EFFICIENT COMPUTATIONAL DESIGN AND OPTIMIZATION OF DIELECTRIC METAMATERIAL DEVICES

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ABSTRACT. Dielectric structures composed of many inclusions that manipulate light in ways the bulk materials cannot are commonly seen in the field of metamaterials. In these structures, each inclusion depends on a set of parameters such as location and orientation which are difficult to ascertain. We propose an optimization-based approach for designing such metamaterials in two dimensions by using a fast integral equation and multiple-scattering solver for a given set of parameters. This approach provides the backbone of an automated process for the design and analysis of metamaterials that does not rely on analytical approximations. We demonstrate the validity of our approach with simulations that converge to optimal parameter values and result in substantially better-performing devices.

1. INTRODUCTION

Over the past decade, interest in metamaterials and specifically in dielectric metamaterials has grown considerably. Typically, metamaterials are defined as large-scale structures of natural materials such that the conglomerate electromagnetic properties are unlike those of the underlying materials. Initially, much of the research efforts were focused on exotic applications attained by negative-index metallic-based metamaterials such as cloaking [1] and perfect lenses [2]. In recent years, much of the focus has shifted to dielectric metamaterials which are better-behaved with respect to power dissipation [3] and are easily fabricated [4, 5].

A prominent example of dielectric metamaterials are the dielectric photonic crystals, which have been intensively investigated over the past thirty years [6, 7]. Photonic crystals are composed of a one- to three-dimensional periodic array of nanostructures, in which a small number of cells may be altered or defective. This structure is designed to allow, alter, or prevent the propagation of light for a selected range of wavelengths. These nanostructures can be round holes, such as in the case of Yablonovite [8], or contain a complex network of nano-engineered rods [9, 10]. Thanks to their ability to control light flow, photonic crystals have promising applications in the developing field of optical computing. Replacing electronic components in integrated circuits with their photonic crystal counterparts will reduce the size and latencies of computer processors, while substantially increasing power efficiency [11, 12].

Dielectric metalenses are another class of successful all-dielectric metamaterials. These metalenses allow manipulation of light for many practical applications, including chirality...
imaging [13], imaging with reduced aberrations [14], and optical fiber coupling [15]. Metalenses are typically comprised of numerous sub-wavelength building blocks arranged on a substrate. The properties of these building blocks dictate which effect the overall metalens has on light passing through it. There are many degrees of freedom in designing metalenses; the size, shape, rotation, and material of each individual building block can be adjusted arbitrarily, yielding a large variety of possible metalenses to meet different objectives [16]. Nevertheless, this freedom creates a large search space in choosing these parameters, which may number in the thousands. See the recent survey by Khorasaninejad and Capasso [17].

In order to analyze and design metamaterials, we need to solve the electromagnetic scattering problems they present. The number of particles or inclusions comprising metamaterial devices is typically much higher than the number of shapes or materials used. We note that we consider differently rotated instances of the same shape composed of the same material to be identical. This scattering problem has been primarily solved using the Finite-Difference Time-Domain method (FDTD) [18, 19], which is both simple to implement and well-established. However, this method does not exploit the shape recurrence nor is it capable of naturally handling smooth curves. Other approaches, such as the Plane-Wave Expansion (PWE) [20] and the Bloch-wave method [21], were developed for the purpose of analyzing periodic structures. These methods are applicable to devices which contain unit cell or supercell periodicity, which is not guaranteed in our context.

We propose a specialized optimization-method for analyzing and designing metamaterials in an automated fashion. In our context, the metamaterials contain a small number of unique prototype inclusions compared to the total number of inclusions, or are circular. We say that differently oriented inclusions of the same shape and material have the same prototype. In our method, we first use a boundary integral equation [22] to discretize each prototype inclusion once and transform it to a compressed cylindrical harmonics representation. It is straightforward to rotate and move this representation. We then apply a multiple-scattering approach (first applied to spheres in [23, 24, 25]) on these representations in order to describe the electromagnetic interactions between the inclusions. Once we solve the arising multiple-scattering problem, we can easily compute the electromagnetic field at any point. This combination of boundary integral equation and multiple-scattering methods was first proposed in 1991 [26] and later developed and applied in [27, 28].

The computational complexity of our method is sufficiently low for employing optimization methods that require many solutions. Our approach is most appropriate for optimizing radii in case of circular inclusions, and for optimizing rotation in case of general inclusions. We demonstrate the benefits of our method for two such scenarios, in which the optimization process converges to a significantly better result than the initial guess.

Our optimization-centric approach is novel. The ability to quickly compute the field at any collection of points makes it simple to define and compute an objective function for minimizing and/or maximizing the field intensity at multiple points. The integral equation approach naturally begets gradient-based optimization, which converges to a locally optimal set of parameters and yields an exact result in each step. This allows us to automate the design process of metamaterials that exhibit desired properties, which has not been previously proposed in this context.

The combined integral equation and multiple-scattering approach has other attractive aspects. This approach takes into account the repetitive nature of many metamaterials. By computing the costly full integral equation solution only once per prototype inclusion, we maintain the accuracy of the full solution while significantly reducing the computational
cost of large-scale problems. This additionally allows us to reuse precomputed data in similar settings, for example, in devices that share prototype inclusions but have different arrangements. Finally, this approach does not require the inclusions to be arranged on a grid.

1.1. Related work. We highlight the differences between our approach and other relevant methods. Optimization methods have been applied to the FDTD method with partial success \cite{29}. However, such methods are unlikely to be practical for more general or larger cases. This restriction is due to the high computational complexity required by the FDTD for precise computation, the need to re-solve the entire problem when changes are made to the parameters, and the lack of an analytic gradient. Optimization of photonic crystal devices was performed \cite{30} by means of transformation optics, but this approach was only demonstrated for circular inclusions. A variety of periodic metamaterial devices were successfully optimized \cite{31} for different properties, where the optimization was performed on the parameters of a single unit cell. In contrast, our approach can optimize multiple different unit cells simultaneously. As for analytic approximations of metamaterial devices, optimization methods may be applied in general, however, these approximations are imprecise and are only available for specific devices. In the field of illumination optics \cite{32}, lenses and mirrors are designed for specific illumination properties by means of optimization or PDE solutions. However, these depend on ray optics and are not suitable for subwavelength structures.

1.2. Organization. The remainder of the paper is organized as follows. The problem description and mathematical formulation used for calculating the fields scattered by a collection of inclusions are presented in detail in Section 2. Section 3 presents our optimization framework for the automated design of metamaterials, which is given as pseudocode in Algorithm 1. Numerical results of both rotation angle and radius optimization are shown in Section 4, as well as a time complexity analysis of our approach. In Section 5 we give concluding remarks.

2. Scattering formulation

In this work, problems are restricted to time-harmonic incident fields scattering off a collection of two-dimensional inclusions in free space, where the variation \( \exp(-i\omega t) \) is assumed and suppressed for a given angular frequency \( \omega \). As any incident plane wave can be trivially separated to TE and TM waves with respect to the infinite axis \( \hat{z} \), we restrict this treatment to TM waves. However, the TE formulation is readily available with small modifications. We assume \( M \) inclusion surfaces \( \Omega_m \) with smooth boundaries \( \partial \Omega_m \), in which the wavenumber \( k_m = \omega \sqrt{\mu_0 \varepsilon_m} \) is real and constant, and \( \Omega_0 \) denotes the open free-space domain. Hence the \( \hat{z} \) component of the electric field is the solution of the Helmholtz equation

\[
\nabla^2 u + k_m^2 u = 0, \quad u = \begin{cases} u^\text{inc} + u^s & \text{in } \Omega_0, \\ u^s & \text{in } \Omega_m \neq 0, \end{cases}
\]

where \( u^\text{inc} \) is the given incident field, \( u^s \) is the scattered field, and the jump in both \( u \) and the normal derivative \( \partial u / \partial n \) is zero across all boundaries, corresponding to continuity of the tangential electric field and the normal magnetic flux density. In addition, the scattered field must satisfy the Sommerfeld radiation condition in \( \Omega_0 \), but this is automatically satisfied due to the integral equation method used here.
2.1. Single inclusion formulation. In this section, we describe the first step of the solution process for a multiple-scattering problem, which includes Nyström discretization of a single prototype inclusion and the transformation of its representation from that of boundary potential densities to cylindrical harmonics.

There are three motivations for this transformation. For smooth inclusions, the number of discretization nodes is dramatically larger than the number of cylindrical harmonics, which allows us to precompute the transformation for each inclusion shape once and only deal with the cylindrical harmonics representation without increasing the error in the electric field. This reduces the computational cost of a multiple-scattering problem by several orders of magnitude, and is particularly helpful when multiple iterations of a scattering problem are required for optimization. The second motivation for this representation is that it enables the use of the multiple-scattering translation, that we will apply to accelerate the solution process. Thirdly, cylindrical harmonics are easily rotated and thus only one transformation needs to be calculated for inclusions that are identical up to rotation. Nonetheless, it is difficult to ascertain a priori what the optimal number of cylindrical harmonics is for a given inclusion in a multiple-scattering problem, as this number depends not only on the type and frequency of the incident wave but also on the shape of the inclusion and the distance between it and its closest neighbor. In the past few years some convergence bounds have been developed [33], but in our examples these proved to be highly shape-dependent and not as accurate in the near field.

One drawback of this transformation is its inability to handle touching or intersecting scattering disks, which are fictitious circles strictly enclosing the inclusions, even if the inclusions themselves are adequately separated. The worst manifestation of this issue would occur with thin and long inclusions whose scattering disks cover a disproportionately large area. However, one can partially overcome this restriction by grouping multiple inclusions in close proximity into one disk and rotating them in unison.

Let $\Omega$ denote an inclusion surface with smooth boundary $\partial \Omega$, filled with material with wavenumber $k_1$ and surrounded by free space with wavenumber $k_0$. For notational simplicity, in this section we assume that $\Omega$ is centered at the origin. Note that although we focus only on smooth shapes, if $\partial \Omega$ is not smooth, the method is still applicable with an appropriate discretization approach [34].

2.1.1. Potential expansion. We utilize a layer potentials formulation [35], wherein a single-layer potential density $\sigma$ and a double-layer potential density $\mu$ are assumed to exist on $\partial \Omega$. These densities have unknown complex amplitudes and give rise to the potential representation

\[
 u^s = \begin{cases} 
 S^{k_1} \sigma + D^{k_1} \mu & \text{in } \Omega, \\
 S^{k_0} \sigma + D^{k_0} \mu & \text{otherwise} 
 \end{cases}
\]

for the $\hat{z}$ component of the scattered electric field, where the single- and double-layer potential operators for wavenumber $k$ are defined by

\[
 S^k \sigma(r) := \int_{\partial \Omega} G^k(r, r') \sigma(r') \, dr', \\
 D^k \mu(r) := \int_{\partial \Omega} \frac{\partial G^k}{\partial n_{r'}}(r, r') \mu(r') \, dr'
\]
and \( G^k(\mathbf{r}, \mathbf{r}') = \frac{i}{4} H_0^{(1)}(k|\mathbf{r} - \mathbf{r}'|) \) is the two-dimensional Green’s function for the Helmholtz equation in a homogeneous material. For a given incident field \( u^{\text{inc}} \), the constant permeability TM \( \mathbf{M} \), boundary discretization yields a formula of the form

\[
S^{k_{0}}\sigma - S^{k_{1}}\sigma + D^{k_{0}}\mu - D^{k_{1}}\mu + \mu = -u^{\text{inc}},
\]

of integral equations which holds for all points \( \mathbf{r} \in \partial \Omega \). This system cannot be solved by directly evaluating the operators on the boundary on account of the singularity in \( G^k \) and the hypersingularity in its second-order derivative. Hence we split each integrand into two terms \([36]\), integrating the first term with the Kussmaul-Martensen quadrature rule and the other with trapezoidal or Gauss-Legendre quadrature. Many other choices for the quadrature rule exist and can be used interchangeably, such as the more sophisticated QBX \([37]\). Denote the values of the potential densities \( \sigma, \mu \) on 2N discretization nodes by \( \sigma, \mu \) respectively. We obtain the system of equations

\[
\mathbf{A} \left( \begin{array}{c} \sigma \\ \mu \end{array} \right) = - \left( \begin{array}{c} u^{\text{inc}} \\ \frac{\partial u^{\text{inc}}}{\partial n} \end{array} \right),
\]

in which \( \mathbf{A} \) is a \( 4N \times 4N \) matrix which includes all potential operators.

2.1.2. Transformation to cylindrical-harmonics representation. In order to expand the potentials in terms of cylindrical harmonics, the system \([4]\) is solved for \( 2P + 1 \) incoming waves sampled on the discretization points of the shape, or \( u^{\text{inc}} = J_{p}(k_{0}|\mathbf{z}|)e^{ip\cdot\mathbf{z}} \) for \( p = -P, \ldots, P \). This yields the single- and double-layer potential density vectors \( \sigma_p, \mu_p \) for the \( p \)-th incident wave. For this solution method to maintain reasonable time complexity, this system should be factorized (e.g. LU) for successive direct solutions, thus requiring \( O(N^3 + (2P + 1)N^2) \) computations in total.

Let \( \mathbf{r} \) be a point that lies strictly outside the inclusion such that \( |\mathbf{r}| > |\mathbf{r}'| \) for any \( \mathbf{r}' \) on the boundary. We apply Graf’s addition theorem for Hankel functions to the integral operator formula for the scattered field given by \([2]\) and obtain the cylindrical harmonics expansion

\[
u^{s}(\mathbf{r}) = \sum_{l=-P}^{P} s_{l,p} H_{l}^{(1)}(k_{0}|\mathbf{r}|)e^{il\hat{\mathbf{n}} \cdot \mathbf{r}},
\]

\[
s_{l,p} := \frac{i}{4} \int_{\partial \Omega} J_{l}(k_{0}|\mathbf{r}'|)e^{-il\hat{\mathbf{n}} \cdot \mathbf{r}'}\sigma_{p}(\mathbf{r}') + \hat{\mathbf{n}} \cdot \nabla \left[ J_{l}(k_{0}|\mathbf{r}'|)e^{-il\hat{\mathbf{n}} \cdot \mathbf{r}'} \right] \mu_{p}(\mathbf{r}') \, d\mathbf{r}'
\]

of the potential operators. Notably, this expansion only holds strictly outside the inclusion, and thus we assume a fictitious scattering disk \( D \) which strictly encloses the inclusion. Inside this disk, the direct integral equation representation is assumed, while outside of it the expansion \([6]\) holds. In this work the diameter of the scattering disks is chosen to be 10% larger than the inclusion diameter. While the diameter of the scattering disk can be reduced if necessary, this typically leads to a dramatic increase in \( P \). Approximating the integral above with the same boundary discretization yields a formula of the form \( s_{l,p} = (\mathbf{A} \sigma_p + \mathbf{B} \mu_p)_l \), which in turn yields the entire scattering matrix \( \mathbf{X}^{(m)} = \mathbf{A} \Sigma + \mathbf{B} \mathbf{M} \) for the \( m \)-th inclusion, where the \( p \)-th column of \( \Sigma \) is \( \sigma_p \) and similarly for \( \mathbf{M} \) and \( \mu_p \).

As mentioned earlier, the process above only needs to be carried out once per inclusion, up to rotation. The representation of an inclusion rotated by an angle \( \varphi_m \) is readily available.
by multiplying the \((l, p)\)-th element of \(X^{(m)}\) by a factor of \(e^{-ip\theta_m(l-p)}\), in other words, by replacing the scattering matrix with \(\Phi X^{(m)}\Phi^*\) for the diagonal matrix \(\Phi_{\beta,p} = e^{-ip\phi_m}\).

Now let \(\Omega_m\) be centered at \(o^{(m)}\) with a local coordinate system \(r^{(m)} = r - o^{(m)}\). In order to use the scattering matrix to solve scattering of an incident field \(u^{inc}\) from the single \(m\)-th inclusion, we first expand \(u^{inc}\) as

\[
u^{inc} = \sum_{p=-P}^{P} \alpha_{p} J_{p}(k_{0}|r^{(m)}|)e^{ip\angle r^{(m)}}.\]

Due to the Jacobi-Anger expansion in the particular case of plane-wave incidence \(e^{ik\cdot r}\) for some \(k = (k \cos \theta_i, k \sin \theta_i)\), we have \(\alpha_{p} = e^{ip(\pi/2-\theta_i)}\) in the local coordinates up to multiplication by a phase constant.

The electric field scattered by the inclusion is given by the outgoing expansion

\[
u^{s} = \sum_{p=-P}^{P} \beta^{(m)}_{p} H_{p}^{(1)}(k_{0}|r^{(m)}|)e^{ip\angle r^{(m)}},\]

that is, a linear combination of the scattering matrix columns, where in this case, \(\beta^{(m)}_{p} = (X^{(m)}\alpha^{(m)})_{p}\).

Note that circular inclusions can be analytically represented using a diagonal scattering matrix by utilizing orthogonality of the basis functions on a circle. For such an inclusion with radius \(R\), the scattering matrix components are readily given by

\[
\beta_{p} = -\alpha_{p} \frac{J_{p}(k_{0}R)J'_{p}(k_{1}R) - J'_{p}(k_{0}R)J_{p}(k_{1}R)}{H_{p}^{(1)}(k_{0}R)J'_{p}(k_{1}R) - H'_{p}^{(1)}(k_{0}R)J_{p}(k_{1}R)},
\]

where \(Z_{p}^{(1)} = k \left( Z_{p-1}(kR) - (p/kR)Z_{p}(kR) \right)\) for \(Z_{p} = J_{p}, H_{p}^{(1)}\).

Two error mechanisms affect the accuracy of the solution beyond the adjustable FMM truncation and quadrature error discussed in Section 2.3. First we have the discretization error due to the finite number of nodes \(2N\) on the inclusion boundary, with the second stemming from the transformation to a cylindrical harmonics formulation. We denote by \(\Delta u\) the normalized RMS errors for these error mechanisms. The discretization error is computed as follows: a fictitious line source is assumed at some point inside the inclusion along with an incident plane wave outside of it. The potential densities \(\sigma, \mu\) on the boundaries \(\partial \Omega\) attained from solving the potential density system \([5]\) induce fields outside the inclusion that are equivalent to those of the line source, up to the error that is measured on the scattering disk \(D\). The cylindrical harmonics transformation error is measured by comparing the field induced by the potential densities to that of the cylindrical harmonics on points distanced \(2D\) from the inclusion center. Fig. 1 shows an example of the relation between \(N\) and \(P\) and their respective errors for two inclusion shapes. Note that not only is \(N\) substantially larger than \(P\) for all values of \(\Delta u\), but the ratio between them continues to grow as the desired errors diminish.

2.2. Multiple-scattering formulation. Here we apply the principles used in the preceding section to a multiple-scattering setting. Previously, the relation between incoming and outgoing coefficients was given by the scattering matrix, however, the incident field of a single inclusion in a multiple-scattering scenario is a combination of the incident field and the fields reflected off all other inclusions. A translation matrix is used to transform
Figure 1. Minimum discretization nodes and cylindrical harmonics for two inclusion shapes. (a) Rounded star with the smooth boundary parametrization \( \mathbf{r}(\theta) = [R + a \cos(5\theta)] (\cos \theta, \sin \theta) \) for \( R = 0.3\lambda_0 \), \( a = 0.1\lambda_0 \), and \( k_1 = 1.5k_0 \), and its scattering disk \( D \). (b) Squircle with \( R = 0.35\lambda_0 \) and \( k_1 = 1.5k_0 \), and its scattering disk \( D \). (c) Minimum values of the discretization nodes \( N \) and number of cylindrical harmonics \( P \) for given discretization and cylindrical transformation error, respectively, for these two inclusions.

the reflected field from the local coordinates of one inclusion to the local coordinates of another \cite{25}.

Let \( \mathbf{r}^{(m)} \) and \( \mathbf{r}^{(m')} \) denote a point in the local coordinates of the \( m \)-th and \( m' \)-th inclusions, respectively, and let \( \mathbf{r}^{(m',m)} \) be the coordinates of the \( m' \)-th inclusion with respect to the center of the \( m \)-th inclusion. Using Graf’s addition formula and truncating the higher-order
elements, we obtain the relation between the two local expansions

$$\sum_{p=-P}^{P} \beta_{p}^{(m)} H_{p}^{(1)}(k_{0}|r^{(m)}|) e^{ip \angle r^{(m)}} =$$

$$\sum_{\mu=-P}^{P} J_{\mu}(k_{0}|r^{(m')}|) e^{i \mu \angle r^{(m')}} \sum_{p=-P}^{P} \beta_{p}^{(m)} \left( T^{(m',m)} \right)_{\mu,p},$$

where $T^{(m',m)}$ with the elements

$$\left( T^{(m',m)} \right)_{\mu,p} = e^{i(p-\mu) \angle r^{(m',m)}} H_{p-\mu}^{(1)}(k_{0}|r^{(m',m)}|)$$

is the translation matrix which translates the outgoing coefficients of one inclusion to the incoming coefficients of another. Summing over the contributions of all the inclusions, we obtain the complete incoming coefficients of the $m'$-th particle

$$\tilde{\alpha}^{(m')} = \alpha^{(m')} + \sum_{m \neq m'} T^{(m',m)} \beta^{(m)}.$$  

Finally, we note that $\beta^{(m')} = X^{(m')} \tilde{\alpha}^{(m')}$ holds for the complete incoming coefficients, and substitute this relation into (12) to obtain

$$\left( X^{(m')} \right)^{-1} \beta^{(m')} - \sum_{m \neq m'} T^{(m',m)} \beta^{(m)} = \alpha^{(m')}.$$  

Thus yielding a system of $(2P + 1)M$ equations, where $M$ is the number of inclusions. A preconditioned scattering system is obtained when multiplying both sides by the block scattering matrix, which we denote in concatenated form by

$$(I - XT) \beta = X \alpha.$$  

2.2.1. Electric field computation. Once the multiple-scattering system (14) is solved, the scattered field at any point outside the scattering disks is readily calculated by summing (8) over all inclusions. Strictly inside the inclusions, the field is given by the discretized integral equation (2), where the densities are

$$\sigma^{(m)} = \Sigma \left( X^{(m)} \right)^{-1} \beta^{(m)}, \quad \mu^{(m)} = M \left( X^{(m)} \right)^{-1} \beta^{(m)}.$$  

These are weighted sums of those $\sigma_{p}$, $\mu_{p}$ obtained from solving (5) for the different incoming waves, as the expansion (8) of the inclusion is not valid inside the scattering disk. Between the $m$-th inclusion and its disk, the scattered field $u^{s}$ is given by summing (8) over all $m' \neq m$ and then adding the direct integral operator for $m$.

2.3. FMM acceleration of the translation. As the computational cost of directly solving (14) becomes prohibitively high for a large number of inclusions, this system should be solved iteratively. While applying the block-diagonal scattering matrix $X$ in each iteration requires only $O(M)$ operations, the translation matrix is almost fully populated and thus requires $O(M^2)$ operations. Therefore, we choose to apply the block translation matrix $T$ using FMM [28], yielding a lower complexity that will be analyzed in the next section. In this section, we shall succinctly describe the FMM process for this problem. Assume a collection of many inclusions, divided into $G$ non-empty $a \times a$ boxes. The FMM process converts the translation matrix to a sequence of operators. These operators aggregate the
translation matrices of multiple inclusions in one box, translate them to a different box and disaggregate them to the inclusions in said box. Note that this process assumes the boxes have some minimal distance between them. For boxes which are closer than this minimal distance, or are the same box, the appropriate blocks of the translation matrix $T$ are directly applied via a sparse near-interaction matrix.

Let the $m$, $m'$-th inclusions which are centered at $o(m)$, $o(m')$ be placed in boxes centered at $c$, $c'$ respectively. Provided $c$, $c'$ are distanced by at least $\sqrt{2}a$, Graf’s addition and Bessel’s integral theorem are applied to the translation matrix in (11), which results in

$$
(T^{(m',m)})_{\mu,p} = \frac{1}{2\pi} \int_0^{2\pi} e^{ik(\alpha(m')-c')} \mathcal{F}_\infty(\theta,c'-c)e^{-ik(\alpha(m)-c)}e^{i(\mu-p)(\pi/2-\theta)} \, d\theta,
$$

where $k = (k \cos \theta, k \sin \theta)$, and the truncated FMM translation function which transmits plane waves from $c$ to $c'$ is defined as

$$
\mathcal{F}_{\text{FMM}}(\theta,x) := \sum_{\xi=-P_{\text{FMM}}}^{P_{\text{FMM}}} H^{(1)}_\xi(k|x|)e^{i\xi(\angle x+\pi/2-\theta)}.
$$

Although this translation function must be truncated for practical computations, the series does not converge for small values of $P_{\text{FMM}}$ and oscillates when it is large, making the optimal choice of $P_{\text{FMM}}$ an extensively-studied, non-trivial problem [33]. Several analytical and empirical formulas have been proposed for this truncation, of which the excess bandwidth formula [39] is used here, such that for $\delta$ digits of accuracy

$$
P_{\text{FMM}} := \sqrt{2}ka + 1.8 \left(\delta^2 \sqrt{2}ka\right)^{1/3}.
$$

Assuming this series truncation, the integral expansion of the Bessel function has finite bandwidth such that a $Q \propto P_{\text{FMM}}$-point quadrature of $[0,2\pi]$ is sufficient. Hence if we define $k_q := (k \cos \theta_q, k \sin \theta_q)$, the translation matrix is approximated as

$$
(T^{(m',m)})_{\mu,n} \approx \frac{1}{Q} \sum_{q=1}^{Q} e^{i\xi \left(\alpha(m')-c'\right)} e^{i\mu(\pi/2-\theta_q)} 
$$

$$
disaggregation

$$
\mathcal{F}_{\text{FMM}}(\theta_q,c'-c)e^{-ik_q(\alpha(m)-c)}e^{-i\pi(\pi/2-\theta_q)}
$$

aggregation

We now construct the FMM matrices used for matrix-vector product acceleration. Denote by $M_g$ the number of inclusions in the $g$-th box, centered at $c_g$. We construct a $1 \times M_g$ block aggregation matrix, containing a block for every inclusion, with the $m$-th block given by

$$
(A^{(m)})_{q,n} := e^{-ik_q(\alpha(m)-c_g)-in(\pi/2-\theta_q)} \quad q = 1, \ldots, Q, \quad n = -P, \ldots, P
$$

Since FMM is applied to every box with respect to every other box, we construct the disaggregation matrix by applying the conjugate transpose to the aggregation matrix.

Finally, for each pair $(g',g)$ of sufficiently distant boxes, a diagonal FMM translation matrix $F^{(g',g)}$ is constructed by

$$
(F^{(g',g)})_{q,q} := \frac{1}{Q} \mathcal{F}_{\text{FMM}}(\theta_q,c_{g'}-c_g), \quad q = 1, \ldots, Q.
$$
2.4. FMM complexity. Complexity analyses for the application of the FMM to various problems are well established, generally leading to a single-level result of $O(N_{\text{dof}}^{1.5})$ and multi-level complexity $O(N_{\text{dof}} \log N_{\text{dof}})$ for $N_{\text{dof}}$ degrees of freedom. However, the relationship between the optimal number of boxes and the wavenumber is different in the multiple-scattering approach, and therefore we find it instructive to briefly analyze the complexity of our FMM application.

Since each aggregation matrix is of dimension $Q \times M_g(2P + 1)$, performing the aggregation of all $G$ boxes has time complexity $O(MQ(2P+1))$, and thus so does the total disaggregation. The time complexity of performing all box-to-box FMM translations is $O(QG^2)$, while the number of nonzero elements in the near-interaction matrix is

$$\sum_{g} M_g^2 + M_g.$$  \hspace{1cm} (22)

Therefore, applying the near-interaction matrix is expected to require $(2P+1)^2 \sum_{g} [M_g^2 + M_g]$ operations. Including the computational cost of applying the scattering and identity matrices, applying the operator $(I - XT)$ using FMM has time complexity

$$O \left( MQ(2P + 1) + QG^2 + (2P + 1)^2 \sum_{g} [M_g^2 + M_g] + M(2P + 1)^2 \right).$$  \hspace{1cm} (23)

Since the quadrature $Q$ is proportional to the diameter of each box, and in two dimensions the area of a box is inversely proportional to the number of boxes, we have $Q \propto G^{-0.5}$. If we assume an approximately constant distribution of inclusions in boxes such that $M_g \approx M/G$, the FMM time complexity expression is simplified to

$$O \left( G^{1.5} + (2P + 1)^2 M^2G^{-1} \right).$$  \hspace{1cm} (24)

We note that while the usual FMM choice $G \propto \sqrt{M}$ yields a complexity of $O(M^{1.5})$, selecting $G = bM^{0.8}$ for a constant $b$ reduces the complexity to $O(M^{1.2})$ per FMM solution with regard to the number of inclusions. In practice, even a choice of $G \propto M$ may be optimal due to the quadratic dependence of the second complexity term on the wavelength. An analogous analysis of a Multi-Level Fast Multipole Algorithm (MLFMA) approach will lead to asymptotic complexity of $O(M)$ \cite{28}, although this is only beneficial in practice for very large values of $M$.

3. Optimization for multiple-scattering features

We give a description of a general optimization problem that is applicable to various metamaterials, where our aim is to provide a template for applying our framework to different devices. We define an objective function that depends on the electric field value at multiple points, develop its gradient, and show how it can be computed in order to find optimal parameters for the overall structure. Let $u$ be the total electric field evaluated at $I$ points of interest $r_i$ that are assumed to lie outside all scattering disks. We may define the objective function

$$f_{\text{obj}} := \sum_{i=1}^{I} |u(r_i)|^2.$$  \hspace{1cm} (25)
Although points inside the scattering disks may also be considered, this complicates and slows down the optimization procedure and thus will not be considered here. Note that whether we are minimizing or maximizing the objective function is immaterial, as maximization problems can be solved by minimizing the negated objective function and again negating the achieved minimum value. Simultaneously minimizing intensity several points while maximizing it at others is achieved by appropriately weighting the objective function. For convenience, we rewrite the field values in the objective function in terms of $\beta$ and obtain the column vector $u = H^{T} \beta + u^{inc}$ and the simplified form $f_{\text{obj}} = \|u\|^2$, where $H$ relates the coefficient solution to the objective function.

At this point we shall derive the objective gradient $g_{\text{obj}} := \nabla f_{\text{obj}}$ in order to utilize gradient-based optimization methods, which are generally superior to their derivative-free counterparts with respect to convergence. Let $w$ denote a vector of $J$ inclusion parameters, where we assume each parameter affects the shape of an inclusion, but not the location of its center, and therefore $H$ remains constant. Then the gradient of our optimization problem is readily shown to be

$$g_{\text{obj}} = \nabla_{w} \sum_{i} |u(r_{i})|^2 = 2\Re \left[ (\nabla_{w} u) \bar{u} \right], \quad \text{(26)}$$

where $\bar{u}$ denotes the complex conjugate of $u$, $\Re(\cdot)$ stands for the real part, and $\nabla_{w} u$ contains the derivatives of the field with respect to the inclusion parameters. Utilizing the simplified form for $u$, it remains to compute $\partial \beta / \partial w_{j}$ for $j = 1, \ldots, J$, which is done by differentiating the multiple-scattering equation (14) with respect to the parameter $w_{j}$ at the optimization point $w$. This yields a system of multiple-scattering equations that we solve with FMM, i.e.,

$$ (I - XT) \frac{\partial \beta}{\partial w_{j}} = \frac{\partial X}{\partial w_{j}} X^{-1} \beta, \quad j = 1, \ldots, J, \quad \text{(27)} $$

where the differentiation can be analytical, as in the examples here, or numerical. All in all, a single evaluation of the objective function and its gradient has the computational cost of $J + 1$ FMM solutions in addition to the right-hand side calculations in (27), and all gradient components can be computed in parallel.

In practice, applications of this optimization technique assume that each parameter $w$ only affects the shape of a single inclusion. Under this assumption, we have that the block matrix $\frac{\partial X}{\partial w_{j}}$ is nonzero only in its $j$-th block $X^{(j)}$, and thus the right-hand side of (27) has $2P + 1$ nonzero elements. Assuming the inverses or factorizations of the scattering matrices are available from earlier stages of our process, the time complexity of calculating all $J$ right-hand sides is $O(J(2P + 1)^2)$. Once all derivatives of $\beta$ are calculated, the gradient (26) can be computed in $O(IJ)$ steps. A description of the complete process of automatically designing a device via our approach is summarized in Algorithm 1. The specifics depend on the optimization method used, where additional evaluations of $f_{\text{obj}}$ might be necessary for the optimization line search.

In this work, we optimize inclusion parameters for which $\nabla_{w} X$ is analytic, such as the rotation angle of an arbitrary inclusion and the radius of a circular inclusion. This significantly simplifies the computation of the gradient. Attempting to optimize parameters that do change the structure of $X$ is more involved, and may require numerical differentiation.
Algorithm 1: Automated design of dielectric metamaterials

Input: initial value \( w = w_1, \ldots, w_J \) for optimization

// Precomputation phase
1 for all distinct non-circular inclusions do
  2 Construct and solve potential density equation (5) for \(-P, \ldots, P\)
end

4 Prepare FMM matrices // using the development in Section 2.3
5 while optimization has not converged do
  6 \( \beta \leftarrow \) solve multiple-scattering equation (14) with FMM
  7 Calculate \( f_{\text{obj}} \) using \( \beta \)
    // Construct gradient:
  8 for \( w_j \in w \) do
    9 Build right-hand side of (27) for \( w_j \) using \( \beta \)
    10 Solve (27) with FMM
    11 Compute \( j\)-th component of \( g_{\text{obj}} \) from (26)
  12 end
  13 \( w \leftarrow \) next optimization point
end

4. Numerical results

In this section, we demonstrate our approach on three examples. First, we study the run time of the multiple-scattering approach for increasingly numerous inclusions. Additionally, we apply the optimization process in its entirety to two practical examples, resulting in improved designs. In what follows, all values of \( 2N \), the number of discretization nodes, and \( P \), the cylindrical harmonics parameter, are chosen to be the minimal values for which an electric field error of \( 10^{-6} \) holds, as explained in Section 2.1.2. All linear systems solved via FMM use GMRES [40] with tolerance \( 10^{-6} \) as the underlying iterative method. All simulations were written in the Julia programming language [41], and run on a 3.4GHz Intel Core i7-6700 CPU with 32GB of memory.

4.1. Complexity of multiple-scattering approach. We examine the run time of the multiple-scattering algorithm for a square \( \sqrt{M} \times \sqrt{M} \) grid of inclusions, and compare it to the theoretical complexity analysis in Section 2.4. Fig. 2 depicts the run time of solving the multiple-scattering equation (14) using FMM for several values of \( M \). The minimal values of \( N \) and \( P \) for \( \Delta u = 10^{-6} \) and this inclusion are \( N = 342 \) and \( P = 10 \). The precomputation of the prototype inclusion for these values was performed once for all simulations and required 0.9s that were not included in the plot. A single matrix-vector product scales almost linearly with the number of inclusions, in accordance with the complexity analysis. The total solution convergence time has complexity \( O(M^{2.1}) \), i.e., the number of iterations depends on the number of inclusions, which is not uncommon when solving electromagnetic equation systems with Krylov subspace methods. Nonetheless, the total solution time is several orders of magnitude below that achievable by a naive method.

4.2. Rotation-angle optimization for arbitrary inclusions. For our first optimization example, we apply our framework to the optimization of inclusion rotation. That is, given an incident wave with wavelength \( \lambda_0 \) scattered by a collection of \( M \) inclusions, we wish to
Figure 2. Run time of the multiple-scattering system solution, as well as of a single matrix-vector product, for different numbers of inclusions. Here an incident plane wave is scattered by a $\sqrt{M} \times \sqrt{M}$ grid of identical rounded stars, randomly rotated. Here the inclusion parameters are $R = 0.3\lambda_0$, $a = 0.1\lambda_0$ and $k_1 = 1.5k_0$, and are distanced $0.9\lambda_0$.

find the optimal rotation angles $\varphi$ of the inclusions such that the field propagation in some desired direction is maximized.

The derivatives of the scattering matrices with respect to the rotation angles are given by

$$
\left( \frac{\partial X^{(m)}}{\partial \varphi_j} \right)_{u,v} = -i\delta_{m,j} (u - v) X^{(m)}_{u,v} = \delta_{m,j} \left( DX^{(m)} - X^{(m)} D \right)_{u,v},
$$

where $(D)_{u,v} = -\delta_{u,v}iu$. This immediately implies that the right-hand side of (27) for the $j$-th derivative of the outgoing coefficients has $2P + 1$ nonzero elements, given by $[D - X^{(j)}D(X^{(j)})^{-1}]\beta^{(j)}$. Since the rotation angles are unconstrained, our choice of optimization method is the Broyden-Fletcher-Goldfarb-Shanno (BFGS) [42] algorithm, which is a quasi-Newton method that locally approximates the objective function as a quadratic. In each iteration, once the descent direction is decided via the gradient, a line search is necessary to determine the step size to the minimum in that direction. While several such line-search methods exist, some require re-computing the gradient which is $M$ times as costly as an objective function evaluation. One method, which only utilizes the objective function and the local gradient, is the backtracking method based on the Armijo-Goldstein condition [43], which is used here.

In Fig. 3, we simulate the case of a $\hat{y}$-traveling plane wave incident upon a collection of $M = 100$ inclusions, randomly positioned in a $21\lambda_0 \times 7\lambda_0$ rectangle such that the scattering disks do not intersect. Inclusions are rounded stars with the same size as in Fig. 1, have wavenumber $k_1 = 3k_0$ and use the minimal parameters $N = 934$, $P = 12$. The objective
function is set as in (25) for $I = 10$ points of interest $\mathbf{r}_i$ located equidistantly along the top boundary of the rectangle. The field amplitude at the points of interest $\mathbf{r}_i$ is substantially larger after convergence of the optimization process. Specifically, the BFGS method converges to an average field magnitude of 1.49 at $\mathbf{r}_i$, up from the initial 0.43 (in the RMS sense). The process required 91 iterations and 21,400 seconds for convergence criterion $\Delta f_{\text{obj}} < 10^{-6}$.

4.3. **Radius optimization for circular inclusions.** We now consider optimization of the radii of circular inclusions, where in contrast to the previous example, both the scattering matrices and their derivatives with respect to the inclusion radius are diagonal and have analytical form. This example is motivated by the photonic crystal implementation of the Luneburg lens. The two-dimensional Luneburg lens [44] is a symmetric circular lens designed such that incoming plane waves are focused to a single point on its rim, and no waves are reflected. This property is achieved by a continuously varying refractive index given by the analytic solution $n(r) = \sqrt{2 - \left(\frac{r}{R_{\text{lens}}}\right)^2}$, where $r$ is the distance from the center of the lens, which has radius $R_{\text{lens}}$. One way of fabricating a Luneburg lens is via long dielectric rods on a glass substrate, which, if long enough, can be assumed to be infinite. Thus the electromagnetic propagation through the device can be treated as a two-dimensional problem. In this setting, the lens is divided into unit cells on a square grid, each with side length $a$. Each unit cell $m$ contains a circular inclusion with the same relative permittivity $\varepsilon_r$ but differing radius $R_m$, such that the effective refractive index in the cell can be approximated analytically for sufficiently small $a/\lambda_0$ [45], and thus the radii are set such that the average permittivity approximates the Luneburg solution.

This implementation of the Luneburg lens begs the question whether the electromagnetic focusing could be improved by sacrificing the rotational symmetry of the device, however, note that the restriction to a square grid has already limited this symmetry. To answer this question, we propose optimizing over the radii of the inclusions to maximize the field amplitude at the focal point. Note that since the inclusions are circular, the computation of the gradient is computationally cheaper than in the previous example, as is applying the diagonal scattering matrix in each FMM iteration. Care must be taken to assure that the computed radii are neither below some non-negative lower practical limit $R_{\text{min}}$ nor above the limit $R_{\text{max}}$ at which they are too close for the multiple-scattering approximation in this work, i.e. 0.45a. Thus unconstrained optimization methods such as BFGS are no longer an option. Fortunately, these so-called box constraints are simple enough to be tackled by the addition of a penalty term which sharpens the constraint from one BFGS run to the next.

In Fig. [4] we consider focusing of an $x$-traveling plane wave to the focal point $(R_{\text{lens}}, 0)$ on the lens rim. In this example, there are 316 circular inclusions with relative permittivity $\varepsilon_r = 4.5$, placed on a square grid with lattice constant $a = 0.2\lambda_0$. The total lens radius is $R_{\text{lens}} = 10a$, while the cylindrical harmonics parameter is $P = 5$, and the initial guess is $R_m = a/4$ for all inclusions. The penalized BFGS algorithm converged to a local maximum of $f_{\text{obj}} = 26.21$ after 123 total iterations and 36,600 seconds, with the convergence criterion $\Delta R < 10^{-6}$. Supplementary Video S1 shows the electric field amplitude throughout the optimization process, where the gradual evolution of the optimized device is clearly visible.

The optimization process yields a device that focuses the incoming electric field substantially better than the Luneburg lens, improving upon the Luneburg design by an amplitude factor of 1.55. Additionally, the optimized design is more intricate than typical intuitive
Figure 3. Optimization of rotation angles. (a) Initial electric field amplitude after scattering by $M = 100$ randomly positioned identical rounded stars with zero rotation, which prevent the $\hat{y}$-traveling plane wave from propagating in its original direction. (b) Electric field amplitude for the same inclusions, with rotation angles optimized to maximize upward scattering. (c) Convergence behavior of the objective function $f_{\text{obj}}$ and its gradient $g_{\text{obj}}$. 
Figure 4. Radius optimization of 316 circular inclusions with $\varepsilon_r = 4.5$ for focusing an $\hat{x}$-traveling plane wave to a single focal point on the lens rim. (a) Initial electric field amplitude. (b) Convergence progress of the objective function and its gradient norm as a function of the penalized BFGS iteration. Markers indicate the beginning of an outer iteration. (c) Electric field amplitude after convergence. (d) Electric field amplitude of the Luneburg lens approximation.

approximations, thus corroborating our promotion of an automated approach. Interestingly, the algorithm produced symmetric radii with respect to the $x$ axis, although this was not an optimization constraint. Applying this constraint, thereby halving the optimization variables, yields a similar result in only 15,000 seconds, less than half of the time required originally.

5. Conclusion

We proposed an automated approach for designing dielectric metamaterials with desired electromagnetic properties. Our approach uses gradient-based optimization that provides quick and reliable convergence as well as a fast boundary integral equation solver for precisely computing the field at any point. The work herein provides a conceptual shift in
the way metamaterials are designed, moving from analytical approximations and manual trial-and-error to rigorous optimization. Our approach should be especially attractive in designing photonic crystals, metalenses, and other devices composed of many substructures whose large number of design parameters would typically render optimal manual design impossible. Although optimization may superficially seem prohibitively expensive for these high-dimensional design problems, our fast solution method makes it practical. We implemented the methods described in this paper for the publicly available open-source software package **ParticleScattering.jl** [46] in the Julia programming language [41], which also includes the examples presented here.

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