is a conic filter with radius $R$,

\[
w_i = \begin{cases} 
\frac{1}{\pi} \left(1 - \frac{|r|}{R}\right), & |r| < R \\
0, & \text{otherwise.}
\end{cases}
\]

(10)

In Eq. 10, $a$ is a normalization factor ($= \pi R^2 / 3$ in the continuum limit), $c_i$ is the centroid of the grid point $i$, and $R$ is the radius of our filter. In this work, $R = L / 10$. The thresholding, $\rho = \check{f}_\gamma(\check{\rho})$, is then carried out using the following function (Wang et al. 2011)

\[
\rho = \frac{\tanh \beta \eta + \tanh (\beta(\check{\rho} - \eta))}{\tanh \beta \eta + \tanh (\beta(1 - \eta))},
\]

(11)

where $\eta$ and $\beta$ are threshold parameters. The resulting field, referred here as “projected” 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 (Hammond et al. 2021), in order to guarantee a good degree of topology variability (especially early on in the optimization process) while ensuring a final binary structure.

In this work, we start with \( \beta = 2 \) and double it every 20 iterations, until convergence is reached.

Once the relationship \( \hat{\rho}(\rho) \) is implemented, we can use the chain rule

\[
\frac{d\hat{\varepsilon}}{d\rho} = \sum_{\mu'c'} G_{\mu'c'}^{\mu c} \frac{\partial \bar{T}_{mc}}{\partial \hat{\rho}_{\mu'c'}} \frac{\partial \hat{\rho}_{\mu'c'}}{\partial \rho} + \sum_{\rho'} \frac{\partial \hat{\varepsilon}}{\partial \hat{\rho}_{\rho'}} \frac{\partial \hat{\rho}_{\rho'}}{\partial \rho},
\]
which is evaluated using reverse-mode automatic differentiation, implemented in JAX (Bradbury et al. 2018). Specifically, for \( \partial \hat{\varepsilon}/\partial \hat{\rho}_{\rho'} \) we use the adjoint method (Strang 2007), which allows to compute such a gradient by solving the linear system

\[
\sum_{\mu'c'} G_{\mu'c'}^{\mu c} \bar{T}_{mc}^{\text{adj}} = P_{mc}^{\text{adj}},
\]

with \( P_{mc}^{\text{adj}} \) defined in Sec. B. In practice, we use the relationship

\[
\bar{T}_{mc}^{\text{adj}} = -\bar{T}_{mc},
\]
derived in Sec. B. Therefore, the adjoint solution is computed by post-processing the solution of Eq. 5, achieving a significant boost in computational efficiency.

Furthermore, as \( \nabla_{\rho} \hat{\varepsilon} \) is available at each iteration while solving the forward problem, we adopt an early termination criteria, based on \( \hat{\varepsilon} \) and \( \nabla_{\rho} \hat{\varepsilon} \). This approach extends Ref. Amir et al. (2010), where early termination strategies were based on the error on the objective function alone. The sensitivity of \( \hat{\varepsilon} \) with respect to the projected density is provided through the custom vector-Jacobian product \( vJ_p(a) = a\partial \hat{\varepsilon}/\partial \rho_p \).

Lastly, we note that for the Fourier solver, the forward and adjoint solutions are related \( \bar{T}_{mc}^{\text{adj}} = -\bar{T}_{mc} \), as derived in Sec. A. Similarly to the BTE case, we use this relationship to avoid solving the adjoint problem.

5 Case I: tailoring the effective thermal conductivity tensor

In this section, we show an example of how topology optimization may be employed to design a periodic material with a prescribed effective thermal conductivity tensor, \( \tilde{\kappa} \), and with a porosity larger than \( \tilde{\phi} \). To this end, we define the objective function

\[
g(\rho) = \| \hat{\varepsilon}(\rho) - \tilde{\varepsilon} \|_{\text{Fro}} = \sqrt{\Delta \kappa_{xx}(\rho)^2 + \Delta \kappa_{yy}(\rho)^2},
\]

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

\[
\tilde{\varepsilon}(\rho) = \left( \begin{array}{cc} \tilde{\kappa}_{xx}(\rho) & 0 \\ 0 & \tilde{\kappa}_{yy}(\rho) \end{array} \right),
\]

is evaluated by solving Eq. 2, for each perturbation direction, after filtering and projecting. The sensitivity of the objective function is

\[
\nabla_{\rho} g(\rho) = g(\rho)^{-1} \left[ \Delta \kappa_{xx}(\rho) \nabla_{\rho} \kappa_{xx}(\rho) + \Delta \kappa_{yy}(\rho) \nabla_{\rho} \kappa_{yy}(\rho) \right].
\]
where the terms $\nabla \rho \tilde{\kappa}_i(\rho)$ are computed using Eq. 12. The above discussion allows us to lay out the optimization algorithm

$$\min_{\rho} g(\rho)$$

$$0 \leq \rho \leq 1$$

$$\text{s.t. } \sum_n \tilde{\rho}_n \leq (1 - \bar{\phi})N,$$

where $N$ is the number of pixels. In this section, the chosen porosity is $\bar{\phi} = 0.25$. As the optimizer, we use an open-source implementation (Johnson 2014) of the method of moving asymptotes (MMA) (Svanberg 2002), which converges globally (i.e. it guarantees to find a local minimum from every starting point).

As a first example, we choose $\tilde{\kappa}_{xx} = \tilde{\kappa}_{yy} = 0.15$. To ensure mesh convergence on a particular local minimum, we use the following algorithm:

1. Optimize a structure at a coarse resolution using a random configuration as the initial structure.
2. Upsample the optimal structure by doubling the resolution.
3. Optimize a structure using the configuration created in step 2 as the first guess. Note that the filter’s radius does not change in physical units, but doubles in pixel units.
4. Repeat from step 2.

Figure 3 illustrates the optimized structures for grid sizes $N = 10 \times 10, 20 \times 20, 40 \times 40$ and $80 \times 80$. For both the Fourier and BTE cases, a shape convergence is achieved. For the rest of this study we adopt a grid of $60 \times 60$, using a random configuration as a first guess. A striking difference between the two solvers is that for the BTE case the pattern is coarser. In fact, phonon size effects are known to be more effective than macroscopic reduction with the same geometric constraints (Sharvin 1965).

We now turn to the design an anisotropic material. 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 (Romano and Kolpak 2017). In this example, we choose $\kappa_{xx} = 0.3$ and $\kappa_{yy} = 0.1$, with the resulting anisotropy $\kappa_{xx}/\kappa_{yy} = 3$.

Convergence is reached within 100 iterations. The final structure, shown in Fig. 4a, is made by two 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. 4b and c, for $\kappa_{xx}$ and $\kappa_{yy}$, respectively. Note that the final values obtained with Fourier’s law are $\kappa_{xx}^F \approx 0.61$ and $\kappa_{yy}^F \approx 0.46$, with anisotropy 1.33, well below the prescribed value.

6 Case II: maximizing phonon scattering

In thermoelectric applications it is desirable to minimize thermal transport while not degrading the electrical conductivity (Rowe 2018). In fact, the thermoelectric figure-of-merit is given by $ZT = TS^2/\sigma/k$, 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.
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(Vineis et al. 2010; Qiu et al. 2015). 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 (Tang et al. 2010; Lee et al. 2017). In passing, we note that macroscopic geometrical effects, often referred to as “porosity factor” (Verdier et al. 2017), in some cases have analytical solutions. For example, in aligned porous systems with circular pores and porosity \( \varphi \), it has the analytical solution

\[
\bar{\kappa}^F = \frac{1}{1 + \varphi} - \frac{1}{1 + \varphi} \approx 0.31
\]

(Hasselman and Johnson 1987). We choose as baseline a porous material with staggered pores of circular shape (Romano and Grossman 2014; Song and Chen 2004; Anufriev and Nomura 2020), as shown in Fig. 5a. The chosen porosity is \( \varphi = 0.5 \), 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:

\[
\min_{\rho} g(\rho)
\]

\[
0 \leq \rho \leq 1
\]

s.t. \( \bar{k}_{xx}^F(\rho) \geq 0.31
\)

(19)

(20)

where

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

(21)

is the cost function to be minimized. We run this optimization problem with \( \gamma = 3 \) (see Sec. A), (smaller values would mostly lead to stagnation). Convergence is reached in 200 iterations, as shown in Fig. 5e. Remarkably, the optimized structure, shown in Fig. 5b, has an isotropic tensor of \( \bar{k} \approx 0.011 \), roughly 4.25 times smaller than that of the baseline; yet, \( \bar{k}^F \) 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. 5d. In passing, we note that it is possible to impose minimum-linewidth and minimum-line-spacing conditions by adding differentiable inequality constraints to the optimization algorithm (Hammond et al. 2021; Zhou et al. 2015), and in the future we plan to optimize the design for specific manufacturing processes in this way. Lastly, we recall that diffusive transport is scale-free, thus in principle we can begin from the staggered configuration and scale it down until we reach the same \( \bar{\kappa} \) obtained from the optimization. However, such a configuration would be much

\[
\frac{1}{\sqrt{2}} \leq \frac{1}{\sqrt{2}}\approx 0.31
\]

\[
0 \leq \rho \leq 1
\]

s.t. \( \bar{k}_{xx}^F(\rho) \geq 0.31
\)

(22)

Fig. 5 The a initial, b optimized and d polished structure in relation to the optimization problem described by Eq. 19. e The evolution of \( \bar{\kappa} \) and \( \bar{\kappa}^F \). c The normalized magnitude of flux when a temperature gradient is applied along the x-axis.
more challenging to be manufactured (it would have several smaller pores) than the one depicted in Fig. 5.

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. 5c 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 (Maxwell 1873) in the diffusive regime, showing that the thermal resistance is proportional to \( 1/a \); on the other side, Sharvin (Sharvin 1965) predicted that in the ballistic regime, i.e. for \( \Lambda \ll a \) (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 (Spence and Moore 2022), 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.

7 Conclusions

In this work, we develop a model, termed the Transmission Interpolation Model (TIM), that is able to smoothly interpolate material properties in the context of nondiffusive heat transport. The key concept behind TIM is that instead of linking a volume-based quantity to the material density, e.g. the bulk thermal conductivity, it parametrizes an interfacial transmission coefficient. Using this approach, TIM recovers the adiabatic hard-wall and no-interface limits. We first apply our methodology to tailoring the effective thermal conductivity, 

\[
\nabla \cdot [\rho(x,y)\nabla T(x,y)] = 0. \tag{A1}
\]

We point out that for numerical reasons, we regularized such expression using a small value, \( \delta \). However, for clarity, we omit it throughout the text. Once Eq. A1 is solved, the normalized effective thermal conductivity is evaluated as

\[
\tilde{k}_{xx} = -\int_{-L/2}^{L/2} \tilde{\rho}(L/2,y)\nabla T(L/2,y) \cdot \tilde{\mathbf{x}} dy. \tag{A2}
\]

To discretize Eqs. A1, A2 we conveniently define the following quantities:

\[
\mathbf{n}_{c,c'} = \begin{cases} 
\text{normal pointing to } c', \text{ if } c \text{ and } c' \text{ are adjacent (including periodicity)} \\
0, \text{ otherwise,}
\end{cases} \tag{A3}
\]

where \( \mathbf{n}_{c,c'} \) and \( \mathbf{K} \) describe connectivity and external perturbation, respectively. We further define \( \mathbf{H} = (\mathbf{K} - \tilde{\mathbf{K}}') \). We discretize Eq. A1 using the finite-volume method, with the material grid being the same as the discretization grid. Upon integrating Eq. A1 over the control volume \( c \), we have

\[
\sum_k \int_{\partial \Omega} \rho(x,y) \frac{\partial T(x,y)}{\partial x_k} n_k dl = \frac{L}{\sqrt{N}} \mathbf{J}_{c,c'} \cdot \mathbf{n}_{c,c'} = \frac{L}{\sqrt{N}} \sum_{c'} u_{c,c'} (\tilde{T}_{c'} + H_{c,c'} - \tilde{T}_c), \tag{A4}
\]

where \( \mathbf{J}_{c,c'} \) is the normalized interfacial thermal flux. To determine \( u_{c,c'} \), we first write the balance equation at the interface between volume \( c \) and \( c' \),

\[
\frac{L}{\sqrt{N}} \mathbf{J}_{c,c'} \cdot \mathbf{n}_{c,c'} = -2\tilde{\rho}_c (\tilde{T}_b - \tilde{T}_c) = -2\tilde{\rho}_c (\tilde{T}_{c'} - \tilde{T}_b), \tag{A5}
\]
where $T_b$ is the temperature at the boundary, shared among both volumes (we assume no thermal boundary resistance.)

After solving for $\tilde{T}$ and, for simplicity, assuming we are at an internal volume, we have $(L/\sqrt{N})\mathcal{J} = \hat{n}$, where

$$u_{cc} = 2\frac{\tilde{\rho} c}{\tilde{\rho} c + \tilde{\rho} c} \mid \hat{n} \mid.$$  

(A6)

In passing, we point out that Eq. A6 is an harmonic average, an approach that has been compared favorably against the arithmetic average, in terms of ability of preventing checkerboard patterns (Gersborg-Hansen et al. 2006). In practice, we use a slightly modified version of Eq. A6, $\tilde{\rho} c = u_{cc}^T$, where $\gamma$ is a tuning parameter. Note that $\tilde{\rho} c = \tilde{\rho} c$. Lastly, Eq. A4 translates into the linear system

$$\sum_{c'} A_{cc'} \tilde{T}_{c'} = b_c,$$

(A7)

where

$$A_{cc'} = \sum_{c''} \tilde{\rho} c_{cc''}(\delta_{c''} - \delta_{c'c''}),$$

$$b_c = \sum_{c''} \tilde{\rho} c_{cc''} H_{c'c''}.$$  

(A8)

Once Eq. A8 is solved, the effective thermal conductivity is evaluated by

$$\hat{k}^F = \sum_{c'} \tilde{\rho} c_{cc'} K_{cc'} \left[ \tilde{T}_{c'} + 1 - \tilde{T}_{c'} \right]$$

$$= \sum_{c'} \tilde{\rho} c_{cc'} K_{cc'} - \sum_c \tilde{T}_{c'} b_c.$$  

(A9)

Depending on the size of $A$, we solve Eq. A7 either using LU decomposition or an iterative solver; in this last case, the operator associated to Eq. A7 is

$$[\mathcal{L}(\mathbf{x})]_c = \sum_{c'} \tilde{\rho} c_{cc'} (x_{c'} - x_c),$$

(A10)

and, similarly to the BTE case, the termination criteria is based on the error on $k^F$ and $\nabla_p k^F$.

### A.1 Gradient of the Fourier solver

Computing the gradient of $k^F$ with respect to the design field translates into the following chained calculations

$$\frac{\partial \hat{k}^F}{\partial \tilde{\rho} p} = \frac{\partial \hat{k}^F}{\partial \tilde{\rho} p} + \sum_c \frac{\partial k^F}{\partial \tilde{T}_c} \frac{\partial \tilde{T}_c}{\partial \tilde{\rho} p}.$$  

(A11)

We employ the adjoint method (Strang 2007), i.e. we differentiate analytically Eq. (A7) and then invert it, obtaining

$$\frac{\partial k^F}{\partial \tilde{\rho} p} = \frac{\partial k^F}{\partial \tilde{\rho} p} + \sum_c \frac{\partial k^F}{\partial \tilde{T}_c} \frac{\partial \tilde{T}_c}{\partial \tilde{\rho} p},$$

where

$$C_{cp} = \sum_{c'} \left[ \frac{\partial h_{cp}}{\partial \tilde{\rho} p} \delta_{c'c} - \tilde{T}_c \frac{\partial A_{cc'}}{\partial \tilde{\rho} p} \right],$$

(A13)

and $\tilde{T}_{adj}$ being the solution of the adjoint problem

$$\sum_{c'} A_{cc'} \tilde{T}_{adj} = \frac{\partial k^F}{\partial \tilde{T}_c} = -b_c.$$  

(A14)

Since $A$ is symmetric,

$$\tilde{T}_{adj} = -\tilde{T}_c,$$  

(A15)

that is, the adjoint solution can be straightforwardly computed using the forward one. A similar result has also been obtained in the context of asymptotic inverse homogenization (Zhou and Li 2008).

To evaluate Eq. A12, we first note that

$$\frac{\partial \tilde{\rho} c_{cc'}}{\partial \tilde{\rho} p} = \gamma \tilde{\rho} c_{cc'}^{-1} \left( r_{cc'} \delta_{cp} + r_{c'} \delta_{cp} \right),$$

(A16)

where

$$r_{cc'} = \frac{1}{2} \left( \frac{\tilde{\rho} c_{cc'}}{\tilde{\rho} c} \right)^2.$$  

(A17)

Then, after some algebra, we have

$$\sum_c \tilde{T}_{adj} \frac{\partial b_c}{\partial \tilde{\rho} p} = \sum_c r_{cp} \left( H_{pc} \tilde{T}_{adj} + H_{cp} \tilde{T}_{adj} \right)$$

(A18)

\begin{equation}
\begin{aligned}
&- \sum_{c'} \tilde{T}_{adj} \frac{\partial A_{cc'}}{\partial \tilde{\rho} p} \\
&= \sum_c r_{cp} \left( \tilde{T}_{c} \tilde{T}_{adj} + \tilde{T}_{p} \tilde{T}_{adj} - \tilde{T}_{p} \tilde{T}_{adj} - \tilde{T}_{c} \tilde{T}_{adj} \right),
\end{aligned}
\end{equation}

(A19)

Putting everything together, we have

$$\frac{\partial k^F}{\partial \tilde{\rho} p} = \sum_c r_{pc} \left[ H_{pc} \tilde{T}_{adj} + H_{cp} \tilde{T}_{adj} + \tilde{T}_{c} \tilde{T}_{adj} - \tilde{T}_{p} \tilde{T}_{adj} - \tilde{T}_{c} \tilde{T}_{adj} + K_{pc} + K_{cp} + H_{pc} \tilde{T}_{adj} - H_{pc} \tilde{T}_{adj} \right].$$

(A20)

Lastly, using Eq. A15 in Eq. A20, we have
\[
d\frac{d\vec{\kappa}}{d\tilde{\rho}} = \sum c \left[ (\vec{T}_p - \vec{T}_r)^2 - 2(\vec{T}_p - \vec{T}_c)(K_{pc} - K_{cp}) + K_{pc} + K_{cp} \right],
\]
where \((x)^+ = \max(0, x), (x)^- = \min(0, x)\), and \(t_{cc'}\) is defined in Eq. (9), and \(H_{cc'}\) is introduced in Sec. A. In Eq. (B25), \(\vec{T}_{cc'}^B\) is obtained by discretizing Eq. (8),
\[
\vec{T}_{cc'}^B = \frac{1}{2} \sum_{\mu} \vec{T}_{\mu}(S_{\mu} \cdot \hat{n}_{cc'})^+.
\]
Combining Eqs. B24, B25 and B26, we have the following matrix linear system
\[
\sum_{\mu'c'} G_{\mu'c'}^\mu \vec{T}_{\mu'c'} = P_{\mu},
\]
with \(c = 1, \ldots, N - 1, \mu = 1, \ldots, M - 1,\) and
\[
G_{\mu'c'}^\mu = \delta_{cc'}\delta_{\mu'\mu'} (1 + D_{\mu'c'} + \delta_{\mu\mu'} A_{\mu'c'} + \delta_{cc'} \left( B_{c\mu'} - \frac{1}{M} \right)).
\]

The notation \(\delta_{cc'}\) refers to the Kronecker delta. The terms in Eq. B28 are
\[
D_{\mu'c'} = \sum_{c''} g_{\mu'c''}^+,
\]
\[
A_{\mu'c'} = t_{cc'} g_{\mu'c'}^-,
\]
\[
P_{\mu} = -\sum_{c'} H_{cc'} t_{cc'} g_{\mu'c'}^-.
\]
\[
B_{\mu'c'} = \sum_{c'} h_{\mu'c'}^+ (1 - t_{cc'}).
\]

where
\[
g_{\mu'c'}^+ = Kn(S_{\mu} \cdot \hat{n}_{cc'})^+,
\]
\[
h_{\mu'c'}^+ = g_{\mu'c''}^- g_{\mu'c''}^- \alpha_{cc'}^-.
\]
In Eq. B30, we defined \(\delta_{cc'} = \sum_{\mu''} g_{\mu''c'}^- g_{\mu''c'}^-\). Lastly, the effective thermal conductivity is computed by discretizing Eq. 4 using a similar procedure, yielding
\[
k = -\frac{1}{f} \sum_{c'} t_{cc'} K_{cc'} [\vec{T}_{\mu} g_{\mu c'}^- + (\vec{T}_{\mu'} + 1) g_{\mu c'}^-] =
\]
\[
= -\frac{1}{f} \sum_{c'} t_{cc'} K_{cc'} g_{\mu c'}^- + \frac{1}{f} \sum_{\mu} P_{\mu'c} \vec{T}_{\mu'},
\]
where \(f = Kn^2 M/2\) and
\[
P_{\mu'c} = -\sum_{c'} t_{cc'} H_{cc'} g_{\mu'c'}^-.
\]
Equation B28 can be 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 a Krylov-subspace, matrix-free approach (specifically, LGMRES Baker et al. 2005) thus \(A\) is never evaluated. To this end, we first implement the linear operator

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\[ X \rightarrow \mathcal{L}(X), \]  
with \( \mathcal{L} : \mathbb{R}^{NM, NM} \rightarrow \mathbb{R}^{NM, NM} \), defined as

\[
[\mathcal{L}(X)]_{c} = D_{\mu c} X_{\mu c} + \sum_{\mu'} A_{\mu c \mu'} X_{\mu' c} + \sum_{\mu'} \left( B_{\mu \mu' c} - \frac{1}{M} \right) X_{\mu' c};
\]

then, we solve the linear system

\[ \tilde{\mathcal{L}}(x) = b, \]

where

\[ \tilde{\mathcal{L}} = \mathcal{F} \circ \mathcal{L}^{-1} : \mathbb{R}^{NM} \rightarrow \mathbb{R}^{NM} \]

\[ b = \mathcal{F}(p). \]

The terms \( \mathcal{F} : \mathbb{R}^{N, M} \rightarrow \mathbb{R}^{NM} \) and \( \mathcal{F}^{-1} : \mathbb{R}^{NM} \rightarrow \mathbb{R}^{N, M} \) are the flattening and reshaping operator, respectively. Lastly, as a first guess to the LGMRES solver, we use the solution from the previous iteration. As a result, we gain a reduction in the number of operator calls of about 30%, 50% and, 70% for grids with \( N = 20 \times 20, 40 \times 40 \) and \( 60 \times 60 \), respectively (based on an exemplary optimization with 50 iterations, \( \beta = 2 \), and \( M = 48 \)).

### B.1 Gradient of the BTE solver

In this section, we detail on the calculation of gradient of \( \delta \) with respect to the projected density \( \tilde{\rho} \). To this end, we conveniently defined (for a reason that will be apparent later) the scaled effective thermal conductivity \( \delta \tilde{\kappa} = f \tilde{\kappa} \), with \( f \) defined in the previous section. Thus, our goal is to evaluate

\[ \frac{d \delta \tilde{\kappa}}{d \tilde{\rho}} = \sum_{\mu c} \frac{\partial \delta \tilde{\kappa}}{\partial \tilde{\rho}} + \frac{\partial \delta \tilde{\kappa}}{\partial \tilde{\rho}}. \]  

(B37)

The calculation of Eq. (B37) is aided by the adjoint method (Strang 2007), which, for our matrix linear system, reads

\[ \frac{d \delta \tilde{\kappa}}{d \tilde{\rho}} = \sum_{\mu c} \tilde{F}^{\text{adj}} C_{\mu c} + \frac{\partial \delta \tilde{\kappa}}{\partial \tilde{\rho}}, \]  

(B38)

where \( \tilde{F}^{\text{adj}} \) is the solution of the matrix linear system

\[ \sum_{\mu' c'} G_{\mu c \mu' c'} \tilde{F}^{\text{adj}} = \frac{\partial \delta \tilde{\kappa}}{\partial \tilde{\rho}} = \tilde{F}_{\mu c}, \]  

(B39)

and

\[ C_{\mu c} = \sum_{\mu' c'} \left( \frac{\partial G_{\mu c \mu' c'}}{\partial \tilde{\rho}} \right). \]  

(B40)

Motivated by the relationship between the forward and adjoint solution of the Fourier solver (Eq. A15), we seek a similar link between \( \tilde{\rho} \) and \( \tilde{F}^{\text{adj}} \). To this end, we first compare the forward and adjoint solvers

\[
\sum_{\mu' c'} \left[ U_{\mu' c'}^{\mu' c} + F_{\mu' c'}^{\mu' c} \right] \tilde{\rho}_{\mu' c'} = - \sum_{c'} t_{c' c} H_{c' c} g_{\mu' c'}, \]

(B41)

\[
\sum_{\mu' c'} \left[ F_{\mu' c'}^{\mu' c} + F_{\mu' c'}^{\mu' c} \right] \tilde{F}^{\text{adj}}_{\mu' c'} = - \sum_{c'} t_{c' c} H_{c' c} g_{\mu' c'}, \]

(B42)

where

\[ U_{\mu' c'}^{\mu' c} = \delta_{c' c} \delta_{\mu' \mu} (1 + D_{\mu c}) + \delta_{\mu' \mu} A_{\mu c} - \delta_{c' c} \frac{1}{M}, \]

\[ F_{\mu' c'}^{\mu' c} = \delta_{c' c} \sum_{c''} A_{c'' c}^{-1} g_{\mu'' c''} \left( 1 - t_{c' c''} \right). \]

(B43)

Combining the first and the third property, we have \( g_{\mu c c} = g_{\mu c c}^{+} \), which translates into \( A_{\mu c c} = A_{\mu c c}^{+} \). Furthermore, \( \tilde{\rho}_{\mu c c} = \tilde{\rho}_{\mu c c}^{+} \), and

\[ D_{\mu c} = \sum_{c'} g_{\mu c c}^{+} = - \sum_{c'} g_{\mu c c}^{-} = \sum_{c'} g_{\mu c c}^{+} = D_{\mu c}, \]  

(B44)

where we use \( g_{\mu c c}^{+} = g_{\mu c c}^{+} \). The last relationship of Eq. B44 can be proved noting that

\[ \sum_{c'} \left[ (S_{\mu} \cdot \tilde{n}_{c c})^* - (S_{\mu} \cdot \tilde{n}_{c c})^* \right] = S_{\mu} \cdot \sum_{c'} n_{c c} = 0, \]  

(B45)

i.e. the sum of the normal to the sides of a square, pointing outward, is zero. Lastly,

\[ p_{\mu c} = - \sum_{c'} t_{c' c} H_{c' c} g_{\mu c c}^{+} = - \sum_{c'} t_{c' c} H_{c' c} g_{\mu c c}^{-} = -P_{\mu c}. \]  

(B46)

Combining these equations leads to

\[ U_{\mu' c'}^{\mu' c} = U_{\mu' c'}^{\mu' c}, \]

\[ F_{\mu' c'}^{\mu' c} = F_{\mu' c'}^{\mu' c}, \]

\[ G_{\mu c c} = G_{\mu c c}, \]  

(B47)

Hence, Eq. B39 becomes

\[ \sum_{\mu' c'} G_{\mu c \mu' c'} \left( - \tilde{F}_{\mu' c'}^{\text{adj}} \right) = P_{\mu c}, \]  

(B48)

from which we deduce that
\[ \tilde{T}_{\mu c} = -\tilde{T}_{-\mu c}. \quad (B49) \]

In light of this result, we can therefore compute the adjoint solution directly from the forward one, without solving a linear system again. Note that by scaling \( \kappa \) we were able to have the forward and the adjoint solution dimensionally consistent.

Let’s now evaluate Eq. B37. We begin by noting that

\[ \frac{\partial T_{c'}^{adj}}{\partial p} = r_{c'} \delta_{cp} + r_{c'} \delta_{c'p}, \tag{B50} \]

where \( r_{c'} = 1/2(t_{c'}/\rho_c)^2 \). We expand the terms appearing in Eqs. B38–B40,

\[ \frac{\partial \kappa^s}{\partial p} = - \sum_{\mu_c} r_{\mu_c} \left( K_{\mu_c} g_{\mu_c} - K_{c\mu_c} \tilde{T}_{-\mu_c} - g_{c\mu_c} \tilde{T}_{-\mu_c} + g_{\mu_c} \tilde{T}_{c\mu_c} \right), \]

\[ \sum_{\mu_c} \tilde{T}_{\mu c} \frac{\partial p}{\partial p} = \sum_{\mu_c} r_{\mu_c} H_{\mu_c} \left( g_{\mu_c} \tilde{T}_{-\mu_c} - g_{c\mu_c} \tilde{T}_{-\mu_c} \right), \]

\[ - \sum_{\mu'c'} \left( \tilde{T}_{\mu c} \tilde{T}_{\mu' c'} + \tilde{T}_{c\mu} \tilde{T}_{c' \mu'} \right) \] \quad (B51)

where we used Eq. B49. Finally, putting everything together, we have

\[ \frac{\partial \kappa^s}{\partial p} = \sum_{\mu_c} r_{\mu_c} \left[ H_{\mu_c} \left( g_{\mu_c} \tilde{T}_{-\mu_c} - g_{c\mu_c} \tilde{T}_{-\mu_c} + g_{\mu_c} \tilde{T}_{c\mu_c} \right) - K_{\mu_c} g_{\mu_c} - K_{c\mu_c} \tilde{T}_{-\mu_c} + \tilde{T}_{-\mu_c} g_{\mu_c} - \tilde{T}_{c\mu_c} g_{\mu_c} \right] \]

\[ - \sum_{\mu'c'} \left( \tilde{T}_{\mu_c} \tilde{T}_{\mu' c'} + \tilde{T}_{c\mu} \tilde{T}_{c' \mu'} \right). \tag{B52} \]

Lastly, we note that thanks to Eq. B46, we can compute \( \kappa^s \) using directly \( P^s \), i.e.

\[ \kappa^s = \sum_{\mu_c} P_{\mu_c} \tilde{T}_{\mu c} - \sum_{\mu c'} I_{c'c} K_{c c'} g_{\mu c'}, \tag{B53} \]

thus sparing the computation of \( P^{adj} \).

**Supplementary Information** The online version contains supplementary material available at https://doi.org/10.1007/s00158-022-03392-w.

**Acknowledgements** This work was partially supported by MIT-IBM Watson AI Laboratory (Challenge No. 2415).

**Funding** Open Access funding provided by the MIT Libraries.

**Declarations**

**Conflict of interest** The authors declare that they have no conflict of interest.

Replication of results The code developed for this work will be made available as free/open-source software in the next release of Romano (2021a).

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