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A non-linear material interpolation for design of metallic nano-particles using topology optimization

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Abstract

This paper discusses a non-linear bi-material interpolation scheme for the relative electric permittivity, ϵ_r , through the refractive index and extinction coefficient. The scheme is tailored for density-based topology optimization of metallic micro- and nano-structures, in electromagnetic problems in the optical wavelength regime. The scheme is shown to exhibit superior properties in the ultraviolet to low infrared wavelength regime, compared to simple linear and inverse interpolation schemes for ϵ_r used in the literature. The superior properties are demonstrated with optimization examples and a physical motivation is provided. Finally, the capability of the scheme is demonstrated by designing a nano-scale Ag antenna-strip providing approximately a 1200 fold spatially-localized enhancement of the electric energy, corresponding to a more than 600% performance improvement over a topology optimized reference design from the literature.

Keywords: material interpolation, electromagnetism, plasmonics, topology optimization, nano-antenna, nano-scale

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1. Introduction

High performance micro- and nano-scale metallic devices and particles designed for specialized interactions with the electromagnetic field utilizing plasmonic and non-plasmonic effects, are of interest for a wide range of applications. Examples include, near-field optical microscopy [1], chemical sensing [2], optically-assisted data storage [3], photovoltaics [4, 5, 6, 7] and photon upconversion [8, 9, 10].

It is possible to design such devices using geometrically and/or physically simplified models which only consider a small number of design variables, hereby enabling designing by parametric studies, see e.g. [8, 11]. To achieve higher geometric freedom one may instead consider a general partial differential equation model which accurately captures the physics and combine it with gradient-based numerical design techniques, like density-based topology optimization. Doing so, enables designing using more than a billion design variables simultaneously [12], which allows for nearly unlimited geometric design freedom, while still capturing the physics accurately. Density-based topology optimization has been applied successfully within nano- and micro-scale electromagnetism on numerous occasions, see e.g. [13, 14] for a few examples and [15] for a review.

The reader is referred to [16] for an in-depth presentation of density-based topology optimization, but for the purposes of this paper the following is briefly remarked. The method is iterative in nature and relies on the introduction of a spatial design field, $\rho(\mathbf{r}) \in [0, 1]$, representing a pixelization of the geometry of the device under design. The design field is used to interpolate the spatial material distribution in the design region between a background and the material constituting the device. Thus non-physically realizable mixtures of materials are allowed in the intermediate stages of the design process. This enables the use of gradient-based algorithms to solve the design problem, saving tremendous computational resources compared to discrete optimization methods [17].

It is the choice of material interpolation scheme when considering metallic materials for certain electromagnetic applications, that is the topic of this paper.

If the interpolation is chosen poorly, a non-physical field amplification can occur in and around spatial regions containing non-physical mixtures of material densities. Such non-physical behaviours of intermediate density regions seem to be unique for the [electromagnetic metallic design problem in wavelength regions where the electric permittivity is negative, and thus has an opposite sign compared to the background material](#). This has created challenges in previous papers on the topic [18, 19, 20]. This is in contrast to simpler structural or thermal problems where the interpolation may have an influence on convergence behaviour but not the physics. The non-physical amplification destroys the stable convergence of the design procedure towards physically admissible designs, thereby reducing the reliability and, hence usefulness of the method. The problem is demonstrated to exist for two well known interpolation schemes and a possible explanation for the behaviour, rooted in physics, is provided. [This paper proposes](#) a physically motivated, non-linear material interpolation scheme for the relative electric permittivity, $\epsilon_r = \epsilon'_r - i\epsilon''_r$, as functions of the refractive index, η , and extinction coefficient, κ . Here, ϵ'_r [constitutes](#) the real part and ϵ''_r the imaginary part of the permittivity [and i the imaginary unit](#). The non-linear scheme is demonstrated to improve the behaviour of the topology optimization method in the ultraviolet to low infrared wavelength regime. The scheme avoids the need for applying auxiliary techniques to stabilize the convergence and does not introduce any case-by-case tuning parameters. Previously used techniques include adding an artificial attenuation term in the material interpolation, [18], adding a term penalizing non-physical mixtures of materials in the objective function, [19] or introducing a tuning parameter into the material interpolation [20].

The capability of the scheme is demonstrated by designing a Ag nano-scale antenna-strip using [dimensions and materials identical](#) to a design proposed recently in [19], yielding a more than 600% performance improvement compared to that design.

2. Physics

The physics under consideration is governed by Maxwell's equations [21]. Under the assumptions of time-harmonic field oscillation, infinite extend of the model problem in the out of plane (transverse) direction, non-magnetic materials, in-plane wave propagation and transverse magnetic field-polarization, the equations reduce to the scalar Helmholtz equation governing the transverse magnetic field-component¹,

$$-\nabla \cdot \left(\frac{1}{\epsilon_r(\mathbf{r})} \nabla H_z(\mathbf{r}) \right) - k_0^2 H_z(\mathbf{r}) = 0, \quad \mathbf{H} = \langle 0, 0, H_z \rangle. \quad (1)$$

Here $\mathbf{H}(\mathbf{r})$ is the magnetic field, $\mathbf{r} \in \mathbb{R}^2$ is the spatial position in 2D, ϵ_r is the relative electric permittivity and $k_0 = \frac{2\pi c}{\lambda_0}$ is the free space wavenumber with λ_0 being the free space wavelength and c the speed of light in vacuum. The electric field, $\mathbf{E}(\mathbf{r})$, is computed from Ampere-Maxwell's law,

$$\mathbf{E}(\mathbf{r}) = -\frac{i}{\omega \epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}), \quad (2)$$

where ω is the angular frequency and i the imaginary unit. From here on, the electric-field energy in a region of space, Ω_t , is calculated from the energy density, $w(\mathbf{r})$, as

$$W = \int_{\Omega_t} w(\mathbf{r}) \, d\mathbf{r} = \int_{\Omega_t} \frac{1}{2} |\epsilon'(\mathbf{r})| \left(\mathbf{E}(\mathbf{r}) \cdot \overline{\mathbf{E}(\mathbf{r})} \right) \, d\mathbf{r}, \quad (3)$$

with $\bar{\bullet}$ denoting the complex conjugate. The amplification of (3) in Ω_t will be used as the performance measure in the following, i.e.

$$\Phi = \frac{W}{W_o}, \quad (4)$$

with W_o being the energy in Ω_t without any design (an empty design domain).

¹Assuming the phase convention, $\exp(i\omega t)$

3. Material interpolations

Density-based topology optimization relies on material interpolation schemes to link a change in the design field to a change in the local spatial material property in the physical model problem. For electromagnetic design problems with dielectric materials, a relatively low material contrast in ϵ_r exists, with all dielectric materials exhibiting a positive and real-valued ϵ_r .² Here a simple linear interpolation in ϵ_r has proven sufficient across numerous works, e.g. [15, 13, 14]. For metals in certain wavelength regions, ϵ_r is complex with negative real part and there is not necessarily a low contrast compared to the background material: facts which potentially makes metallic design problems harder to treat.

Nonetheless material interpolations for design problems concerning metals have in previous work been expressed directly in the electric permittivity interpolated linearly [14] or inversely [19]. For a two material setup these interpolation schemes are given by Eq. (5a) and Eq. (5b), respectively,

$$\epsilon_r(\rho) = \epsilon_{r_{M_1}} + \rho(\epsilon_{r_{M_2}} - \epsilon_{r_{M_1}}), \quad (5a)$$

$$\frac{1}{\epsilon_r(\rho)} = \frac{1}{\epsilon_{r_{M_1}}} + \rho\left(\frac{1}{\epsilon_{r_{M_2}}} - \frac{1}{\epsilon_{r_{M_1}}}\right), \quad (5b)$$

where $M_{[]}$ denotes material 1 and 2, respectively.³

In certain wavelength regions, a high permittivity contrast exists between the metallic device and the background material(s). This increases the sensitivity of the physics towards changes in material densities, since a small change in the design field, $\rho(\mathbf{r})$, causes a large change in $\epsilon_r(\rho(\mathbf{r}))$. While potentially problematic, this issue can be mitigated by imposing tight restrictions on the variation of ρ in each design iteration. Two other more crucial differences from the dielectric case exist. Firstly, the real part of ϵ_r , denoted ϵ'_r , is negative and

²Assuming a negligible material loss, which is most often done in practice.

³Note that in other topology optimization applications, e.g. in elasticity, it is common to penalize intermediate design variable values by raising ρ in (5a) or (5b) to exponent n , thereby making intermediate densities uneconomical in the presence of a global volume constraint. Here, no volume constraint is imposed (nor inherently meaningful), rendering such penalization obsolete. This observation is supported by numerical experience in connection with previous works and lab studies.

as ρ is varied from 0 to 1 introduces an unavoidable crossing of 0 when going from a dielectric to a metallic behavior. Secondly, the attenuation introduced by metals in the form of absorption losses, which are related to the non-zero imaginary part of ϵ_r , denoted ϵ_r'' . As will be demonstrated in the following, when using either interpolation (5a) or (5b) for a metallic design problem, non-physical field amplification can occur at intermediate values of ρ . That is, field amplifications which are not generated by a physically admissible design. These amplifications may destroy the smooth convergence towards a high performance, physically admissible design, when solving the optimization problem. Various mitigations of the problems described above have been utilized in the literature as noted in the introduction, see e.g. [18, 19, 20].

As an alternative to interpolating directly in ϵ_r one can utilize the existing relationship between the refractive index, η , extinction coefficient, κ , and electric permittivity, given as: $\epsilon_r = (\eta^2 - \kappa^2) - 2i\eta\kappa$ [22], to formulate the following non-linear interpolation scheme for ϵ_r ,

$$\begin{aligned}\epsilon_r(\eta(\rho), \kappa(\rho)) &= (\eta(\rho)^2 - \kappa(\rho)^2) - i(2\eta(\rho)\kappa(\rho)), \\ \eta(\rho) &= \eta_{M_1} + \rho(\eta_{M_2} - \eta_{M_1}), \\ \kappa(\rho) &= \kappa_{M_1} + \rho(\kappa_{M_2} - \kappa_{M_1}),\end{aligned}\tag{6}$$

with,

$$\eta_{M_i} = \sqrt{\frac{|\epsilon_{r_{M_i}}| + \epsilon'_{r_{M_i}}}{2}}, \quad \kappa_{M_i} = \sqrt{\frac{|\epsilon_{r_{M_i}}| - \epsilon'_{r_{M_i}}}{2}}, \quad i \in \{1, 2\}.\tag{7}$$

Here η and κ are both interpolated linearly in the design field, after which ϵ_r is interpolated non-linearly in η and κ . As is demonstrated in the following, this alternative interpolation scheme behaves significantly better than (5a) and (5b) in the majority of the considered wavelength interval.

Figure 1 illustrates the difference in behaviour of the real and imaginary part of (5a), (5b) and (6) when interpolating between vacuum and Ag at $\lambda_0 = 413$ nm using material parameter values from [23].

It is noted that the shape of the graphs for (5b) and (6) has a strong

Figure 1: Graphs of the interpolations (5a), (5b) and (6) as a function of ρ using vacuum and Ag at $\lambda_0 = 413$ nm as the two materials. (i) Real part of ϵ_r ; ϵ_r' . (ii) Imaginary part of ϵ_r ; ϵ_r'' . (color online)

dependence on the values of ϵ_r, η and κ , which changes with wavelength and choice of metal.

4. Interpolation Behaviour

The model problem sketched in Figure 2, consists of a cross section of an infinitely long out-of-plane square rod in a vacuum background. This model problem is used to investigate the behaviour of the three interpolation schemes; (5a), (5b) and (6), as the design field value, ρ , is varied from 0 to 1 in Ω_d .

Figure 2: Model domain, Ω , for scan of λ_0 and ρ . ρ varies in Ω_d . The electric-field energy amplification, (3), is evaluated in Ω_t . The model is truncated using PML in Ω_{PML} . $\mathbf{k}$: wave vector, $\mathbf{H}$: magnetic field, $\mathbf{E}$: electric field.

The model consists of the following domains; a sub-domain in which the design field is varied uniformly from 0 to 1, Ω_d , embedded in an evaluation sub-domain, Ω_t , further embedded in the full model domain $\Omega \cup \Omega_{\text{PML}}$, the last two

of which contain vacuum, i.e. $\rho(\mathbf{r}) = 0 \quad \forall \quad \mathbf{r} \in \Omega_t \cup \Omega \cup \Omega_{\text{PML}}$. The physics of the model is governed by (1) and the model is excited by an incoming linearly H_z -polarized plane wave propagating from left to right. The model is truncated using perfectly matched layers (PMLs) around Ω to minimize reflections from the boundaries.

The model problem is solved for pairs of λ_0 - and ρ -values in the intervals $\lambda_0 \in [200 \text{ nm}, 1900 \text{ nm}]$ and $\rho \in [0, 1]$, respectively. This is done for each of the three interpolation schemes, (5a), (5b), and (6) using the finite element method (FEM) in COMSOL Multiphysics 5.3 [24]. The wavelength dependent material properties in Ω_d are interpolated between vacuum and each of three noble metals used in plasmonic applications; silver (Ag), gold (Au), and copper (Cu) [23]. The resulting electric-field energy amplifications in Ω_t , (3), for Ag are presented in figure 3(i-iii) and discussed in the following, while the results for Au and Cu are provided in Appendix A.

From figure 3i it is observed that interpolating linearly in ϵ_r results in a band of significant artificial field enhancement at intermediate values of ρ , i.e. for non-physically admissible values of ρ , from the ultraviolet and well into the infrared spectrum, $400 \text{ nm} \leq \lambda_0 \leq 1800 \text{ nm}$. From figure 3ii it is seen that interpolating inversely in ϵ_r reduces and shifts the span of densities at which the non-physical field enhancement is seen to a narrow band at higher ρ -values. Finally, from figure 3iii one observes that the non-linear interpolation is less prone to large field enhancements (observed in figure 3i) and to sudden jumps in the field enhancement for intermediate design field values (observed in figure 3iii). The exception being a narrow wavelength and density band at approx. $400 \text{ nm} \leq \lambda_0 \leq 500 \text{ nm}$ and $0.7 \leq \rho \leq 1.0$.

A possible explanation of the observed behaviours may be found by considering the following physical quantities: the polarizability of a particle, α , (a bulk resonance condition), the conditions for a surface plasmon at a metal/dielectric interface, and the value of the imaginary part of interpolated material parame-

Figure 3: Maps of quantities as a function of λ_0 and ρ for the three interpolation schemes between Ag and vacuum for the model problem sketched in figure 2. The maximum values of the color bars are truncated to improve comparability across interpolations. (i)-(iii): Maps of the electric-field energy amplification, (4), in Ω_t by introducing the particle in a vacuum background. (iv)-(vi): Maps of (8). (vii)-(ix): Binary maps of the condition (9), red is true, blue is false. (x)-(xii): Maps of ϵ''_r . (color online)

ter, ϵ''_r .

For a cylindrical needle (length/diameter $\rightarrow \infty$), in the quasi-static limit where the diameter is much smaller than wavelength of the driving field, an in-plane polarizability condition is presented in [25]. Further, two surface plasmon material interface conditions from [26] are considered. These are,

$$\alpha = 2 \frac{\epsilon_{r_{M_a}} - \epsilon_{r_{M_b}}}{\epsilon_{r_{M_a}} + \epsilon_{r_{M_b}}} \quad [\text{polarizability, needle (bulk condition)}], \quad (8)$$

$$\epsilon_{r_{M_a}} + \epsilon_{r_{M_b}} < 0, \quad \epsilon_{r_{M_a}} \epsilon_{r_{M_b}} < 0 \quad [\text{surface plasmon conditions}], \quad (9)$$

where M_a and M_b denotes the particle and background materials, respectively. Although (8) is derived for a circular needle the expression still provide ample qualitative insight for the behaviour of the infinitely extruded square "needle" considered here, as will be seen in the following.⁴ The absolute value of (8) is evaluated for the three interpolation cases as a function of λ_0 and ρ using the interpolated material as M_a and vacuum as M_b . The results are plotted in figure 3(iv-vi). For the surface plasmon conditions the procedure in [26] is followed (the imaginary part of ϵ_r is omitted when evaluating the binary conditions in (9)). The results of which are plotted in figure 3(vii-ix), red being used to indicate the region where the condition is fulfilled. Finally the magnitude of the imaginary part of ϵ_r for each interpolation is plotted in figure 3(x-xii).

Consider first the linear interpolation, i.e. the first column of figure 3. Here a region of large field amplification is observed in figure 3i, which coincides with the ridge of high polarizability in figure 3iv. Simultaneously, the region also overlaps with the region in which the surface resonance condition is fulfilled, seen in figure 3vii, as well as residing in a region with a low value of ϵ_r'' as seen in figure 3x. Hence it is possible to select non-physical material mixtures for a wide range of wavelengths for which both bulk and surface resonances can occur, while simultaneously experiencing low attenuation. The result of which being a non-physical field amplification.

Consider next the inverse interpolation, i.e. the second column of figure 3. From figure 3v it is seen that the interpolation exhibits a low polarizability in almost the entire mapped parameter region. From figure 3viii it is seen that

⁴Both a square and a circular case have been investigated, yet only the former is included due to its similarity to the design problems considered later in the paper.

the surface plasmon condition is only fulfilled in a smaller parameter region. When inspecting figure 3xi, it is clear that ϵ_r'' is close to zero in a large region of the parameter map. This effectively renders the non-physical material mixture semi-transparent to the electromagnetic field by making it behave as a dielectric instead of a metal. Hence it is possible to select a material mixture for which the field can propagate through regions of the material without experiencing any attenuation.

Finally, consider the non-linear interpolation, i.e. the third column of figure 3. From figure 3vi it is seen that this interpolation exhibits a low polarizability in nearly the entire mapped parameter region. From figure 3ix it is seen that the surface plasmon condition is fulfilled in a large parameter region. However, figure 3xii shows that almost the entire parameter region have a high value of ϵ_r'' , hence any field propagating into the particle will be attenuated significantly. The attenuation at intermediate ρ -values, coupled with the lack of polarizability, reduces the existence of non-physical field enhancements, as observed from figure 3iii.

Figure 4: Electric-field norm, $|\mathbf{E}|$, in and around the Ag particle in vacuum background at $\lambda_0 = 1000$ nm for different values of ρ and different interpolations. (i) $\rho = 0$. (ii) The linear interpolation, (5a), at $\rho = 0.04$. (iii) The inverse interpolation, (5b), at $\rho = 0.96$. (iv) For the non-linear interpolation, (6), at $\rho = 0.29$. (v) $\rho = 1$. (color online)

In addition to studying the maps in figure 3 there is also insight to be gained by observing the field in and around the square particle at selected ρ -values. Figure 4 shows snapshots of the electric-field magnitude for $\lambda_0 = 1000$ nm at the ρ -values for which maximal amplification is observed for each interpolation scheme along with the field for $\rho = 0$ and $\rho = 1$. It is seen that the field profile for the linear and inverse interpolation schemes are significantly different from each other, and more crucially from the profile for $\rho = 1$. This is not the case

for the non-linear interpolation. Here the field profile is close to the profile for the pure Ag particle, meaning that the change from the non-physical material mixture form $\rho = 0.29$ to pure Ag ($\rho = 1$) has little influence on the field profile.

In summary, the factors found to determine the success/failure of an interpolation scheme for metallic design problems in the optical wavelength regime are found to be the presence of attenuation at intermediate densities and crucially the (in)admissibility of bulk and surface plasmons at intermediate densities.

5. Design problem

The rest of the paper concerns the design of nano-scale metallic particles placed in a vacuum background, $\epsilon_{r_{\text{vacuum}}} = 1$. The aim of which is to amplify Φ in Ω_t when the particles are illuminated by an external Hz-polarized field at a specified angle. The design problem is formulated as an optimization problem where the metallic particles are modelled using the design field, $\rho(\mathbf{r})$, and Φ is sought maximized over $\rho(\mathbf{r})$.

$$\max_{\rho(\mathbf{r})} \Phi = \frac{W}{W_o}, \quad (10)$$

$$\text{s.t.} \quad 0 \leq \rho(\mathbf{r}) \leq 1, \quad (11)$$

with the constraint that $\mathbf{H}$, used for calculating $\mathbf{E}$, is a solution to (1) for all permissible realizations of $\rho(\mathbf{r})$. Filtering techniques are applied to $\rho(\mathbf{r})$ and the resulting field is introduced into the physics through ϵ_r in (1), (2) and (3) using either interpolation (5a),(5b) or (6) to interpolate between the metallic particle and vacuum background.

Figure 5 illustrates the model domain, Ω [200 nm x 1000 nm], with Ω_d denoting the design domain of width $w_d = 100$ nm and height $h_d = 100$ nm with a hole at its centre consisting of the target domain, Ω_t , of width $w_t = 10$ nm and height $h_t = 10$ nm.

Figure 5: Model problem and design domain. Ω : Model domain, Ω_d : Design domain, Ω_t : Target domain, Γ_F : Fourier boundary, Γ_P : Periodic boundary, $\mathbf{k}$: wave vector, $\mathbf{H}$: Magnetic field, $\mathbf{E}$: electric-field.

$\mathbf{H}$ is obtained by solving the model problem using a first order finite element scheme on a mesh consisting of 1 nm square elements covering the entire modelling domain. A free space radiation condition on Γ_{F} is approximated using a plane wave expansion based method [27] and periodicity is imposed on Γ_{P} using a Floquet-Bloch boundary condition [14].⁵

The design field is discretized into a piecewise constant field coinciding with the FEM mesh on which the model problem is solved with one design variable, ρ_i , assigned to each element. A density filter [28] using a smoothing radius of $R = 2.5$ nm is applied to $\rho(\mathbf{r})$ for all cases, yielding a smoothed design field, $\tilde{\rho}(\mathbf{r})$. In cases 2 and 3, a projection operator [29, 30] is applied to $\tilde{\rho}(\mathbf{r})$ yielding the projected design field $\bar{\rho}(\mathbf{r})$, using the projection level $\eta_p = 0.5$ and a continuation scheme for the projection sharpness β_p . $\tilde{\rho}(\mathbf{r})$ (case 1) and $\bar{\rho}(\mathbf{r})$ (cases 2 and 3) is used to interpolate the material parameters using (5a), (5b) and (6), respectively. An initial guess of $\rho(\mathbf{r}) = 0.5$, $\forall \mathbf{r} \in \Omega_d$ is used in all cases. The sensitivities $\frac{d\Phi}{d\rho_i}$ are calculated using adjoint sensitivity analysis [31]

⁵The use of a different numerical model from the previous study does not influence the interpolation behaviour.

and (10)-(11) are solved using the Method of Moving Asymptotes (MMA) [32].

6. Design cases

Three design cases are considered in the following. The first two are used to illustrate the different behaviours of (5a), (5b), (6). The third concerns the design of a physically admissible nano-scale antenna-strip device using (6) with model parameters taken from [19]. In the first two cases the three metals Ag, Au and Cu are considered. The results for Ag are presented and analysed in the following, while the results for Au and Cu are provided in Appendix A.

6.1. Case 1: Gray scale designs (no projection during optimization)

Gray scale designs for Ag particles are optimized using each of the interpolation schemes (5a), (5b) and (6). To do so, the optimization problem (10)-(11) is solved using a fixed number of 400 design iterations, for the wavelengths $\lambda_0 \in \{200 \text{ nm}, 250 \text{ nm}, \dots, 1900 \text{ nm}\}$, with the density filter applied to $\rho(\mathbf{r})$. Note that the projection operator is not applied in this case. The final smoothed design field, $\tilde{\rho}_{\text{final}}(\mathbf{r})$, is projected to $\rho = 0$ and $\rho = 1$ around $\rho = 0.5$ using a Heaviside step function. This is done to recover a physically admissible design consisting purely of Ag and vacuum. The performance of the recovered design is plotted in figure 6i on a logarithmic base 10 scale.

From figure 6i it is seen that for $\lambda_0 \leq 300 \text{ nm}$ the design obtained using each of the three interpolations perform similarly. For $1400 \text{ nm} \leq \lambda_0$ the linear interpolation performs equally to or better than the non-linear interpolation, up to a maximum of a factor of 1.5 at $\lambda_0 = 1900 \text{ nm}$, while the inverse interpolation consistently show poorer performance. For $350 \text{ nm} \leq \lambda_0 \leq 1400 \text{ nm}$ the picture is different, however. In this range the non-linear interpolation consistently outperforms both of the other interpolations. In the interval $350 \text{ nm} \leq \lambda_0 \leq 950 \text{ nm}$ the difference in performance ranges from nearly one order of magnitude up to almost two orders of magnitude for all but a single design (at $\lambda_0 = 550 \text{ nm}$).

The observed performance differences may be understood by inspecting the final smoothed and projected design fields, along with the corresponding spatial electric-field energy amplification. This is illustrated for each interpolation scheme at the excitation wavelengths $\lambda_0 = 250$ nm and $\lambda_0 = 500$ nm in figure 6(ii-iii) and figure 6(iv-v), respectively. Note that $\tilde{\rho}_{\text{final}}(\mathbf{r})$ is plotted using a white, yellow, red and black colour map to enhance the visibility of regions with $0 < \tilde{\rho}_{\text{final}}(\mathbf{r}) < 1$.

Consider first the case of $\lambda_0 = 250$ nm shown in figure 6(ii-iii). Here similar designs with similar energy profiles exhibiting similar performance are seen across the three interpolations. The designs all have features in the form of a vertical bar and two symmetrically placed lumps of material and the performance difference is within 10%, with the projected designs all performing better than the gray scale designs.

Consider next the case of $\lambda_0 = 500$ nm shown in figure 6(iv-v). Here it is seen that the three gray scale designs exhibit several differences and by extension so do the projected designs. It is also observed that Φ decreases from the gray scale designs to the projected designs for both interpolation (5a) and (5b) while it increases for (6).

For interpolation (6) the gray scale design is close to the final projected design, with only the gray scale along the edges being removed by the projection. These gray-scale regions has a width of less than 1% of the considered wavelength. Hence the truncation of the gray scale has a negligible effect on the phase of the field. Meanwhile any gray scale removed by the projection reduces the attenuation of the field, thereby leading to an increase in the total energy in the system. This effect can be observed by looking at the electric-field energy amplification in figure 6v. For interpolation (5b) the gray scale design has large areas of intermediate densities which allows the electromagnetic field to propagate through the design without attenuation (see figure 3xi) while simultaneously influencing the phase of the field causing favourable interference, effectively acting as a dielectric. Once the Heaviside step function is applied, however, the intermediate densities disappear and so does their effect on the

field, hereby degrading the performance of the design by almost two orders of magnitude. Again, this effect is observable by considering the electric-field energy amplification in figure 6v. Finally, consider the gray scale designs for the design obtained using interpolation (5a). Here, two narrow horizontal channels of $\tilde{\rho} \approx 0.7$ and a vertical variation in $\tilde{\rho}$ between 0.8 and 0.9 in the left part of the gray scale design are seen to be present. This allows the field to propagate through this part of the design with lower attenuation than would be the case for $\tilde{\rho} = 1$ (see figure 3x). As $\tilde{\rho}$ is projected, the regions of intermediate values of $\tilde{\rho}$ disappear and the field is forced to propagate through the Ag barrier, losing intensity while simultaneously not experiencing artificial amplification. From figure 6v one can observe the local artificial field amplification in several spatial regions for both interpolation (5a) and (5b).

Figure 6: (i) electric-field energy amplification (Φ) as a function of wavelength for pure Ag/vacuum designs obtained using the three interpolation schemes. Column 1 of (iii) and (iv) shows the final smoothed design fields, $\tilde{\rho}_{\text{final}}(\mathbf{r})$, in a $[120 \text{ nm} \times 120 \text{ nm}]$ spatial region, for each interpolation scheme at $\lambda_0 = 250 \text{ nm}$ and $\lambda_0 = 500 \text{ nm}$, respectively. Column 2 of (iii) and (iv) shows the pure Ag/vacuum-projection around $\rho = 0.5$ of $\rho(\mathbf{r})$ from column 1. The six images in (ii) and (v) show the point wise electric-field energy amplification corresponding to the plots in (iii) and (iv), respectively, on a logarithmic base 10 scale. (color online)

6.2. Case 2: Designing for physical admissibility (using projection in optimization)

Three Ag particles are designed using the interpolation schemes (5a), (5b) and (6) respectively for the excitation wavelength, $\lambda_0 = 500$ nm. This is done by solving the optimization problem (10)-(11) using a fixed number of 2400 design iterations, applying both the smoothing and projection operators to obtain the final design field, $\bar{\rho}_{\text{final}}(\mathbf{r})$. A β_p -continuation scheme is used for the projection operator where β_p is increased by a factor of 1.5 for every 400 design iterations starting at $\beta_p = 1$ and ending at $\beta_p \approx 7.6$ after 2000 iterations. This procedure results in designs with $> 99\%$ of all design variables attaining the value of 0 or 1.

Figure 7 shows $\bar{\rho}_{\text{final}}(\mathbf{r})$ as well as the evolution of Φ during the optimization for each interpolation scheme.

Figure 7: (i)-(iii) Final Ag distribution (black) in vacuum background (white) for the three interpolation schemes at $\lambda_0 = 500$ nm, shown in a $[120 \text{ nm} \times 120 \text{ nm}]$ spatial region. (iv)-(vi) Φ as a function of design iteration for the three interpolation schemes, (note the different scale on Φ -axis).

Comparing the geometry of the designs in figure 7(i-iii), it is seen that the design created using interpolation (6) has a simpler topology than the designs created using interpolation (5a) and (5b). Turning the attention to figure 7(iv-vi) it is seen that the objective increases monotonously for the design created using interpolation (6). In contrast, Φ is seen to exhibit an oscillatory behaviour with drops at each β_p -increase for the designs created using interpolation (5a)

and (5b). The [design performance](#) is seen to decrease by several orders of magnitude for the inverse interpolation as β_p is increased towards its final value.

While this example only considers $\lambda_0 = 500$ nm, similar conclusions regarding the design topology and objective evolution have been reached for $\lambda_0 \in [350 \text{ nm}, 1400 \text{ nm}]$.

6.3. Case 3: Designing a physically admissible antenna

In [19] a 2D nano-scale antenna is designed using a hybrid two-stage optimization scheme [with the intent of maximizing the field enhancement of the antenna. This is done by introducing a target enhancement in the optimization problem formulation and aiming to match or exceed this target by solving the optimization problem.](#) The first stage consists of using density-based topology optimization with explicit penalization of intermediate material densities in the design problem, a smoothing operation on the design field and inverse interpolation of ϵ_r using (5b). The second stage consists of a shape optimization using the final densities from the first stage to compute the initial shape. Using this approach an electric-field energy amplification of 193 compared to the background field was reported for an antenna with 0.5 nm design field resolution.

The pure density-based topology optimization scheme outlined previously is used in the following. The excitation wavelength, material parameters, design dimensions and resolution as well as the design region and target region, are chosen to match those used in [19]. This allows for a direct comparison of the resulting designs. The smoothing operator is applied to the design field using the radius $R_s = 2.5$ nm and a continuation scheme is applied to the projection sharpness, β_p , performing 50 design iterations between increases in β_p by a factor of 1.5 starting from 1.

Figure 8 shows a graph of the objective function as a function of design iteration along with the evolving design field and corresponding electric-field energy amplification plotted on a logarithmic base 10 scale for eight select iterations during the design process. It is seen that the design evolves from

Figure 8: Φ as a function of design iteration with snapshots of the design field, $\bar{\rho}$, and spatial electric-field energy amplification on a logarithmic base 10 scale. Both fields are shown in a $[105 \text{ nm} \times 105 \text{ nm}]$ spatial region. (color online)

$\bar{\rho}(\mathbf{r}) = 0.5 \quad \forall \mathbf{r} \in \Omega_d$ into an nearly pure Ag/vacuum design. It is noted from the graph that Φ is monotonically increasing for the entire design procedure. The slow monotone increase of Φ between β_p -increases suggest that it is possible to reduce the number of design iteration, to save computational resources, without affecting the final design performance.

Figure 9: (i) Final design field for the nano-scale antenna-strip, black is Ag and white is vacuum. (ii) spatial electric-field energy amplification on a logarithmic base 10 scale. Both fields are shown in a $[105 \text{ nm} \times 105 \text{ nm}]$ spatial region. (color online)

The final posts processed, physically admissible design, obtained using a Heaviside step function around $\bar{\rho} = 0.5$ is shown in figure 9i. The design is evaluated in COMSOL Multiphysics [24] using a model with PML boundary conditions and a continuous Lagrange FEM formulation with quadratic basis functions on a triangular mesh with a maximum element size of 1 nm. Here, a value of $\Phi \approx 1254$ is obtained⁶, i.e. a more than three orders of magnitude amplification in the localized electric-field energy, a map of which is shown in figure 9ii. This value constitutes a more than 600% increase compared to the reference design from [19].

The final design is interesting and possibly non-intuitive, consisting of a closed cavity with an elaborate outer profile and a horn antenna like inner profile. The roughly 12 nm thick front wall of the cavity allows the electric-field to penetrate inside, as Ag has a skin depth at normal incidence, of ≈ 29 nm at $\lambda_0 = 413$ nm. The field is then guided into Ω_t where it is concentrated and amplified.

It is noted that the antenna-strip design has features below current standard production tolerances using e.g. EBL nano-lithography, leaving little hope of its immediate realization using present day production tools. Although, it can be argued that a production technique like helium ion deposition [33] might be able to achieve the required resolution. Further, the utilization of established robust optimization techniques [29, 34, 35] enable the design of devices which are robust towards manufacturing errors, thus facilitating the design of producible particles. However, since the purpose of this example is to demonstrate the benefits of applying the new non-linear interpolation scheme, the issue of fabrication is not of interest and thus not addressed in this work.

⁶The reason for the increase in Φ from the non-projected final design shown in figure 8 to the projected final design in figure 9 is, as in both cases 1 and 2, the removal of gray scale along the solid feature edges.

7. Conclusion

This paper has demonstrated superior properties of a new non-linear material interpolation scheme for performing density-based topology optimization of metallic particles for electromagnetic design problems in the ultraviolet to low infrared wavelength regime. The scheme was used to design a Ag antenna-strip yielding a more than 1200 fold field enhancement, a more than 600% increase in performance compared to a reference design from the recent literature.

An in-depth analysis of the scheme was provided and examples of applying the scheme to the design of nano-particles using density-based topology optimization were presented and analysed. Two alternative interpolation schemes, previously used in the literature, were considered for comparison. The non-linear scheme was demonstrated to consistently produce designs with higher performance and simpler topologies over a wide wavelength range compared to the references. Further, the convergence of the objective function over the course of the optimization was shown to be significantly smoother using the non-linear interpolation. This shows that no auxiliary techniques are needed to stabilize the convergence of the optimization problem, hence no arbitrary tuning constants are introduced.

It is noted that for all cases considered in this work the final sharp projection of the optimized designs for the non-linear interpolation performed better than the optimized gray-scale designs. It would be trivial to execute the optimizations with a higher value for the maximal projection strength, β_p , and/or using an adaptive scheme for increasing β_p , thereby assuring that a (near) perfect discreteness is achieved in the optimization. An adaptive approach was indeed tested for several designs using interpolation (6) and in all cases it was found that the final geometry and performance did not vary significantly from the sharply projected final designs.

While this paper focusses on the two dimensional case, the authors have also successfully utilized the non-linear interpolation scheme for three dimensional design problems and are confident that the conclusions drawn from the results

in this paper extend directly to three dimensions.

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Appendix A. Results and Data for Au and Cu

Maps of the energy amplification (3), polarizability (8), surface plasmon conditions (9) and imaginary part of the electric permittivity for the three interpolations (5a), (5b), and (6) interpolating between Cu and vacuum in figure A.10 and Au and vacuum in figure A.11. These maps illustrate similar tendencies to those shown in figure 3 for Ag and vacuum, consequently similar conclusions may be drawn.

Figure A.12 and figure A.13 show results for design case 1 for Cu and Au, respectively. These corresponds to the results presented in figure 6 for Ag. The superiority of the non-linear interpolation in a wide wavelength region is demonstrated for both Cu and Au. The wavelength region is shifted upwards compared to the Ag case and the difference in performance is up to one order of magnitude between the three interpolations compared to two orders of magnitude for Ag. The illustrations of the final and project design field and corresponding electric energy amplification (at $\lambda_0 = 250$ nm and $\lambda_0 = 700$ nm) for each of the three interpolations, reveal the same tendencies as those discussed for the Ag case.

Figure A.14 and figure A.15 show results for design case 2 for Cu and Au, respectively, attained for $\lambda_0 = 700$ nm. These figures corresponds to figure 7 for Ag. Analysing the data in figure A.14 and figure A.14 result in similar conclusions regarding the topology of the final designs and the behaviour of Φ as a function of design iteration, as those reached for Ag.

Figure A.10: Maps of quantities as a function of λ_0 and ρ for the three interpolation schemes between Cu and vacuum for the model problem sketched in figure 2. The maximum values of the color bars are truncated to improve comparability across interpolations. (i)-(iii): Maps of the electric-field energy amplification, (4), in Ω_t by introducing the particle in a vacuum background. (iv)-(vi): Maps of (8). (vii)-(ix): Binary maps of the condition (9), red is true, blue is false. (x)-(xii): Maps of ϵ_r'' . (color online)

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Figure A.11: Maps of quantities as a function of λ_0 and ρ for the three interpolation schemes between Au and vacuum for the model problem sketched in figure 2. The maximum values of the color bars are truncated to improve comparability across interpolations. (i)-(iii): Maps of the electric-field energy amplification, (4), in Ω_t by introducing the particle in a vacuum background. (iv)-(vi): Maps of (8). (vii)-(ix): Binary maps of the condition (9), red is true, blue is false. (x)-(xii): Maps of ϵ_r'' . (color online)

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Figure A.12: (i) electric-field energy amplification (Φ) as a function of wavelength for pure Cu/vacuum designs obtained using the three interpolation schemes. Column 1 of (iii) and (iv) shows the final smoothed design fields, $\rho_{\text{final}}(\mathbf{r})$, in a $[120 \text{ nm} \times 120 \text{ nm}]$ spatial region, for each interpolation scheme at $\lambda_0 = 250 \text{ nm}$ and $\lambda_0 = 700 \text{ nm}$, respectively. Column 2 of (iii) and (iv) shows the pure Cu/vacuum-projection around $\rho = 0.5$ of $\rho(\mathbf{r})$ from column 1. The six images in (ii) and (v) show the point wise electric-field energy amplification corresponding to the plots in (iii) and (iv), respectively, on a logarithmic base 10 scale. (color online)

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Figure A.13: (i) electric-field energy amplification (Φ) as a function of wavelength for pure Au/vacuum designs obtained using the three interpolation schemes. Column 1 of (iii) and (iv) shows the final smoothed design fields, $\hat{\rho}_{\text{final}}(\mathbf{r})$, in a $[120 \text{ nm} \times 120 \text{ nm}]$ spatial region, for each interpolation scheme at $\lambda_0 = 250 \text{ nm}$ and $\lambda_0 = 700 \text{ nm}$, respectively. Column 2 of (iii) and (iv) shows the pure Au/vacuum-projection around $\rho = 0.5$ of $\rho(\mathbf{r})$ from column 1. The six images in (ii) and (v) show the point wise electric-field energy amplification corresponding to the plots in (iii) and (iv), respectively, on a logarithmic base 10 scale. (color online)

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Figure A.14: (i)-(iii) Final Cu distribution (black) in vacuum background (white) for the three interpolation schemes at $\lambda_0 = 700 \text{ nm}$, in a $[120 \text{ nm} \times 120 \text{ nm}]$ spatial region. (iv)-(vi) The Φ -evolution during the design process for the three interpolation schemes, note the different scale on the Φ -axes.

Figure A.15: (i)-(iii) Final Au distribution (black) in vacuum background (white) for the three interpolation schemes at $\lambda_0 = 700 \text{ nm}$, in a $[120 \text{ nm} \times 120 \text{ nm}]$ spatial region. (iv)-(vi) The Φ -evolution during the design process for the three interpolation schemes, note the different scale on the Φ -axes.

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