MetaDesigner: A web app-based design tool powered by deep learning inverse models for accelerated design of metamaterials

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Abstract

The ever-evolving field of materials design and discovery has been revolutionized by the emergence of data-driven algorithms for generative designs of materials and explorations of structure-property relationships. In particular, AI-guided design frameworks have been successfully applied to the field of artificially structured electromagnetic composites known as metamaterials where their use has not only alleviated the computational burden associated with simulations based on first principles but also facilitated faster, more efficient sampling of vast parameter spaces to converge on a solution. MetaDesigner is a user-friendly web application which simplifies and automates the inverse design of metamaterials, i.e., it is a tool powered by generative and discriminative deep learning models for enabling 'design-by-specification'. The practical application of this framework is exemplified by the successful end-to-end design of a metamaterial broadband absorber as well as the demonstration of plasmonic metasurface for generating structural color 'at will'. We envision that MetaDesigner's user-friendly interface will accommodate users with varying levels of expertise by providing access to multiple inverse algorithms and play a pivotal role in expediting the design and exploration of metamaterial-based devices. As this work is still under development and the technologies underpinning its development are expected to change over time, this abstract is aimed primarily at explaining the overall philosophy and design goals of this project.

Introduction

Metamaterials and metasurfaces (the 2D planar equivalent of metamaterials), are artificially crafted, composite materials designed to support unique, highly customizable interactions with incoming electromagnetic (EM) waves. Over the past decade, these engineered materials have garnered tremendous attention owing to their ability to demonstrate remarkable, seemingly anomalous phenomena such as negative refraction and cloaking which are unattainable using naturally occurring substances (Cai etal. 2007; Pendry 2000). The fundamental building block of metamaterials are referred to as meta units or 'meta-atoms' which essentially mimic atoms in conventional materials. The physical dimensions of meta-atoms are designed to be smaller than the interaction wavelengths of interest. Their electromagnetic responses are dictated primarily by the size, shape, and geometry of their meta-atoms as opposed to the fundamental properties of their constituent materials and therefore, artificial structuring provides an intriguing pathway to tweak the material responses 'by specification'. The capability to control EM waves unconventionally, coupled with the compact size and reduced environmental impact of metamaterials, has rendered them an appealing choice for replacing traditional electro-optic components in a wide range of systems. Examples of their applications include innovative 'meta' lenses that are essentially flat films capable of replacing conventional bulky and expensive lens assemblies in imaging devices (e.g., cameras, smartphones). Additionally, metamaterial-based antennas have the potential to replace conventional phased arrays in next generation communication systems. Metamaterials are typically fabricated using fairly complex, labour-intensive methods (typically top-down lithographic techniques) and therefore, there is a real need for digital rapid prototyping tools that support a significant degree of automation and have the ability to accurately define topological parameters before proceeding towards actual fabrication. At this juncture, it is useful to quickly review the landscape of open source as well as commercially available design and simulation packages for metamaterials. The major stages involved in the simulation and design of metamaterials include defining the problem (e.g., how do I want my material to 'behave' or respond), choosing the base materials in terms of properties such as the conductivity, electric permittivity, magnetic permeability etc. This is followed by the first major design step wherein which the geometry of the unit cell or meta-atom is defined via relevant geometrical parameters. Up till this stage, the design process is guided mainly by knowledge, domain experience and intuition of the user. Once the meta-atom is defined, a set of excitation conditions are set up (akin to a virtual experiment) and the electromagnetic response of the material is simulated, typically using iterative, numerical full wave simulations such as the finite difference time-domain (FDTD) and finite element method (FEM). There are multiple commonly used engineering simulation packages that support capabilities for modelling the structure → property relationships but not the inverse. As the complexity of the metamaterial structures increases, so does the demand on user expertise, design timescales and computational resources. The area of materials design and discovery is therefore, ideally primed for data-driven, AI-guided methods. For metamaterials in particular, deep learning-based design frameworks have been the go-to approach for navigating complex structure ↔

property relationships. In general, a deep learning-aided design process can be approached in two different ways:

- **Forward 'Predictors'**: The input is provided in terms of the geometrical parameters describing the meta-atom structure and the model is trained to predict attributes such as the spectral response (amplitude, phase) or the distribution of scattered electric fields etc. In other words, the structure (geometry) → property (electromagnetic response) relation is mapped using data-driven techniques.
- **Inverse Design**: these models are typically for scenarios where the solution cannot be obtained analytically; they treat the desired EM response as an objective function which needs to be optimized in accordance with appropriate constraints, e.g., by using the target functionalities and leveraging neural networks to yield the topological parameters of the metamaterial.

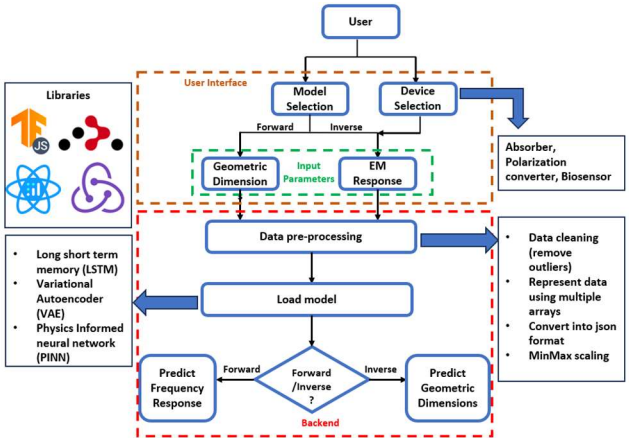


Figure 1: Flowchart illustrating the workflow of the designed web application

We describe our approach for developing a web application named "MetaDesigner" which offers users both forward as well as inverse design capabilities using multiple deep learning models (described in the next section). This tool is intended to provide an easy-to-use interface to users for designing devices such as near-unity absorbers, highly sensitive biosensors, polarization converters for next generation communication systems etc. Perhaps one of the biggest bottlenecks standing in the way of a wider adoption of technologies based on metamaterial platforms is the lack of easy-to-use design 'co-pilot' tools that offer a degree of automation and guidance for users thereby obviating the need for extensive trial-and-error parameter scans as well as domain expertise. As with the materials informatics field in general, there have been multiple efforts at various scales to build and deploy web-based toolboxes that can democratize the design process for users (Horton etal. 2023; http://materialsatlas.org/). Inverse designing in particular, has been a long sought after goal for real-world applications that require ways to 'reverse engineer' composite designs for yielding 'on-demand' functionalities.

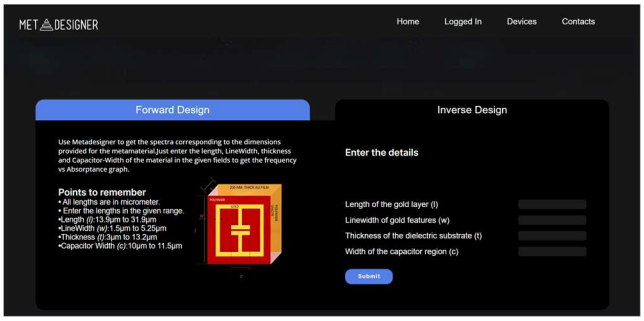
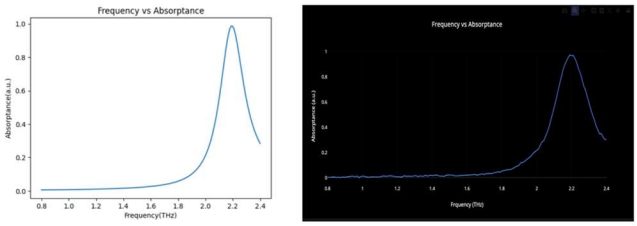


Figure 2: UI for accepting geometrical parameters for the forward predictor

Methodology

We have conceptualized, trained and validated multiple inverse architectures and integrated them into MetaDesigner. Here, it must be mentioned that the web app is work in progress and we are continuing to expand the library of devices the tool can handle as also seamlessly integrate more and more deep learning models into it. Here, we describe some of the tool's current capabilities; one is to design broadband metamaterial absorbers that demonstrate near-unity absorption at specified frequencies (Tao etal. 2008; Pillai etal. 2021). This functionality comprises of forward and inverse prediction blocks. (target performance → structural parameters). The underlying model is based on a forward predictor. This is based on a dual-model framework comprising a forward predictor that is trained using the meta-atom geometry as the input and the corresponding spectral response as the output and an inverse problem is dealt as a single-input, multi-output model using a tandem decoder-encoder architecture based on a long short-term memory (LSTM) network. The EM response plots are treated as sequential data and the LSTM is used to identify relevant pieces from the input EM data sequences. We created the training dataset which consisted of >5000 candidate geometries whose responses were simulated using a widely used, commercially available FEM solver. This dataset was subsequently split into training, validation, and test sets in the ratio 0.7:0.15:0.15. The weights of the decoder were saved from the pre-trained forward model. The network was trained for 1000 epochs with mean square error chosen as the loss function. A fivefold cross-validation was also performed to ensure that the model was generalized. The time taken for generating the training dataset was around 55 hours on a standard Intel Core i5-8250U CPU @ 1.60 GHz with 8 GB RAM,

the training for the forward model took approximately 6 hours and the total time to predict the spectral responses for the test set (~450 designs) took less than a second. This serves as a benchmark measure for demonstrating how well the forward predictor alleviates the computational burden for designing these devices. Additional details of this functionality are beyond the scope of this abstract. We pose our spectrum-design-spectrum problem as a sequence-to sequence learning task.

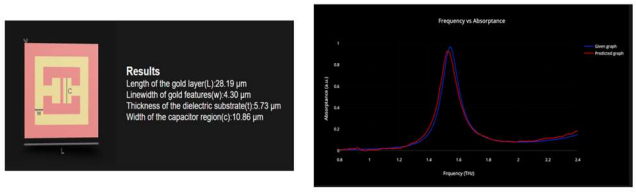


(a) (b)

Figure 3: Comparison of the FEM Simulated (left) and model-predicted (right) absorptance plot for a candidate absorber design

Another instance of MetaDesigner's ability to digitally 'rapid prototype' a metamaterial device without using rule-based numerical methods is exhibited by the successful demonstration of the design of plasmonic metasurfaces that demonstrate structural color specified by the user. These surfaces have carefully designed nanoscale features that selectively absorb or reflect specific wavelengths (dictated by the nanoscale geometry) thereby displaying selective coloration and are being increasingly considered as an environment-friendly, sustainable alternative to chemical dyes and pigments (Pillai etal. 2023). Here, the generated color is expressed in terms of the CIE 1931 color coordinate system wherein any color on the CIE chromaticity chart can be expressed as x and y coordinate pairs based on the three CIE primaries. In our design capability, we have used equally spaced polydimethylsiloxane (PDMS) nanopillars coated with a uniform aluminum layer as our candidate surface. For this particular device, we chose an approach wherein we generated a limited dataset comprising of the chromaticity coordinates corresponding to nanopillars of varying dimensions. As this dataset was unevenly distributed, we further pre-processed the data to remove clustering. The inverse model, which empowers the user to specify a target color and retrieve the nanopillar dimensions that will generate that color, is based on a modified variational autoencoder (VAE). VAEs are generative models that can stochastically output multiple different predictions given the same input; this is particularly critical for actual fabrication scenarios wherein the robustness of design models to variations within fabrication tolerances becomes imperative. This model has been particularly optimized for situations where the training data is limited (as is typically the case for plasmonic nanostructured materials).

We have used React (Meta Inc.) which is an open-source front-end JavaScript library for building our user interface. All the data, such as JSON files, bin files, and images, are stored locally for faster use. To handle page routing, we have used useNavigate, useLocation, Link, HashRouter, Routes, Route and useLocation functions from the "react-router-dom" package. useSelector function from Redux stored the states in react.js. The most crucial part of developing this server-rendered web application is the integration of the forward and inverse models with the web page. This is done using tensorflow.js (version 4.8.0) library. Here, it is imperative to use the exact same version of the package in both ReactJS and Google Collaboratory. The flowchart explaining the workflow of the forward and inverse model is illustrated in figure 1. In the forward model, the user is prompted to enter the geometrical parameters required for their desired meta-atom structure. As an example, the 'forward design' functionality for generating the spectral response of a gold-on-dielectric metamaterial absorber (Tao etal. 2008) is shown in figure 2, the input parameters required from the user include the length(l) and linewidth (w) of the gold layer, dielectric substrate thickness(t) and width of the capacitor region(c) in the respective textboxes (figure 2). The model computes the absorptance vs frequency response plot. Also, if the user enters any invalid text or layer dimensions exceeding the permissible range, an error message is displayed. A comparison between the FEM simulated (top) and predicted (bottom) plots for l = 21.9 μm, w = 3.75 μm, t = 6 μm and c = 11 μm is shown in figure 3.



(a) (b)

Figure 4: (a) Comparison between the user defined absorptance plot and the plot corresponding to the parameters inversely predicted by the model (b) Geometrical parameters inversely predicted by the model

In the inverse model, we upload our desired absorptance spectra as a csv file and the model outputs the l, w, t and c values of the absorber structure. In figure 4(a), the blue colored plot is the user defined desired response uploaded as csv file, where the first and second columns are frequency and absorptance respectively. Based on that input, the model predicts the geometrical parameters as shown in figure 4(b). To validate the prediction, we performed a forward simulation (based on first principles) of the struc-

ture with the parameters given by the model and the response is shown in red color (figure 4(a)). It can be observed from figure 3 and 4 that both the forward and inverse models perform very well in predicting the response and structural parameters.

Discussion and Future Work

Data-driven methods and algorithms have been at the frontier of materials design and discovery in recent years. In spite of the increasing availability of data and source codes of these algorithms, considerable expertise is required for their implementation and deployment thereby impeding widespread adoption. Web-based applications have been widely acknowledged as an effective approach for enhancing the accessibility of these algorithms to users of all experience levels. The MetaDesigner web application is to the best of our knowledge – the very first tool that provides a user-friendly interface for designing metamaterial-based functional devices in an intelligent, automated and expedited manner. As the development of this web app is still under progress, several functionalities will be made available soon (in addition to the capabilities we have demonstrated till date). The future scope includes the inclusion of a performance measure to indicate the prediction confidence of the models via a wide array of analysis tools, an expanded library of meta atoms and build templates, comprehensive documentation for assisting users (we have already implemented a feature wherein relevant publicly available literature can be accessed from the query pages), integration of additional AI-assisted 'click-and-run' algorithms, utility tools for enhancing interactive explorations and pipelines for users to upload their datasets along with a recommendation engine for suggesting which pre-built models they can utilize based on target specifications. A short video demonstrating MetaDesigner's capabilities can be accessed at: https://youtu.be/Uy7TirvPvGk

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