Cascaded Metasurface Design Using Electromagnetic Inversion with Gradient-Based Optimization

Trevor Brown and Puyan Mojabi, Member, IEEE

Abstract—This paper presents an electromagnetic inversion algorithm for the design of cascaded metasurfaces that enables the design process to begin from more practical output field specifications such as a desired power pattern or far-field performance criteria. Thus, this method combines the greater field transformation support of multiple metasurfaces with the flexibility of the electromagnetic inverse source framework. To this end, two optimization problems are formed: one associated with the interior space between two metasurfaces, and the other for the exterior space. The cost functionals corresponding to each of these two optimization problems are minimized using the nonlinear conjugate gradient algorithm with analytic expressions for the gradient operators. The numerical implementation of the developed design procedure is presented in detail, including a total variation regularizer that is incorporated into the optimization procedure to favour smooth field variations from one unit cell to the next. The capabilities of the method are demonstrated by converting the produced surface susceptibilities into three-layer admittance sheet models, which are simulated in several two-dimensional (2D) examples.

Index Terms—Electromagnetic metasurfaces, inverse problems, inverse source problems, optimization, pattern synthesis.

I. INTRODUCTION

METASURFACES offer a level of systematic control over electromagnetic fields not typically possible with conventional materials [1]–[6]. They have several applications such as radiation pattern control [7], polarization control [8], [9], impedance matching [10], cloaking [11], and others. Fabrication of these metasurfaces is often much simpler than bulk metamaterials, typically using established printed circuit board (PCB) techniques and materials. Metasurface design can be decomposed into two distinct steps: macroscopic and microscopic [12]. The first step, macroscopic design, is to determine a homogenized representation of the metasurface that is able to effectively model the desired field transformation, e.g., via surface susceptibilities [13]. The second step, microscopic design, is to determine physical unit cell structures that exhibit the behaviour of the metasurface model [14], [15]. Microscopic design, although important, is not considered in the work presented here.

Several macroscopic metasurface design methods can be found in recent literature [12], [13]; however, most methods require knowledge of both the incident and the desired transmitted field on the metasurface itself. While the incident field is either known analytically or easily measured, an analytical representation of the transmitted field is typically only possible in ideal cases involving plane waves or other simple fields. We recently presented a macroscopic design method that allows for more practical design criteria, such as far-field (FF) performance criteria (e.g., main beam direction, half-power beamwidth (HPBW), null locations, etc.) [16]–[18]. Since this method is based on solving an electromagnetic inverse source problem, we have referred to this approach as an electromagnetic inversion algorithm for metasurface design. Subsequently, in [19], we modified this inversion method by augmenting its associated cost functional to enforce local power conservation (LPC) [20], [21] which ensures the resulting metasurfaces can be implemented using passive, lossless, and reciprocal elements. While practically necessary, the drawback of enforcing LPC is that the supported field transformations are restricted. One possible solution is to utilize multiple metasurfaces in succession, as described in [7], [22]–[27]. In this scenario, the field transformations at each metasurface still satisfy LPC, but the transmitted field from the last metasurface no longer has to have the same power distribution as the field incident on the first metasurface. This extra freedom can support a greater variety of output fields by allowing for a redistribution of the incident field power onto the final (output) metasurface. Considering the cascaded metasurfaces as a single structure, total power is still conserved from incident to output fields but the power is redistributed locally.

The design methods presented in [7], [22]–[27] utilize metasurface pairs to perform field transformations that would not be possible with a single metasurface. Similar to the macroscopic design methods mentioned above, these methods often require explicit knowledge of the transmitted field on the output metasurface. Alternatively, antenna array synthesis techniques have also been used to find the required tangential fields [24], [28]. These array synthesis techniques are powerful, well-established, and provide a great deal of insight; however, they have their own limitations. For example, they are mostly concerned with linear or planar structures which could limit their application to non-planar metasurfaces. In addition, some synthesis techniques are applicable to field pattern synthesis (desired amplitude and phase) which could then limit their application to the design of intensity distributions such as those reported in [29]. On the other hand, while more general shaped beam power pattern synthesis techniques exist, some
approaches are more suitable for particular cases such as patterns with equal side lobe levels or equally spaced linear arrays [30]. As described in [31], the inverse problem formulation of the antenna synthesis problem can serve as a unified framework to accommodate various forms of power and field pattern syntheses. In addition, as shown by the antenna characterization community, the inverse source formulation can be applied to surfaces of arbitrary shapes, can take into account surface truncation, and can be used for both near-field and far-field data; e.g., see [32], [33]. Consequently, the inverse formulation can offer the same benefits for the design of metasurfaces to achieve desired field patterns, power patterns, near-field distributions, or FP performance criteria. Finally, the inversion approach can be augmented by different constraints to favor a trade-off between achieving desired pattern features and other design parameters [19]. To this end, the aim of this paper is to adapt the electromagnetic inversion metasurface design method to the design of cascaded metasurfaces (in our case, two metasurfaces) to allow for more general output field specifications.

Herein, we cast the design problem as two optimization problems. The first problem aims to infer the required tangential fields on the output surface of the second metasurface so as to meet the field specifications. The second problem is concerned with finding the tangential fields in the interior space between the two metasurfaces. It is worth noting that while in [19] we used a stochastic method (particle swarm) to enforce LPC in the inversion process, in this work we use gradient-based optimization for improved convergence. Furthermore, we introduce regularization into the optimization process based on the $L^2$-norm total variation (TV) regularizer commonly used for the inverse problem associated with microwave imaging [34], [35]. This regularizer has a smoothing effect on the achievable solution which translates into less field variations from one unit cell of the metasurface to the neighbouring unit cell. This results in several benefits which will be discussed in the paper.

We begin with a description of the problem statement followed by a high-level overview of the proposed methodology. We then explain the numerical implementation of each step of the method in detail. This is followed by a series of full-wave simulated examples in both 2D transverse magnetic and transverse electric cases. Lastly, we present our conclusions and identify the existing limitations of the proposed method.

II. PROBLEM STATEMENT

We consider the design of a pair of metasurfaces, denoted respectively as $\Sigma_1$ and $\Sigma_2$ as shown in Figure 1. In this paper we restrict our discussion to that of planar, parallel metasurfaces separated by a distance $d$, but the theory presented is consistent with more complicated geometries. A known electromagnetic source produces an incident field $\Psi_{\text{inc}}$ where $\Psi \in \{ \vec{E}, \vec{H} \}$ that impinges on the input metasurface, $\Sigma_1$. The interaction of this incident field with the pair of metasurfaces will create a reflected field $\Psi_{\text{ref}}$ (which may be zero) emanating from $\Sigma_1$ and a transmitted field $\Psi_{\text{tr}}$ emanating from the output metasurface, $\Sigma_2$.

It is important to note that this design method does not require prior knowledge of $\Psi_{\text{tr}}$ as is common in alternative methods, but rather a set of user-defined field specifications, denoted as $f$ on some region of interest $S$. As noted in [17], the field specifications could be provided in any of the following forms:

- Complex fields (amplitude and phase information) in either the near-field (NF) or far-field (FF) region,
- Phaseless fields (amplitude-only) in either the NF or FF region. If the desired phaseless fields are specified in the FF zone, they will be equivalent to a desired power pattern. To emphasize that the desired phase data have not been provided to the algorithm, $|f|^2$ is used in the remaining of this paper to represent the amplitude-only specification for such cases. ($|\cdot|$ denotes the amplitude operator), or
- FF performance criteria such as main beam directions, half-power beamwidth (HPBW), and null locations. (These performance criteria are first converted to a desired power pattern and are then incorporated into the inversion algorithm.)

The goal of the design procedure is then to find passive, lossless, and reciprocal surface susceptibility profiles for each metasurface such that, when illuminated with the given incident field, produce a transmitted field that closely satisfies the field specifications.
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III. METHODOLOGY

This section provides a high-level overview of the procedure employed to design the cascaded metasurface pair. The goal of this procedure is to define the tangential electric and magnetic fields on either side of both metasurfaces, from which the susceptibility profiles can be calculated [13]. That is, we need to determine

- tangential output fields, \( \vec{E}^+_2 \) and \( \vec{H}^+_2 \), on \( x = 0^+ \),
- tangential input fields, \( \vec{E}^-_2 \) and \( \vec{H}^-_2 \), on \( x = -d^- \), and
- tangential interior fields, \( \vec{E}^+_1 \) and \( \vec{H}^+_1 \), on \( x = -d^+ \), and \( \vec{E}^-_2 \) and \( \vec{H}^-_2 \) on \( x = 0^- \).

Noting Figure 1, we refer to \( x = 0^+ \) and \( x = 0^- \) as \( \Sigma_2^+ \) and \( \Sigma_2^- \) respectively, and we refer to \( x = -d^+ \) and \( x = -d^- \) as \( \Sigma_1^+ \) and \( \Sigma_1^- \) respectively.

A. Finding the Tangential Output Fields (on \( \Sigma_2^+ \))

The first step involves determining tangential electric and magnetic fields on the output side of the second (output) metasurface. This step is formulated as an inverse source problem as shown in Figure 2, in which the unknowns are equivalent electric and magnetic currents, \( \vec{J}_2 \) and \( \vec{M}_2 \). A cost-functional is minimized to find \( \vec{J}_2 \) and \( \vec{M}_2 \) such that these equivalent currents:

- produce electromagnetic fields that satisfy the user-defined specifications \( \mathbf{f} \) on the region of interest \( S \), and
- satisfy Love’s equivalence condition (i.e., produce null fields on the input side of \( \Sigma_2 \)).

Noting that Love’s condition is enforced, the resulting equivalent currents will be related to the required tangential electric and magnetic fields as

\[
\vec{H}^-_2 = -\alpha \hat{n} \times \vec{J}_2 \quad \text{and} \quad \vec{E}^-_2 = \alpha \hat{n} \times \vec{M}_2,
\]

where \( \hat{n} \) is the unit outward normal to \( \Sigma_2 \) (i.e., towards the output side) and \( \alpha \) is a real-valued scaling factor. (\( \hat{n} = \hat{x} \) in Figure 1.) The choice of \( \alpha \) does not affect the normalized output field. As will be seen, we select \( \alpha \) to ensure that total power is conserved across the cascaded metasurface structure.

B. Tangential Input Fields (on \( \Sigma_1^- \))

Since the cascaded metasurface system is assumed to be reflectionless, the tangential fields on the input side of the first metasurface (i.e., at \( x = -d^- \)) are assumed to be the same as the known incident field (i.e., the tangential components of \( \vec{E}^{\text{inc}} \)). Thus, \( \vec{E}^+_1 \) and \( \vec{H}^+_1 \) are known.

C. Finding the Tangential Interior Fields (on \( \Sigma_1^+ \) and \( \Sigma_2^- \))

The next step is to determine the tangential electric and magnetic fields in the interior region between the two metasurfaces. This is accomplished by formulating and solving a second inverse source problem, as shown in Figure 3. In this step, the goal is to find equivalent currents \( \vec{J}_1 \) and \( \vec{M}_1 \) on \( \Sigma_1^+ \) such that

- their corresponding fields satisfy LPC on both metasurfaces, and
- they satisfy Love’s condition (i.e., produce null fields on the input side of \( \Sigma_1 \)).

On \( \Sigma_1 \), satisfying LPC means that the time-averaged real power density in the \( \hat{x} \) direction of \( \vec{E}^+_1 \) and \( \vec{H}^+_1 \) must be locally (i.e., at each unit cell) equal to the real power density of \( \vec{E}^-_1 \) and \( \vec{H}^-_1 \) in the \( \hat{x} \) direction. Since Love’s condition is enforced the necessary fields are related to the equivalent currents as

\[
\vec{H}^+_1 = -\hat{n} \times \vec{J}_1 \quad \text{and} \quad \vec{E}^+_1 = \hat{n} \times \vec{M}_1.
\]

On \( \Sigma_2 \), the LPC condition is between the previously defined output fields, \( \vec{E}^+_2 \) and \( \vec{H}^+_2 \) (Section III-A) and the fields \( \vec{E}^-_2 \) and \( \vec{H}^-_2 \) that are computed from the equivalent currents using

\[
\vec{E}^-_2 = B_1 \left( \vec{J}_1, \vec{M}_1 \right) \quad \text{and} \quad \vec{H}^-_2 = B_2 \left( \vec{J}_1, \vec{M}_1 \right)
\]

where \( B_1 \) and \( B_2 \) are electric and magnetic field integral equation operators, respectively [36].

D. Computing the Susceptibility Profiles

Once the tangential fields on either side of both metasurfaces have been found, we can apply the generalized sheet transition conditions (GSTCs) [37], [38] to compute the surface susceptibility profiles required to support the two intended field discontinuities. Assuming a planar metasurface on the \( zy \) plane for convenience, adopting a time-dependency of \( e^{j\omega t} \), and neglecting the normal component of the polarization

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\( x = 0 \)

\( \vec{E}^+_2 = \alpha \hat{n} \times \vec{M}_2 \)

\( \vec{H}^+_2 = -\alpha \hat{n} \times \vec{J}_2 \)

\( \Sigma_2 \)

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\( x = -d^- \)

\( \vec{E}^-_1 = \hat{n} \times \vec{M}_1 \)

\( \vec{H}^-_1 = -\hat{n} \times \vec{J}_1 \)

\( \Sigma_1 \)

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\( x = 0^+ \)

\( \vec{E}^+_2 = B_1 \left( \vec{J}_1, \vec{M}_1 \right) \)

\( \vec{H}^+_2 = B_2 \left( \vec{J}_1, \vec{M}_1 \right) \)

\( \Sigma_2^- \)
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where the superscript ‘T’ denotes the transpose operator. Metasurfaces are parallel to the $yz$ plane. (A TM$_{1}$ unit cell and a TM$_{2}$ unit cell for the second metasurface, then $x_2 \in \mathbb{R}^{4N}$. Thus, we now have two vectors of unknowns: $x_1$ and $x_2$.

### B. Forming a Data Misfit Cost Functional with Respect to $x_2$

The first step involves forming a cost functional with respect to $x_2$ representing the discrepancy between the field specifications $f$ on $S$ and those generated by a predicted $x_2$. Let us assume that the desired specifications are amplitude-only fields on $S$. That is, let the field specifications be $|f|^2$, a vector of squared field amplitude at the discrete points of $S$. The data misfit cost functional is then a mapping from $\mathbb{R}^{4N}$ to $\mathbb{R}$, and is expressed as

$$C_f(x_2) = \left\| |f|^2 \right\|_{S}^{-2} \left\| A_f x_2 \right\|_{S}^2 - \left\| |f|^2 \right\|_{S}^2$$

where $A_f$ is the discretized integral operator that produces $H_z$ (due to TE$_z$ assumption) at the locations of the field specifications in $|f|^2$ from the equivalent currents $x_2$. In addition, $\left\| . \right\|_{S}$ denotes the $L^2$-norm over $S$. Later on in Section V-B, we will also consider a case where the field specifications are instead FF performance criteria such as main beam directions, HPBW, and null locations. In such cases, these performance criteria need to be first converted to a desired power pattern $|f|^2$. The procedure to perform this conversion can be found in [17].

In addition, we note that Love’s condition is enforced by adding ‘virtual’ data to $|f|^2$. This is done by augmenting $|f|^2$ with a vector of zeros associated with the locations at which the null field is desired [17], [36]. In this case, these nulls are enforced on a line which is an inward offset of $\Sigma_2^x$. Similarly, the matrix $A_f$ needs to be augmented such that when it operates on $x_2$, the operation results in the fields produced by $x_2$ in the region of interest $S$ and in the domain at which null fields are desired.

### C. Forming a Total Variation Regularizer for $x_2$

We now introduce an additive regularization term based on the $L^2$-norm total variation (TV) regularizer. This functional, denoted as $C_{TV}(x_2)$, penalizes solutions with rapid variations from cell to cell and is given by

$$C_{TV}(x_2) = w_{TV} \left\| D_y(x_2) \right\|_{\Sigma_2}^2$$

where $w_{TV}$ is a real-valued weighting parameter. The operator $D_y(x_2)$ applies a derivative with respect to $y$ (i.e., along the metasurface) to the individual current components of $x_2$ separately, explicitly stated as

$$D_y(x_2) \triangleq \left[ \frac{\partial}{\partial y} J_{2,1} \frac{\partial}{\partial y} J_{1,1} \frac{\partial}{\partial y} M_{1,2} \frac{\partial}{\partial y} M_{1,1} \right]^T.$$ (10)

This regularization term biases the solution towards a higher degree of continuity in the equivalent currents (and therefore
fields) from unit cell to unit cell. This is especially important because in Section IV-F we attempt to enforce LPC at each unit cell on $\Sigma_2$, and rapidly varying output fields could make this more difficult or even practically impossible given the finite size of the metasurfaces. A secondary benefit of this regularization is apparent when considering microscopic metasurface design, i.e., physical unit cell design. The typical procedure is to design and simulate each unit cell independently while assuming infinite periodicity. When each unit cell is then placed in the final metasurface structure, the periodicity assumption no longer holds and the behaviour of each unit cell will deviate from what was expected. The inclusion of the TV regularizer reduces the variation from cell to cell, thereby reducing the error in the periodicity assumption.

D. Iterative Minimization to Determine $x_2$

Combining (8) and (9) results in the total cost functional (or, regularized cost functional) that is minimized during the first optimization step, explicitly written as

$$C_2(x_2) = C_{FP}(x_2) + C_{TV}(x_2).$$

Minimization is performed in an iterative fashion using the nonlinear conjugate gradient (CG) method. At the $k$th iteration, the solution update is

$$x_{2,k+1} = x_{2,k} - \beta_k v_k,$$

where $\beta_k$ is the real-valued step length. The vector $v_k$ is the CG direction at the $k$th CG iteration computed using Polak-Ribiére formula [40]

$$v_k = g_{2,k} + \frac{(g_{2,k} - g_{2,k-1})^H g_{2,k}}{g_{2,k-1}^H g_{2,k}} v_{k-1},$$

where the superscript ‘H’ denotes the Hermitian operation (complex conjugate transpose) and $g_{2,k}$ and $g_{2,k-1}$ are the gradients of (11) with respect to $x_2$ at iterations $k$ and $k - 1$, respectively. As derived in Appendix A, the gradient of (11) is the sum of the gradients of (8) and (9), the first of which is

$$g_{F}(x_2) = 4 \left\| f \right\|^2_s \Re \left\{ A_F^H (r_F \circ A_F x_2) \right\},$$

where “$\circ$” indicates a Hadamard (element-wise) product of two vectors, ‘$\Re$’ denotes the real-part operator, and $r_F$ is the residual vector of (8) defined as

$$r_F = \left| A_F x_2 \right|^2 - \left| f \right|^2.$$

The gradient of (9) is

$$g_{TV}(x_2) = -2w_{TV} D_{2,y}^2(x_2),$$

where $D_{2,y}^2(x_2)$ computes the second derivative with respect to $y$ of the individual current components of $x_2$ as

$$D_{2,y}^2(x_2) = \begin{bmatrix} \frac{\partial^2}{\partial y^2} J_{2,R} & \frac{\partial^2}{\partial y^2} J_{2,I} & \frac{\partial^2}{\partial y^2} M_{2,R} & \frac{\partial^2}{\partial y^2} M_{2,I} \end{bmatrix}^T.$$

Both (10) and (17) are evaluated numerically using a central difference approximation. The gradient required to update the search direction $v_k$ in (13) can then be computed as

$$g_{2,k} = g_{F,k} + g_{TV,k},$$

The iterative procedure is terminated when the percent change in $x_2$ from one CG iteration to the next drops below a preset tolerance, typically $10^{-6}$. Finally, in the CG algorithm, the unknown equivalent currents are initialized using the known incident field, i.e., $J = \hat{n} \times \vec{H}_{11}$ and $M = -\hat{n} \times \vec{E}_{11}$.

E. Enforcing Total Power Conservation to Find $\vec{E}_{12}^+$ and $\vec{H}_{12}^+$

Upon convergence, the above iterative minimization will yield an appropriate $x_2$. Subsequently, we need to compute the corresponding output tangential fields on $\Sigma_2^+$ using (1). However, we first need to compute the scaling factor $\alpha$ needed to ensure that total power is conserved across the cascaded metasurface structure. To do so, we define $p_m \in \mathbb{R}^N$ as the vector containing the time-average real power density of $\vec{E}_{11}^-$ and $\vec{H}_{11}^-$ normally incident on $\Sigma_1^+$, with the $i$th element of $p_m$ defined as

$$p_{m,i} = \frac{1}{2} \Re \left( \vec{E}_{11}^- \times \vec{H}_{11}^- \right)_{\text{unit cell } i}.$$

Since we are concerned with the design of reflectionless metasurfaces, $p_m$ can be calculated with knowledge of the incident field only. Thus, the total incident power will be the summation of the elements of the vector $p_m$, denoted by $\text{sum}(p_m)$.

The time-average real power density of the output field can be written in terms of the equivalent currents as [19]

$$p_{\text{out}} = \frac{\alpha^2}{2} (J_{2,R} \circ M_{2,R} + J_{2,I} \circ M_{2,I}).$$

Note that since we have already determined $x_2$ in the previous step, we also know $J_{2,R}, J_{2,I}, M_{2,R},$ and $M_{2,I}$. If we now select $\alpha$ to be

$$\alpha = \left( \frac{\text{sum}(p_m)}{\frac{1}{2} \text{sum}(J_{2,R} \circ M_{2,R} + J_{2,I} \circ M_{2,I})} \right)^{\frac{1}{2}},$$

the total output power will be equal to the total input power, i.e., $\text{sum}(p_{\text{out}}) = \text{sum}(p_m)$, thus satisfying TPC. Finally, having found $\alpha, J_{2,R}, J_{2,I}, M_{2,R},$ and $M_{2,I}$, we can now use (1) to determine $\vec{E}_{12}^+$ and $\vec{H}_{12}^+$ on $\Sigma_2^+$. 

F. Forming the Cost Functional with Respect to $x_1$

The goal of this step is to determine the fields between the two metasurfaces that result in the intended field transformation while satisfying LPC on both metasurfaces. This involves finding a set of equivalent electric and magnetic currents $x_1$ on $\Sigma_1^+$, as defined in (7). The cost functional that is minimized in this step is a mapping from $\mathbb{R}^{4N}$ to $\mathbb{R}$, and consists of the following four terms

$$C_1(x_1) = C_{L_1}(x_1) + C_{p_{\text{LPC on } \Sigma_1}} + C_{p_{\text{LPC on } \Sigma_2}} + C_{\text{smoothness}}.$$  

The first term is defined as

$$C_{L_1}(x_1) = \left\| Lx_1 \right\|^2_{\Sigma_1},$$

where $L$ is a discretized integral operator that produces $H_z$ (or $E_z$ for TM$_z$ polarization) at the locations where Love’s
condition is enforced for \( \Sigma_1 \). (The discrete integral operator \( \mathbf{L} \) is constructed in the same manner as \( \mathbf{A}_F \).) Minimizing \( \mathcal{C}_L(\mathbf{x}_1) \) ensures that \( \mathbf{x}_1 \) produces null fields on the \( x = -d^- \) side of \( \Sigma_1 \) and allows us to eventually calculate the tangential fields using (2).

The second term in (22) is used to enforce LPC on \( \Sigma_1 \) as originally derived in [19], defined as
\[
\mathcal{C}_{P_1}(\mathbf{x}_1) = \frac{\| \frac{1}{2} (\mathbf{J}_{1,R} \odot \mathbf{M}_{1,R} + \mathbf{J}_{1,I} \odot \mathbf{M}_{1,I}) - \mathbf{p}_m \|^2}{\| \mathbf{p}_m \|_{\Sigma_1}}
\] (24)

which quantifies the difference between the real power density of \( \mathbf{E}^{+}_{1_2} \) and \( \mathbf{H}^{+}_{1_2} \) and the known incident power \( \mathbf{p}_m \) in the \( x \) direction at each unit cell on \( \Sigma_1 \). The real-valued weighting parameter \( w_1 \) is included to balance the contribution of \( \mathcal{C}_{P_1}(\mathbf{x}_1) \) to the overall functional.

The third term in (22) is used to enforce LPC on \( \Sigma_2 \). In terms of the tangential fields, this condition can be explicitly written as
\[
\frac{1}{2} \Re \left( \mathbf{E}^{-}_{1_2} \times \mathbf{H}^{+*}_{1_2} \right)_{\text{unit cell } i} = \frac{1}{2} \Re \left( \mathbf{E}^{+}_{1_2} \times \mathbf{H}^{+*}_{1_2} \right)_{\text{known from Section IV-E}}
\] (25)

which must hold at each unit cell on \( \Sigma_2 \). Analogously to (19), we evaluate the right-hand side of (25) for each unit cell to generate the vector \( \mathbf{p}_{\text{out}} \) containing the local real power densities of the fields \( \mathbf{E}^{+}_{1_2} \) and \( \mathbf{H}^{+}_{1_2} \). We also define discretized integral operators \( \mathbf{B}_1 \) and \( \mathbf{B}_2 \) corresponding to (3), which respectively produce the tangential electric and magnetic fields at each unit cell on \( \Sigma_2 \) from the equivalent currents \( \mathbf{x}_1 \). We can then write \( \mathcal{C}_{P_2}(\mathbf{x}_1) \) as
\[
\mathcal{C}_{P_2}(\mathbf{x}_1) = \frac{w_2 \| \frac{1}{2} \Re (\mathbf{B}_1 \mathbf{x}_1 \odot \mathbf{B}_2 \mathbf{x}_1) - \mathbf{p}_{\text{out}} \|^2}{\| \mathbf{p}_{\text{out}} \|_{\Sigma_2}^2}
\] (26)

where \( w_2 \) is a real-valued weighting parameter. The final term of (22), \( \mathcal{C}_{TV}(\mathbf{x}_1) \), performs the same operation previously defined in (9) (but operating on \( \mathbf{x}_1 \) instead of \( \mathbf{x}_2 \)).

At this point, it is worthwhile to discuss the existence of an appropriate solution \( \mathbf{x}_1 \) for given (i) desired output field specifications, (ii) separation distance, and (iii) incident field, is the existence of a solution guaranteed? Currently, we do not have a definitive answer for this question; but the following can be stated. As the separation distance \( d \) gets electrically smaller, \( \frac{1}{2} \Re (\mathbf{B}_1 \mathbf{x}_1 \odot \mathbf{B}_2 \mathbf{x}_1) \) in (26) becomes more similar to \( \mathbf{p}_{\text{in}} \). This will then create problems in minimizing (26) if the desired output power profile \( \mathbf{p}_{\text{out}} \) is significantly different than the input power profile \( \mathbf{p}_{\text{in}} \). This shows that the separation distance needs to be sufficiently large for this approach to work. (In [22], the importance of this separation distance is lessened by taking advantage of multiple reflections between the metasurface pair for reshaping the power profile.)

**G. Iterative Minimization to Determine \( \mathbf{x}_1 \)**

The cost functional in (22) is minimized using the nonlinear CG method with update equations similar to (12) and (13). As derived in Appendix B, the gradient of \( \mathcal{C}_L(\mathbf{x}_1) \) is
\[
\mathbf{g}_L(\mathbf{x}_1) = 2 \Re \left( \mathbf{L}^H \mathbf{L} \mathbf{x}_1 \right)
\] (27)

and the gradient of \( \mathcal{C}_{P_1}(\mathbf{x}_1) \) is
\[
\mathbf{g}_{P_1}(\mathbf{x}_1) = \frac{w_1}{\| \mathbf{p}_m \|_{\Sigma_1}} \begin{bmatrix} \mathbf{r}_1 \odot \mathbf{M}_{1,R} \\ \mathbf{r}_1 \odot \mathbf{M}_{1,I} \\ \mathbf{r}_1 \odot \mathbf{J}_{1,R} \\ \mathbf{r}_1 \odot \mathbf{J}_{1,I} \end{bmatrix}
\] (28)

where the residual vector \( \mathbf{r}_1 \) is defined as
\[
\mathbf{r}_1(\mathbf{x}_1) = \frac{1}{2} (\mathbf{J}_{1,R} \odot \mathbf{M}_{1,R} + \mathbf{J}_{1,I} \odot \mathbf{M}_{1,I}) - \mathbf{p}_m.
\] (29)

In addition, the gradient of \( \mathcal{C}_{P_2}(\mathbf{x}_1) \) is
\[
\mathbf{g}_{P_2}(\mathbf{x}_1) = \frac{w_2 \Re \left[ \text{diag} (\mathbf{B}_1 \mathbf{x}_1) \mathbf{B}_2^* + \text{diag} (\mathbf{B}_2^* \mathbf{x}_1) \mathbf{B}_1 \right]^{\top} \mathbf{r}_2}{\| \mathbf{p}_{\text{out}} \|^2_{\Sigma_2}}
\] (30)

where the ‘\( \text{diag} (\cdot) \)’ operator generates a diagonal matrix from a vector. The residual vector \( \mathbf{r}_2 \) is defined as
\[
\mathbf{r}_2(\mathbf{x}_1) = \frac{1}{2} \Re \left( \mathbf{B}_1 \mathbf{x}_1 \odot \mathbf{B}_2 \mathbf{x}_1 \right) - \mathbf{p}_{\text{out}}.
\] (31)

The gradient of \( \mathcal{C}_{TV}(\mathbf{x}_1) \) is computed in the same way as (16) but now operates on \( \mathbf{x}_1 \). In addition, the iterative procedure is terminated in the same way as in Section IV-D, when the solution stagnates as determined by a preset tolerance.

Finally, once we have a solution for \( \mathbf{x}_1 \), we use (2) to compute the tangential fields \( \mathbf{E}^{+}_{1_1} \) and \( \mathbf{H}^{+}_{1_1} \). We then use (3) to compute the tangential fields \( \mathbf{E}^{-}_{1_2} \) and \( \mathbf{H}^{-}_{1_2} \). Let us also remind ourselves that we have already determined \( \mathbf{E}^{+}_{1_2} \) and \( \mathbf{H}^{+}_{1_2} \) in Section IV-E, and we already know \( \mathbf{E}^{-}_{1_1} \) and \( \mathbf{H}^{-}_{1_1} \) from Section III-B. Therefore, we now know the tangential fields on both metasurfaces, and can therefore determine the required surface susceptibility profiles for both of these metasurfaces.

Note that since we have enforced LPC for each individual metasurface, we can implement the desired transformation using lossless and passive metasurfaces.

**H. Susceptibility Profile Calculation**

Once the tangential fields have been determined on both sides of \( \Sigma_1 \) and \( \Sigma_2 \) we can apply the GSTCs to determine the required susceptibility profiles to support the two field discontinuities. For 1D metasurfaces along \( y \) with TE\(_y\) fields, (4) at a given unit cell simplifies to
\[
- \Delta H_z = (j \omega \varepsilon_0 E_{y,av}) \chi_{yy}^{yz} + (j \omega \sqrt{\mu_0} H_{z,av}) \chi_{yz}^{yzz}.
\] (32a)
\[
- \Delta E_y = (j \omega \mu_0 H_{z,av}) \chi_{zz}^{yy} + (j \omega \sqrt{\varepsilon_0} E_{y,av}) \chi_{zz}^{yyz}.
\] (32b)

In order to ensure that the susceptibilities are passive, lossless, and reciprocal, we follow the procedure in [19] which stipulates that \( \chi_{yy}^{yz} \) and \( \chi_{zz}^{yy} \) are purely real (\( \mathbb{R} \)) while \( \chi_{yz}^{yzz} \) and \( \chi_{zz}^{yyz} \) are purely imaginary (\( \mathbb{I} \)). This restriction allows (32) to be solved analytically on each metasurface, with a unique solution for each unit cell.\(^2\) (Any field transformation that satisfies

\[^2\text{Note that (32) represents two complex equations which are equivalent to four real equations. Since } \chi_{yy}^{yz}, \chi_{yy}^{yz}, \chi_{zz}^{yy}, \chi_{zz}^{yyz} \in \mathbb{R} \text{ and } \chi_{yz}^{yzz}, \chi_{zz}^{yyz} \in \mathbb{I} \text{ we essentially have four real unknowns as well.}\]
LPC can be supported in this manner due to the inclusion of magnetoelectric coupling [20]. Note that since (i) we have already satisfied LPC in Section IV-F, and (ii) \( \chi_{ee}^{yy} \in \mathbb{R} \) and \( \chi_{mm}^{zz} \in \mathbb{R} \) cannot create any loss, this will inherently result in the losslessness condition \( \chi_{me}^{zy} = (\chi_{em}^{yz})^* \) [41, Appendix B] being satisfied. Finally, the stipulation \( \chi_{me}^{zy} \in \mathbb{I} \) and \( \chi_{em}^{yz} \in \mathbb{I} \) causes the relation \( \chi_{me}^{zy} = (\chi_{em}^{yz})^* \) to be equivalent to \( \chi_{me}^{zy} = -\chi_{em}^{yz} \), which is the condition for reciprocity [41, Sec. 2.2], and therefore the resulting metasurface is also reciprocal. Thus, in the next section, we have substituted \( \chi_{me}^{zy} \) with \( -\chi_{em}^{yz} \).

I. Conversion to the Three-Layer Model

In order to simulate the metasurfaces using commercial software, we employ a three-layer admittance sheet topology [24, 42]–[44] for each unit cell (based on the local periodicity approximation [45]) as shown in Figure 4. The conversion from the susceptibility profiles to the admittance sheet model is performed using the procedure in [46]. At a given unit cell, we start by rearranging (32) into the ABCD representation of a two-port network as

\[
\begin{bmatrix}
\hat{E}_{-t_i} \\
\hat{H}_{t_i}
\end{bmatrix} =
\begin{bmatrix}
A & B \\
C & D
\end{bmatrix}
\begin{bmatrix}
\hat{E}_{+t_i} \\
\hat{H}_{-t_i}
\end{bmatrix},
\]

(33)

where \( i = 1, 2 \) for the first and second metasurfaces respectively. This results in the following ABCD parameters

\[
A = G^{-1} \left[ \frac{k_0^2}{4} \chi_{ee}^{yy} \chi_{mm}^{zz} - \left(1 - \frac{jk_0}{2} \chi_{em}^{yz} \right)^2 \right]
\]

(34a)

\[
B = G^{-1} \left[ -j\omega \mu_0 \chi_{mn}^{zz} \right]
\]

(34b)

\[
C = G^{-1} \left[ -j\omega \epsilon_0 \chi_{ee}^{yy} \right]
\]

(34c)

\[
D = G^{-1} \left[ \frac{k_0^2}{4} \chi_{ee}^{yy} \chi_{mm}^{zz} - \left(1 + \frac{jk_0}{2} \chi_{em}^{yz} \right)^2 \right]
\]

(34d)

where \( G \) is

\[
G = -\left( \frac{k_0}{2} \chi_{em}^{yz} \right)^2 - \frac{k_0^2}{4} \chi_{ee}^{yy} \chi_{mm}^{zz} - 1.
\]

(35)

It is worthwhile to note that \( AD - BC = 1 \) (reciprocal network). In addition, note that since \( \chi_{ee}^{yy} \in \mathbb{R} \), \( \chi_{mm}^{zz} \in \mathbb{R} \) and \( \chi_{em}^{yz} \in \mathbb{I} \), then we will have \( A \in \mathbb{R} \), \( D \in \mathbb{R} \), \( B \in \mathbb{I} \), and \( C \in \mathbb{I} \), which further indicates a lossless two-port network.

The \( ABCD \) parameters of the three-layer admittance sheet topology can be computed using the transmission line theory [42] and equated with (34), allowing the three admittance sheet values \( Y_1 \), \( Y_2 \), and \( Y_3 \) to be calculated as

\[
Y_1 = \frac{D - jZ_0 \sin (\beta l) \cos (\beta l) Y_2 - \cos^2 (\beta l) + j\sin^2 (\beta l)}{2jZ_0 \sin (\beta l) \cos (\beta l) - Z_0^2 \sin^2 (\beta l) Y_2}
\]

(36a)

\[
Y_2 = \frac{B - 2jZ_0 \sin (\beta l) \cos (\beta l)}{Z_0^2 \sin^2 (\beta l)}
\]

(36b)

\[
Y_3 = \frac{A - jZ_0 \sin (\beta l) \cos (\beta l) Y_2 - \cos^2 (\beta l) + j\sin^2 (\beta l)}{2jZ_0 \sin (\beta l) \cos (\beta l) - Z_0^2 \sin^2 (\beta l) Y_2}
\]

(36c)

where \( Z_0 \), \( \beta \), and \( l \) are the characteristic impedance, propagation constant, and thickness of the substrate layers, respectively. (Similar relations can also be found in the Supplemental Material of [24].) Since \( A \) and \( D \) are purely real and \( B \) and \( C \) are purely imaginary and noting that \( Z_0 \) and \( \beta \) are purely real (assuming a lossless substrate), we will have purely imaginary \( Y_1 \), \( Y_2 \) and \( Y_3 \). In the next section, we calculate \( Y_1 \), \( Y_2 \), and \( Y_3 \) for each unit cell on each metasurface, and subsequently simulate our cascaded metasurface system in ANSYS HFSS.

V. Full-Wave Simulated Examples

The examples presented here use ANSYS HFSS to simulate the cascaded metasurfaces designed using the proposed procedure along with the three-layer admittance sheet topology for each unit cell.

A. Phaseless Far-Field Power Pattern

In the first example we design a pair of metasurfaces to produce a desired FF power pattern from a normally incident TE\(_2\) plane wave (i.e., only \( E_x \), \( E_y \), and \( H_z \) field components) at 10.5 GHz. We assume 2D field propagation in the \( xy \) plane with 1D metasurfaces placed along \( x = 0 \) and \( x = -1.5\lambda \), where \( \lambda \) denotes the free space wavelength. The metasurfaces are both 5\( \lambda \) in length and each metasurface is discretized into 30 unit cells of width \( \lambda / 6 \). While the normally incident plane wave requires periodic boundaries (implemented through the use of master/slave boundaries in HFSS), the designed metasurface will actually be aperiodic. To accommodate the simulation of an aperiodic structure within periodic boundary conditions, we add absorbing elements in-line with both metasurfaces that extend out a distance of two wavelengths from either end. These absorbers ensure that the fields close to the metasurfaces are not affected by the adjacent “images” of the structure due to the periodic boundaries.

The field specifications consist of the phaseless FF power pattern shown in Figure 5, specified for the angular range \(-90^\circ \leq \varphi \leq 90^\circ \). In the first optimization step, we use \( w_{\varphi TVR} = 10^{-12} \) and a step length of 100 and minimize (11) to determine the equivalent currents \( x_0 \) on the output metasurface located at \( x = 0 \). The tangential output fields are then computed and scaled to match the total incident field power using (1) and (21). The normalized FF power pattern that would be produced by these tangential output fields is shown in Figure 5 for reference. The second optimization step is then performed to minimize (22). The weighting parameters used
in this step are \( w_1 = 0.5 \), \( w_2 = 0.7 \), and \( w_{TV} = 8 \times 10^{-10} \), and a step length of 1 is used. Once \( x_3 \) is determined, the remaining tangential fields are found using (2) and (3) and the susceptability profiles can be computed using (32).

In this design, we use the Rogers RO3010 substrate (\( \varepsilon_r = 10.2 \), \( \tan \delta = 0.0022 \)) for each of the two layers, each with a thickness of 1.27 mm (50 mil). We now calculate the admittance sheet values \( Y_1 \), \( Y_2 \), and \( Y_3 \) for each unit cell using (36). (Since the substrate’s loss tangent is small, it has not been taken into account in the calculation of the required admittances; however, the loss tangent will be taken into account in ANSYS HFSS simulations.) The admittance sheets are then implemented in the HFSS simulation using impedance boundary conditions, with metallic baffles placed between each of the unit cells as in [14]. The real part (absolute value) of the total electric field in the simulation domain is shown in Figure 6. The FF pattern generated from this simulation (using a NF to FF transformation) is shown in Figure 5, in which the simulated pattern exhibits excellent agreement with the desired pattern within the main beam. Although the generated sidelobes are not exactly matched with the desired sidelobes, the generated sidelobe level (SLL) remains almost below \(-20 \) dB. The overall transmission efficiency, which we define as the ratio between the total real power of the output field to the total real power of the incident field, is 77.76% in this example.

**B. Far-Field Performance Criteria**

In the second example, the goal is to design a cascaded metasurface structure that produces a FF pattern that satisfies a collection of performance criteria. The only change required to support this type of field specifications is to replace the functional in (8) with

\[
C_{\text{FF}}(x_2) = \|W|f|^2\|_S^2 - \|W|A_F x_2|^2 - W|f|^2\|_S^2
\]

(37)

where \( W \) is a diagonal prescaling matrix used to balance the relative contributions of the various performance criteria, calculated as in [17]. The details on converting the FF performance criteria into \(|f|^2\) can also be found in [17]. For this example the target FF performance criteria are shown in Table I, which consist of two identical main beams (in different directions), each with the same HPBW and associated nulls. A visual representation of these performance criteria can be seen in Figure 7, in which the elements of \(|f|^2\) are plotted using red circular markers. In particular, note the eight red circular markers on the \(-60 \) dB line specify the desired null locations.

We adopt the same geometry and incident field as the previous example. In the first optimization step, we use parameters of \( w_{TV} = 10^{-9} \) and a step length of 10, and in the second optimization step we use weighting parameters \( w_1 = 0.5 \), \( w_2 = 0.7 \), \( w_{TV} = 8 \times 10^{-10} \), and a step length of 0.1. The normalized FF power pattern that would be produced by the tangential output fields \( E_{12}^t \) and \( H_{12}^t \) found during the first optimization step is shown for reference in Figure 7 (dashed black curve). The impedance values of \( Z_1 \), \( Z_2 \), and \( Z_3 \) (used to implement the corresponding admittance sheets \( Y_1 \), \( Y_2 \), and \( Y_3 \)) are shown in Figure 8 for each unit cell and each metasurface. The real part (absolute value) of the total electric field resulting from simulating the designed
metasurfaces in HFSS is shown in Figure 9, while the resulting FF is shown in Figure 7 (solid blue curve). The produced FF pattern has two main beams at $\varphi = \pm 33^\circ$ with HPBWs of 15.5° and 15.2°, exhibiting excellent agreement with the field specifications. The eight desired pattern nulls are also visible, although they deviate from the intended directions by up to 5°. In addition, although we did not achieve very deep nulls (set to −60 dB level in the specifications), all the generated nulls are still below −20 dB with the best null being below −50 dB. Finally, the transmission efficiency observed in this case is 83.31%. For reference, we also designed a single metasurface to perform the same field transformation using the procedure described in [19], and the FF pattern produced by simulating this single metasurface in HFSS is also shown in Figure 7 (dotted green curve). As can be seen, the single metasurface is constrained by the input power distribution and does not have enough degrees of freedom to satisfy the FF performance criteria as accurately as the cascaded metasurface structure.

C. Comparison to a Single Metasurface

The goal of this example is to demonstrate a scenario in which the ability of a cascaded metasurface to redistribute power offers an advantage compared to a single metasurface. To this end, we attempt to produce a FF power pattern with low side lobe levels as shown in Figure 10 (red curve) from the same normally incident plane wave as in previous examples. In conventional antenna array design, creating such a pattern generally requires a “tapered” element amplitude distribution, such as a ‘cosine’ taper. Generating this pattern using metasurfaces will require a similarly tapered output power distribution.

For the cascaded metasurface, we use the same geometry as the previous examples. We use the proposed procedure to design the cascaded metasurface, with $w_{TV} = 10^{-12}$ and a step length of 100 in the first optimization step. In the second optimization step we use $w_1 = 0.5$, $w_2 = 0.7$, and $w_{TV} = 8 \times 10^{-10}$, and a step length of 1. Additionally, we attempt to design a single metasurface using the procedure in [19] to produce a satisfactory FF pattern from the same incident field. The real part (absolute value) of the total electric field in the simulation domains for the single metasurface and cascaded metasurface system are shown in Figures 11(a) and (b), respectively. Noting Figure 11(b), we can clearly see the creation of an amplitude taper on $\Sigma_1^2 (x = 0^\circ)$ for the cascaded metasurface system that enables side lobe suppression. In addition, the corresponding FF patterns for the single metasurface (dashed black curve) and cascaded metasurface system are shown in Figures 11(a) and (b), respectively, compared to the target of $51\%$ and $5\%$, respectively, $\Sigma_1^2 (x = 0^\circ)$.

For the cascaded metasurface, we use the same geometry as the previous examples. We use the proposed procedure to design the cascaded metasurface, with $w_{TV} = 10^{-12}$ and a step length of 100 in the first optimization step. In the second optimization step we use $w_1 = 0.5$, $w_2 = 0.7$, and $w_{TV} = 8 \times 10^{-10}$, and a step length of 1. Additionally, we attempt to design a single metasurface using the procedure in [19] to produce a satisfactory FF pattern from the same incident field. The real part (absolute value) of the total electric field in the simulation domains for the single metasurface and cascaded metasurface system are shown in Figures 11(a) and (b), respectively. Noting Figure 11(b), we can clearly see the creation of an amplitude taper on $\Sigma_1^2 (x = 0^\circ)$ for the cascaded metasurface system that enables side lobe suppression. In addition, the corresponding FF patterns for the single metasurface (dashed black curve) and cascaded metasurface system are shown in Figure 10. While the single metasurface has a similar transmission efficiency to the cascaded metasurface pair (81.72% and 83.51%, respectively), the FF pattern produced by the cascaded metasurfaces is closer to the target pattern. The cascaded metasurface and single metasurface FF patterns exhibit half-power beamwidths of 11.7° and 10.1°, respectively, compared to the target of 11.5°. Furthermore, the side lobe level of the cascaded metasurface FF pattern is 7.6 dB lower than the single metasurface FF pattern. The low side lobe levels require a tapered output power distribution, which a single metasurface is unable to produce because it is constrained by the uniform input power distribution provided by the incident plane wave. In the cascaded scenario, the first metasurface is able to ‘redirect’
produced by this source are TMz away from the input metasurface at 10.5 GHz. The fields current line source (infinite in the D. TMz create the intended output field.

normally incident plane wave.

HFSS simulations using (a) a single metasurface and (b) two metasurfaces

Fig. 11. Absolute value of the real part of the total electric field of the HFSS simulations using (a) a single metasurface and (b) two metasurfaces to produce the desired far-field power pattern shown in Figure 10 with a normally incident plane wave.

The power such that the second metasurface can more easily create the intended output field.

D. TMz Fields

We now change the incident field to that of an electric current line source (infinite in the z direction), placed λ/3 away from the input metasurface at 10.5 GHz. The fields produced by this source are TMz (i.e., Ez, Hx, and Hy only). Each metasurface consists of 50 unit cells of λ/10 width and the thickness of the Rogers RO3010 substrate has been decreased to 0.254 mm (10 mil). Absorbing elements and periodic boundary conditions are not needed with this incident field, and so the simulation domain is bounded by an appropriate perfectly matched layer. (PEC boundary conditions are applied on the faces perpendicular to the z axis to support the TMz fields and 2D nature of the simulation.)

The field specifications consist of a FF power pattern with a main beam at ϕ = −15° as shown in Figure 12 (red curve). We design a cascaded metasurface structure with wTV = 10−5 and a step length of 0.005 in the first optimization step. In the second optimization step we use w1 = 25, w2 = 25, and wTV = 5 × 10−11, and a step length of 1. We also design two different single metasurfaces to perform the same transformation. The first single metasurface is placed at the location of the first metasurface from the cascaded structure at x = −1.5λ, while the second single metasurface is placed at the location of the second metasurface from the cascaded structure at x = 0. The real part (absolute value) of the total magnetic field in the simulation domains for the single metasurfaces and the cascaded metasurface system are shown in Figures 13(a), (b), and (c), while the corresponding FF patterns are shown in Figure 12. In this case, the single metasurface at x = −1.5λ is unable to produce the desired FF pattern accurately. The narrow beamwidth requires a rather uniform field amplitude distributed over a large aperture, but the single metasurface at x = −1.5λ is constrained to the ‘focused’ input power distribution generated by the line source. However, the FF pattern produced by the cascaded metasurfaces is only slightly closer to the target pattern compared to the FF pattern produced by the single metasurface at x = 0. Increasing the distance between the line source and the single metasurface results in a more uniform input power distribution, and thus the LPC constraint does not hinder the ability of the single metasurface at x = 0 to meet the desired FF pattern. This shows that the added flexibility of a second metasurface may not always be needed in scenarios where the input and output power distributions are relatively similar. Additionally, while the single metasurface at x = 0 has a higher transmission efficiency than the cascaded metasurfaces (90.96% compared to 72.36%), the output power of the cascaded metasurfaces is actually 21.68% higher than the single metasurface at x = 0. This is mainly due to the fact that the input power to the single metasurface at x = 0 is much lower since it is further away from the source, while the first metasurface in the cascaded structure receives more input power and is able to ‘focus’ the field on the second metasurface.

VI. CONCLUSION

A framework for the design of passive, lossless, and reciprocal cascaded metasurfaces structures was presented. The framework utilizes electromagnetic inversion to allow for the flexibility to specify the desired output field in a variety of ways, including complex fields (amplitude and phase), phaseless fields (amplitude-only), or even in terms of far-field performance criteria such as main beam directions, half-power beamwidths, and null locations. This framework allows for full generality with respect to metasurface geometry and the locations at which the field specifications are defined. Local power conservation is enforced at each metasurface during the two-step optimization procedure, and we have introduced a total variation regularizer to improve the continuity of the
incorporating reflections into the model can allow for smaller large enough such that reflections can be neglected. However, into account, and currently require that the separation be we have not yet taken reflections between the two metasurfaces resulting fields from unit cell to unit cell. Several designed metasurfaces were simulated in ANSYS HFSS using a three-layer admittance sheet topology to demonstrate the validity and flexibility of the method.

The main limitation of the proposed design method is that we have not yet taken reflections between the two metasurfaces into account, and currently require that the separation be large enough such that reflections can be neglected. However, incorporating reflections into the model can allow for smaller separation between the metasurfaces and improve the transmission efficiency, as shown in [22] and [23]. A secondary limitation is that the CG step length and functional weighting parameters are determined in an ad-hoc fashion, and require some tuning to ensure convergence.

The next logical step is to physically implement the designed metasurfaces using metallic ‘dogbone’ structures [14], [15] or some other unit cell design. The main challenge concerning the physical implementation is compensating for the mutual coupling between the layers of each unit cell. To this end, an iterative method for tuning unit cells to account for mutual coupling was recently presented in [47]. However, a method of this nature may not be practical for the large number of unique unit cells required for the aperiodic designs presented here.

APPENDIX A
 REQUIRED GRADIENTS WITH RESPECT TO $x_2$

We begin by deriving the gradient of $C_{TV}(x_2)$ using standard vector differentiation rules as

$$
\mathbf{g}_F(x_2) = \left\| \mathbf{f} \right\|^2 \left( \frac{\partial}{\partial x_2} \right) \left\| \mathbf{A}_F x_2 \right\|^2 - \left\| \mathbf{f} \right\|^2 
$$

$$
= 2 \left\| \mathbf{f} \right\|^2 \left( \frac{\partial}{\partial x_2} \right) \left( \mathbf{A}_F x_2 \right) \circ \left( \mathbf{A}_F x_2 \right)^* - \left\| \mathbf{f} \right\|^2 \mathbf{r}_F 
$$

where $\mathbf{r}_F$ is given in (15). To evaluate the derivative in (38), we use the identity

$$
\frac{\partial}{\partial \mathbf{x}} (\mathbf{A} \circ \mathbf{B}) = \text{diag}(\mathbf{A}) \mathbf{B} + \text{diag}(\mathbf{B}) \mathbf{A}. 
$$

Noting that $x_2$ and $\mathbf{r}_F$ are purely real vectors, the use of (39) in conjunction with (38) results in

$$
\mathbf{g}_F(x_2) = 4 \left\| \mathbf{f} \right\|^2 \left( \frac{\partial}{\partial x_2} \right) \text{Re} \left\{ \mathbf{A}_F^H (\mathbf{r}_F \circ \mathbf{A}_F x_2) \right\}. 
$$

Next, consider the gradient of the total variation regularizer given in (9). As an analogous derivation, we instead consider the functional

$$
\tilde{C}_{TV}(u(y)) = \left\| \nabla_y u(y) \right\|^2_{\Sigma_2}
$$

in which $u(y)$ is a continuously defined real-valued function of $y$ on $\Sigma_2$ and the norm is defined as

$$
\left\| \tilde{f}(y) \right\|^2_{\Sigma_2} = \left\langle \tilde{f}(y), \tilde{f}(y) \right\rangle_{\Sigma_2} = \int_{\Sigma_2} \tilde{f}(y) \cdot \tilde{f}(y) \, dy. 
$$

Note that since we are dealing with real-valued functions (i.e., the continuous form of the real-valued $x_2$ vector), the presence of the complex conjugate operator has been dropped in the above norm definition.\(^3\) For the sake of notational simplicity, the $y$ dependency of $u$ will be implied from now on. We start by finding the first variation of $\tilde{C}_{TV}(u)$ when $u$ is slightly varied by some function $\psi$ (which is defined on the same domain as $u$)

$$
\frac{\partial \tilde{C}_{TV}}{\partial \varepsilon} \left|_{\varepsilon=0} \right. \psi = \lim_{\varepsilon \to 0} \frac{\tilde{C}_{TV}(u + \varepsilon \psi) - \tilde{C}_{TV}(u)}{\varepsilon}
$$

$$
= \lim_{\varepsilon \to 0} \frac{\left\| \nabla_y (u + \varepsilon \psi) \right\|^2_{\Sigma_2} - \left\| \nabla_y u \right\|^2_{\Sigma_2}}{\varepsilon}. 
$$

\(^3\)For a similar derivation in the complex domain, see [48, Appendix D.3].
Using the definition of the norm in (42) and applying the divergence theorem, we can simplify (43) as
\[
\partial \tilde{C}_{TV} = 2 \int_{\Sigma_2} (\nabla_y u) \psi \cdot \hat{t} dy - 2 \int_{\Sigma_2} \psi \nabla_y \cdot (\nabla_y u) \; dy \tag{44}
\]
where \(\partial \Sigma_2\) refers to the edges of the metasurface. We assume that the function \(u\) vanishes on the boundary, i.e., \(u (y \in \partial \Sigma_2) = 0\), which is equivalent to assuming that the equivalent currents are assumed to be zero on the edges of the metasurface in our case. Since \(\psi\) exists in the same function space as \(u\), then \(\psi (y \in \partial \Sigma_2) = 0\). Subsequently, (44) simplifies to
\[
\partial \tilde{C}_{TV} = -2 \int_{\Sigma_2} \psi \nabla_y \cdot (\nabla_y u) \; dy = \left\langle -2 \nabla_y^2 u, \psi \right\rangle_{\Sigma_2}. \tag{45}
\]
If we were to discretize (41) such that the functional operates on the equivalent currents in \(x_2\) as in (9), and considering the regularization weight \(w_{TV}\), the corresponding discrete gradient vector \(g_{TV}(x_2)\) [49], [50] assuming identical unit cell sizes can then be written as
\[
-2w_{TV} \begin{bmatrix} \frac{\partial}{\partial y^2} J_{2,R}^1 & \frac{\partial}{\partial y^2} J_{2,I}^1 & \frac{\partial}{\partial y^2} M_{2,R}^1 & \frac{\partial}{\partial y^2} M_{2,I}^1 \end{bmatrix}^T. \tag{46}
\]
\[\text{APPENDIX B}
\]
\[\text{REQUIRED GRADIENTS WITH RESPECT TO } x_1\]

The gradient of \(C_1(x_1)\) can be derived using vector differentiation rules as
\[
g_1 = \frac{\partial}{\partial x_1} \left\| Lx_1 \right\|_{\Sigma_1}^2 = \frac{\partial}{\partial x_1} \left\| x_1^T L^H Lx_1 \right\|
= \left(L^H L + L^* L\right)x_1 = 2 \text{Re} \left(L^H L x_1\right) \tag{47}
\]
To derive the gradient of \(C_{P_1}(x_1)\), we first find the gradient of \(C_{P_1}(x_1)\) with respect to \(J_{1,R}\) as
\[
\frac{\partial C_{P_1}}{\partial J_{1,R}} = \frac{\partial}{\partial J_{1,R}} \left\| \frac{1}{2} \left( J_{1,R} \odot M_{1,R} + J_{1,I} \odot M_{1,I} \right) - p_m \right\|_{\Sigma_1}^2
= 2w_1\frac{\partial}{\partial J_{1,R}} \left( \frac{1}{2} \left( J_{1,R} \odot M_{1,R} + J_{1,I} \odot M_{1,I} \right) - p_m \right) r_1
= \frac{w_1}{\left\| p_m \right\|_{\Sigma_1}} r_1 - \frac{w_1}{\left\| p_m \right\|_{\Sigma_1}} r_1 \odot M_{1,R} \tag{48}
\]
where \(r_1\) is given in (29). Performing a similar derivation for the gradients with respect to \(J_{1,I}, M_{1,R},\) and \(M_{1,I}\) and concatenating the results according to the order of (7) produces the final gradient with respect to \(x_1\), which is given in (28).

We now derive the gradient of \(C_{P_2}(x_1)\) as
\[
g_{P_2} = \frac{\partial}{\partial x_1} \left\| \frac{1}{2} \text{Re} \left( B_1 x_1 \odot B_2^* x_1 \right) - p_{out} \right\|_{\Sigma_2}^2 \tag{49}
\]
Using the identity in (39) this simplifies to
\[
g_{P_2} = \left[ \text{Re} \left( B_1 x_1 \odot B_2^* x_1 \right) - p_{out} \right]^T r_2 \frac{2}{\left\| p_{out} \right\|_{\Sigma_2}}. \tag{50}
\]
Finally, similar to (46), \(g_{TV}(x_1)\) will be
\[
-2w_{TV} \begin{bmatrix} \frac{\partial}{\partial y^2} J_{1,R}^1 & \frac{\partial}{\partial y^2} J_{1,I}^1 & \frac{\partial}{\partial y^2} M_{1,R}^1 & \frac{\partial}{\partial y^2} M_{1,I}^1 \end{bmatrix}^T. \tag{51}
\]

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Trevor Brown (S’12) received the B.Sc., M.Sc., and Ph.D. degrees in electrical engineering from the University of Manitoba, Winnipeg, MB, Canada, in 2014, 2016, and 2020 respectively. His current research interests include applied and computational electromagnetics, electromagnetic metasurface design, inverse problems, optimization techniques, and phaseless nearfield antenna measurement techniques.

Dr. Brown received the IEEE Antennas and Propagation Society Eugene F. Knott Memorial Prize in 2017, the Canadian Geophysical Union Scholarship in 2018, and the Canadian Geophysical Union Gold Medal in 2019. He has also received the Natural Sciences and Engineering Research Council (NSERC) Postgraduate Scholarship from 2016 to 2019. He also served as the Secretary of the IEEE Winnipeg Section from 2015 to 2020.

Puyan Mojabi (S’09–M’10) Puyan Mojabi received the B.Sc. degree from the University of Tehran, Iran, in 2002, the M.Sc. degree from Iran University of Science and Technology, Tehran, Iran, in 2004, and the Ph.D. degree from the University of Manitoba, Winnipeg, MB, Canada, in 2010, all in Electrical Engineering.

He is currently an Associate Professor and a Canada Research Chair (Tier 2) in the Department of Electrical and Computer Engineering at the University of Manitoba, and is a registered Professional Engineer in Manitoba, Canada. His current research interests include applied and computational electromagnetics, electromagnetic metasurface design, inverse problems, optimization techniques, and phaseless nearfield antenna measurement techniques.

Dr. Mojabi is a recipient of the University of Manitoba’s Falconer Emerging Researcher Rh Award for Outstanding Contributions to Scholarship and Research in the Applied Sciences category and two Excellence in Teaching Awards from the University of Manitoba’s Faculty of Engineering as well as a University of Manitoba Graduate Students Association Teaching Award. He has also received three Young Scientist Awards from the International Union of Radio Science (URSI), and has served as an Early Career Representative of URSI’s Commission K, and as the Chair of the IEEE Winnipeg Waves Chapter.