Inverse design of 2D wave devices with optimization

Egor E. Nuzhin[1]†, I. - B. Minin[1, 2] and A. X. Boyko[1]

[1]Computational and Data-Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Building 3, Russian Federation

[2]Department of Physical and Quantum Electronics, Moscow Institute of Physics and Technology, 9 Institutskiy per., Dolgoprudny, Moscow Region, 141700, Russian Federation

(Received xx; revised xx; accepted xx)

The optimization techniques used in coupled with ab-initio solver for wave physics to obtain optimal shape of a device. The simplified version of the problem, showing applicability of optimization methods to inverse design of some optical devices has been considered.

Key words: Topology optimization, solver, generalized minimal residual method, numerical linear algebra, gradient, Jacobi matrix, complex functions.

1. Team

- **Egor**: He has implemented two topology optimization solvers based on the non-gradient (broadcasting on the edge of the homogeneous substance) and the gradient implementations. Both solvers use Greedy algorithm. He has tried to implement this problem as locally convex and to resolve this problem using CVXPY but it hasn't been successful. He has implemented Jacobi matrix for computing the mask gradient of maximum of field vector. He has produced and programmed (in Python) easily computed formula for calculating **row** of Jacobi matrix using 2D FFT-matvec. He has implement topology optimization problem using built-in *scipy*−optimizer.
- **Iurii**: He has designed main idea of stable version of topology optimization solver and described it theoretically. He has produced formula for the easily-computable diagonal of Jacobi matrix and programmed it in Python. He has implemented solver of linear equations systems based on GMRES-solver, organized this function with features that have user-friendly interface with flags of outputing data, for example, on convergence of solution, residuals, etc. He has tested program and organized output results using .png format, has collected output data, created this report.
- **Alexey**: He has provided group with formulas of field vector distribution in 2D space, using Helmholtz equation, Hankel function, Green function, debugged errors that have been appeared during the programming. He has reviewed the code of program. He has checked results of program for physical principles compliance.

† Email address for correspondence: egor.nuzhin@skoltech.ru

2. How should it be used?

Optimization of geometry of acoustic, photonic or nanooptical devices numerically, as opposed to analytically, is a modern direction in engineering in acoustics, optics, photonics and metamaterial science.

It is practical because new generation of computational devices will require photonics components on silicon chips. To make such devices to operate properly one needs to do careful and precise design. The full version of it is a promising way to design actual nanophotonic devices.

3. Problem formulation

- Modeling of interaction of electromagnetic waves in conducting medium
- Representation of electromagnetic waves animations
- Topological optimization of electromagnetic wave based devices

Problem, that we solved, it is : Modeling and Representation of interaction of electromagnetic waves in conducting medium, And Topological optimization of material for wave based devices.

To mathematically formulate an optimization problem, and especially topology optimization problem based on the generic functional obtained from an integral equation is by itself a part of our research.

The approximate formulation is the following - to explore how various optimization methods and formulations work in conjunction with FFT-GMRES Volume Integral Equation solver

3.1. *Existing methods to resolve this problem:*

- Direct solution of Maxwell equations
- Experimental observing
- Numerical methods

Actually, this problem solved Numerically, since to compute field analytically for complex forms is very hard.

3.2. *Data*

Input parameters - some 2D distribution of material as a binary mask. Output parameters - complex-valued electric acoustic field distribution in the device, obtained from physics solver. Cost function - some functional of the quality of the device of the electric field, depending on the device. For example, in case of simple devices such as lens, parabolic reflectors or optical systems the cost function will the the focus power.

3.3. *Scope*

Creation of a software capable to return an optimal shape of a certain type of wave - device, for example, a light reflector, optical lens or a wave splitting grating.Due the novelty of the problem it is not known in advance which types of devices may be effectively optimized using standard techniques.

4. Who cares

- Physics based studying of electromagnetic waves entity
- Radio photonics
- Topological optimization of size and performance of photonics devices:

- ◦ HUAWEI
- ◦ CISCO
- ◦ INTEL
- ◦ SAMSUNG
- ◦ IBM

Our work may be interested for physics based studying (when we can see or may be touch field by hand). Radio phoenix is also important area, where such research are often used. And most important sub topic is topological optimization of size and performance of photonics devices. Such companies like HUAWEI, CISCO, INTEL, SAMSUNG, IBM preform such studies intensively.

5. Main wave integral equations

5.1. *Helmholtz equation*

Our project is based on the following integral equation. This formula represent real field E in some area with dielectric constant distribution ε, if in a vacuum it was represented by F.

$$E(x) - k^2 \int G(x - \tilde{x}) \left(\{\varepsilon(\tilde{x}) - 1\}\right) E(\tilde{x}) d\tilde{x} = F(x), \tag{5.1}$$

where $E(x)-$is required field, $G(x-\tilde{x})-$is Green function, $k-$ is the wave number, $\varepsilon(\tilde{x})-$is the dielectric constant, $f(x)-$ is the electromagnetic intensity distribution in vacuum.

Green function $G(r)$ is represented by the Hankel-function H_α that is the complex superposition of Bessel functions of of the first kind J_α and of the second kind Y_α, where α is complex number, the the order of the Bessel function. The $\alpha = 0$ with first kind of Hankel-function $H_0^{(1)}$ has been used in this research :

$$H^{(1)}_{\alpha=0} = J_{\alpha=0} + iY_{\alpha=0} \leftrightarrow H_0^{(1)} = J_0 + iY_0 \tag{5.2}$$

Green-function has been represented using the Hankel-function in the following way:

$$G(r) = \frac{i}{4} H_0^{(1)}(k \cdot r) \tag{5.3}$$

6. Wave equation discretization (Vacuum with homogeneous substance is considered)

One resolves the following linear equations system:

$$Ax = f, \tag{6.1}$$

where

$$\begin{cases} A = I - k^2(\varepsilon - 1)G \cdot diag(m) \\ x = vect(E) \\ f = vect(F) \end{cases}, \tag{6.2}$$

where m is mask: $\{0, 1\}$

This system may be discretized and, in our partition case for constant epsilon and arbitrary mask, expressed in the following vectorized format.

Here one set the problem to maximize the maximal field vector $E(x)$ in whatever point of the 2D space by varying the mask m of the 2D space. Mask m of this space determines the location of homogeneous substance in the 2D space: $m_{ij} = 1$ means that homogeneous substance is present in the $i, j-$th pixel of the 2D space, otherwise: $m_{ij} = 0$ means there is the vacuum in the $i, j-$th pixel of this 2D space.

7. Topology optimiztion problem statement

Now we can formulate optimization problem. We want to maximize power of electromagnetic wave in some point. This problem is discrete, so o solve it using continuous optimize we need to relax it.

Maximization the maximal field vector $E(x)$ in whatever point of the 2D space by varying the mask m of the 2D space is the following:

$$\max_m \|x(m)\|_\infty \textbf{Subject to} \begin{cases} A = I - k^2(\varepsilon - 1)G \cdot diag(m) = f \\ m \in \{0, 1\} \end{cases} \tag{7.1}$$

This problem is non-convex because there is a lot of local optimums may be achieved in this statement because of big freedom degree of 2D space.

8. Penalization of optimization problem

$$\max_m \|x(m)\|_\infty - c \cdot m^T(1 - m) \textbf{Subject to} \begin{cases} A = I - k^2(\varepsilon - 1)G \cdot diag(m) = f \\ 0 \leqslant m \leqslant 1 \end{cases} \tag{8.1}$$

9. Acceleration of optimization problem provided by Jacobi matrix

To solve this problem fast we have coupled Jacobian:

$$A \cdot J_m(x) = BA = I - k^2(\varepsilon - 1)G \cdot diag(m) = fB = k^2(\varepsilon - 1) \cdot diag(m) \tag{9.1}$$

10. FFT matvec for G matrix product

Problem is that size of G matrix is $n^2 \times n^2$. Usual matrix-by-matrix multiplication requires $\mathcal{O}(n^2)$, but for a 2D FFT one have to do $m \times 1D$ FFTs in each axis so that's $\mathcal{O}(2n^2 \log n) = \mathcal{O}(n^2 \log n)$. Thus 2D FFT has been implemented to create matrix G by vector P multiplication where in the case of the given problem matrix G is the the Green matrix (Toeplitz matrix). Since G is Toeplitz matrix, fast FFT matvec has been implemented in this problem. In addition, there is another problem with matrix G. It is the capacity of storage of this matrix. For example, to storage of the $G-$matrix that corresponds to the mask of n^2-elements requires n^4 float elements that corresponds to 2 gigabytes of Random-Access Memory. However, in this research this problem has been resolved using FFT matvec linear operator that corresponds to the storage of n^2 elements. This linear operator convert each ith $1 \times n^2$ row of $G-$ matrix G_i into ith $n \times n$ matrix that in the next step will be converted using FFT. Next, the mask-vector $1 \times n^2$ $M-$ converts into $n \times n$ $m-$ matrix and then, after FFT on m, the inverse FFT on multiplication of $FFT_{2D}(G_i)$ and $FFT_{2D}(m)$ is calculated. Result of this operation returns the part of product of matrix G by matrix M multiplication:

$$G_i \cdot m = IFFT_{2D}[FFT_{2D}(G_i) \cdot FFT_{2D}(m)] \tag{10.1}$$

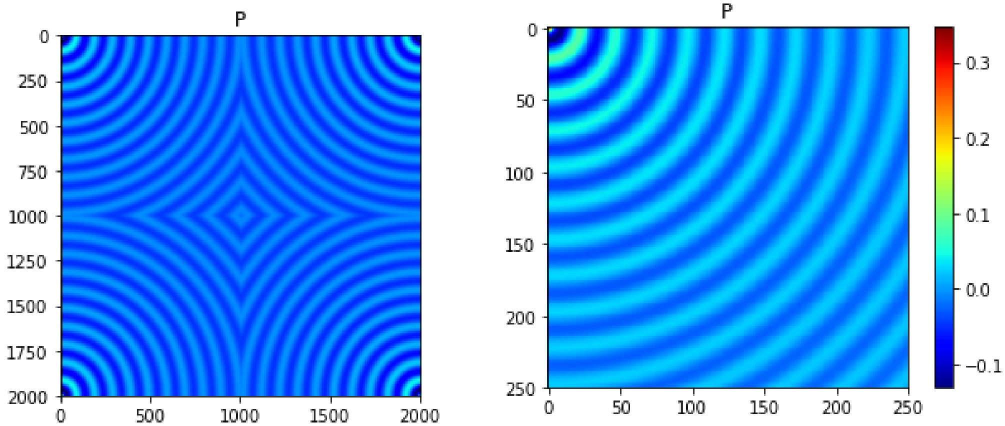


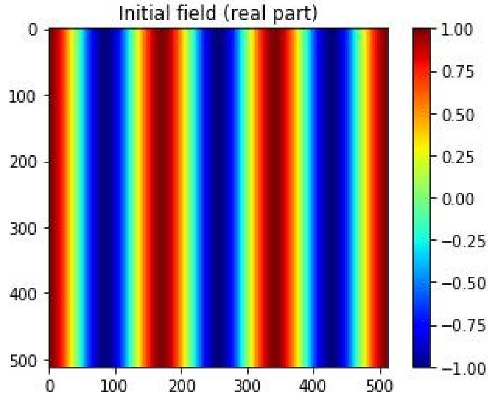
FIGURE 1. in the left: circulant matrix (Surrogate of G); in the right: Toeplitz block of G

11. Examples of work of the solver

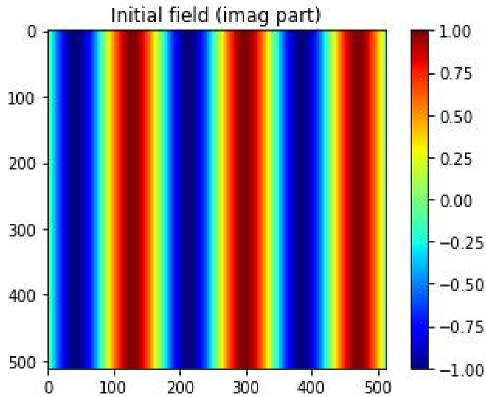
The solver is in Python (programming language). In initial vector of wave intensity that corresponds to the case when there is now homogeneous substance and there is only vacuum in all $n \times n$ 2D space is represented by its real part and its imaginary part:

The **number of periods of electromagnetic wave** on this planes= $\frac{\textbf{the length of the plane}}{\textbf{the wave length}}$

[h]



Initial field (real part)

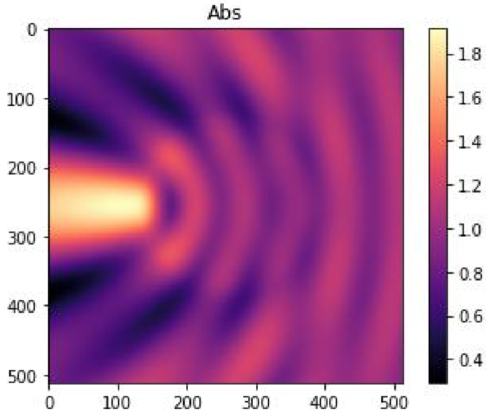


Initial field (imaginary part)

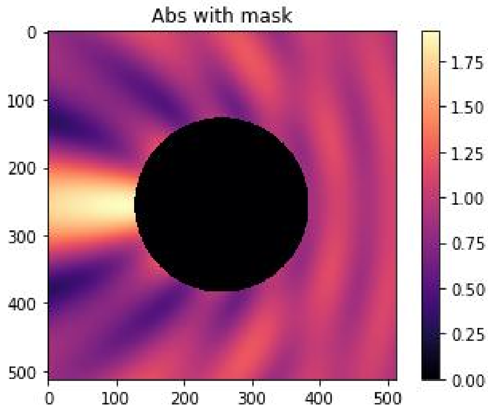
FIGURE 2. Initialization

11.1. *Circular mask ($\varepsilon = 1.5$)*

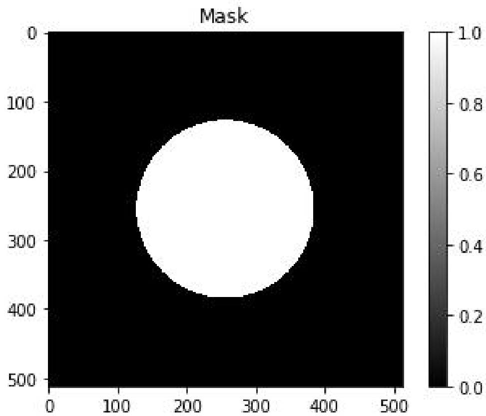
[h]



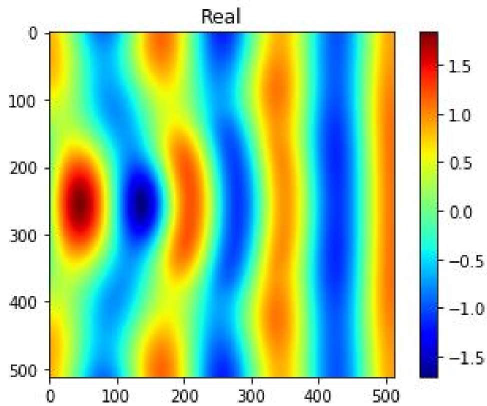
Absolute value on field vector x



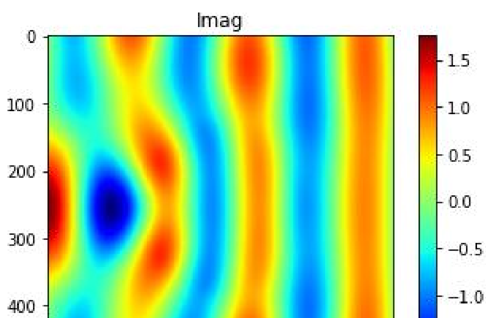
Absolute value on field vector x with mask m



Circular mask m of grid. Black means $m_b = 0$, white means $m_w = 1$

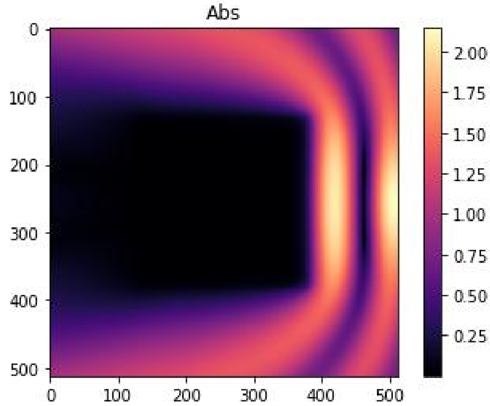


Real part of solution (field vector x)

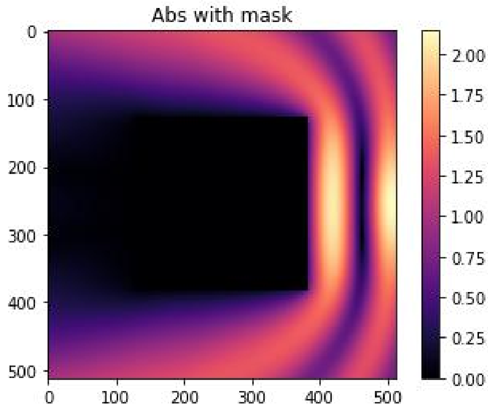


11.2. *Rectangular mask (* $\varepsilon = -10$*)*

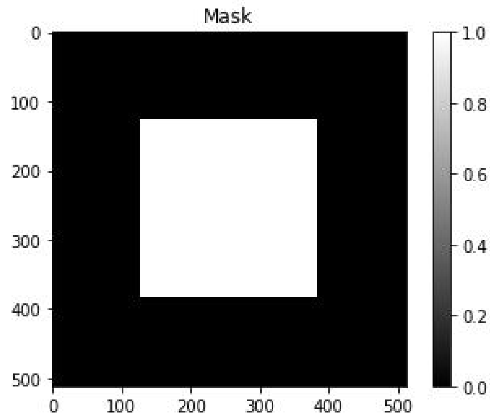
[h]



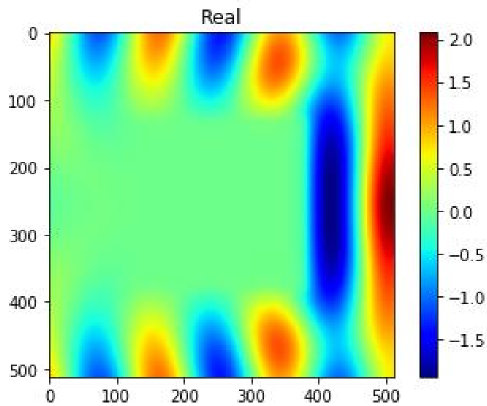
Absolute value on field vector x



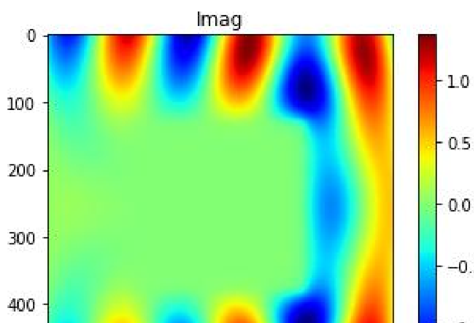
Absolute value on field vector x with mask m



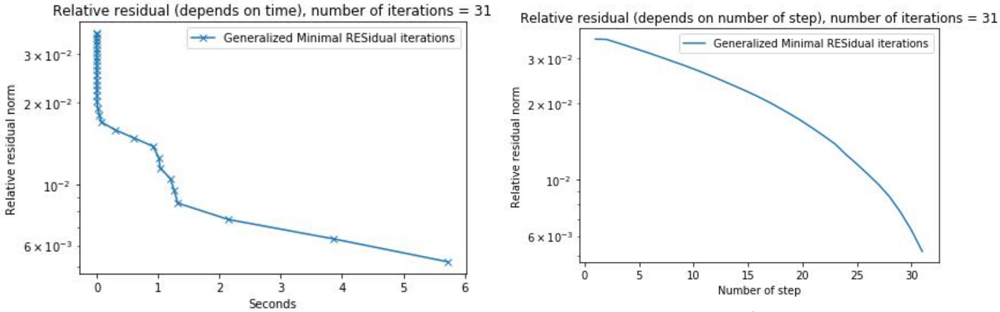
Rectangular mask m of grid. Black means $m_b = 0$, white means $m_w = 1$



Real part of solution (field vector x)



[h]

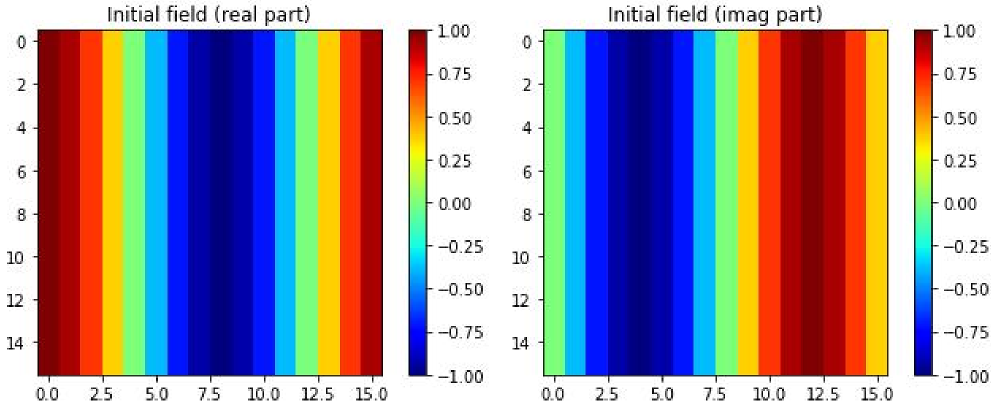


Relative residuals (depend on time), number of iterations = 31

Relative residuals (depend on the step number), number of iterations = 31

FIGURE 5. Convergence of GMRES Solver (grid 512×512)

[h]



Real part of discretized field vector

Imaginary part of discretized field vector

FIGURE 6. Initialization of topology optimization for 16×16 grid with 1 wavelength per domain

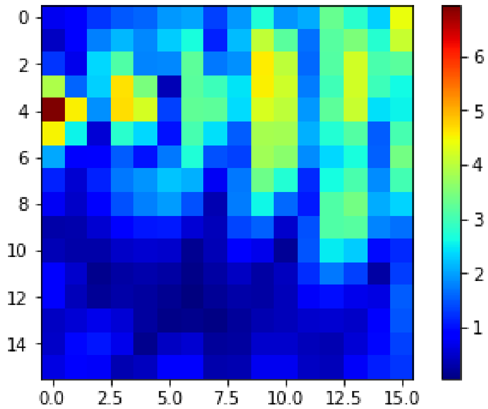
11.3. *Convergence of GMRES Solver (grid* 512×512*)*

12. Results of optimization

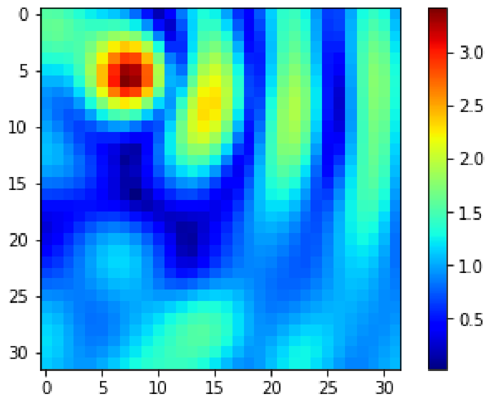
12.1. *Initialization*

For this task grid 16×16 has been used, since optimization is more hard computing task.

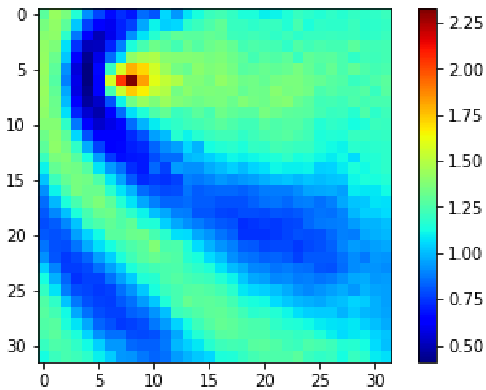
[h]



Real part of discretized field vector



Imaginary part of discretized field vector

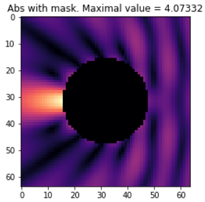


Imaginary part of discretized field vector

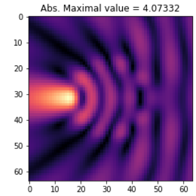
FIGURE 7. Initialization of topology optimization for 16 × 16 grid with 1 wavelength per domain

12.2. *Optimization examples on continuous ε grid*

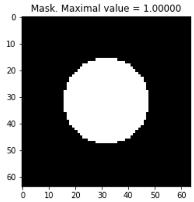
[h]



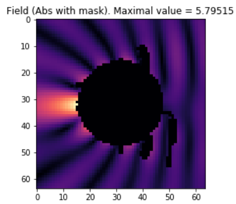
Absolute value of field vector with mask



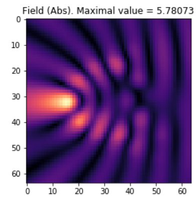
Absolute value of field vector



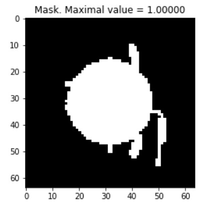
Mask



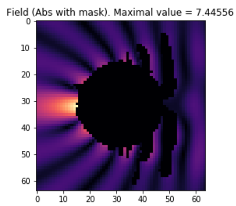
Absolute value of field vector with mask



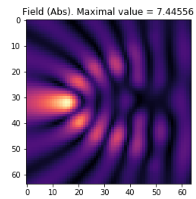
Absolute value of field vector



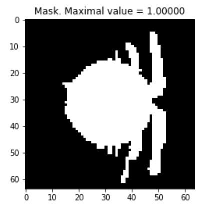
Mask



Absolute value of field vector with mask



Absolute value of field vector



Mask

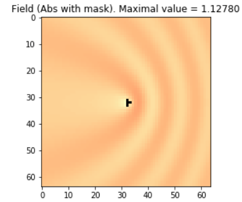
FIGURE 8. Topology optimization of circular mask

12.3. *Optimization examples on discrete ε grid*

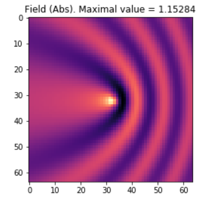
12.3.1. *Using Gradient solver*

In this case the gradient-solver has been programmed. Initial point has been circle mask. In addition, only the principle of the building neighbors has been implemented in this topology optimization solver. The neighbors with the biggest gradient has been masked (mask on this neighbors with 0 mask changes and becomes to be equal to 1).

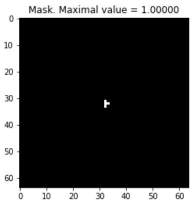
[h]



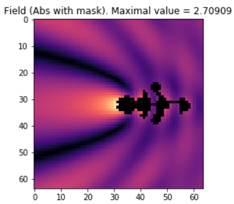
Absolute value of field vector with mask



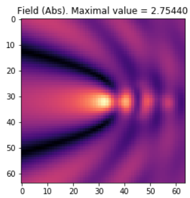
Absolute value of field vector



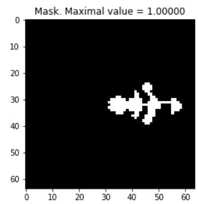
Mask



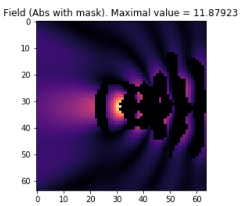
Absolute value of field vector with mask



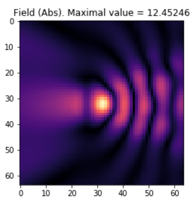
Absolute value of field vector



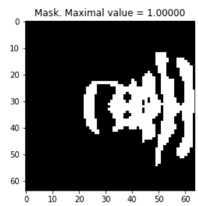
Mask



Absolute value of field vector with mask



Absolute value of field vector



Mask

FIGURE 9.

12.3.2. *Using non-gradient method*

In this case the non-gradient-solver has been programmed. Initial point has been the central point of the grid. In addition, only the principle of the building neighbors has been implemented in this topology optimization solver. But it has used broadcasting principle. Program tries to assign the 1 value in the cells of grid that are neighbors of the cells that are equal to 1. Next, program chooses the broadcasting of the biggest objective function.

[h]

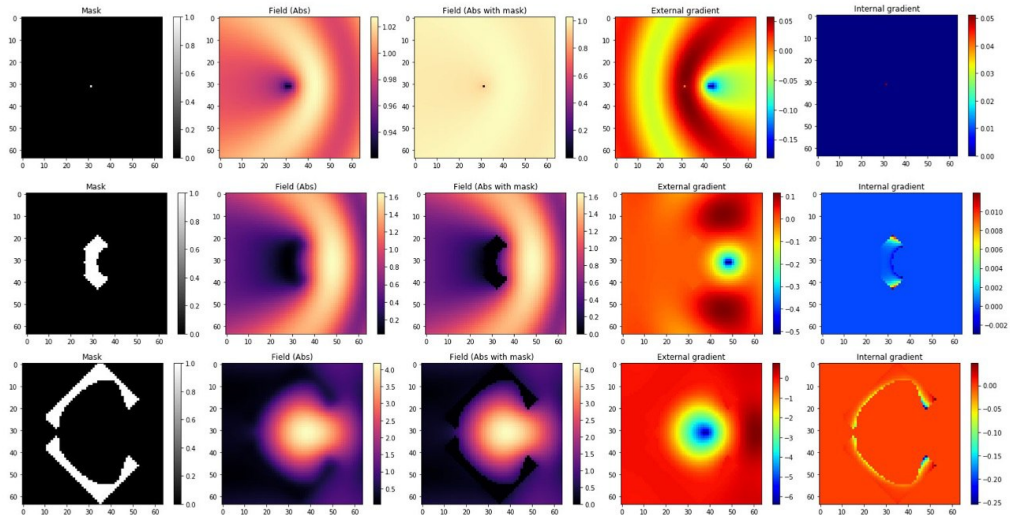


FIGURE 10.

[h]

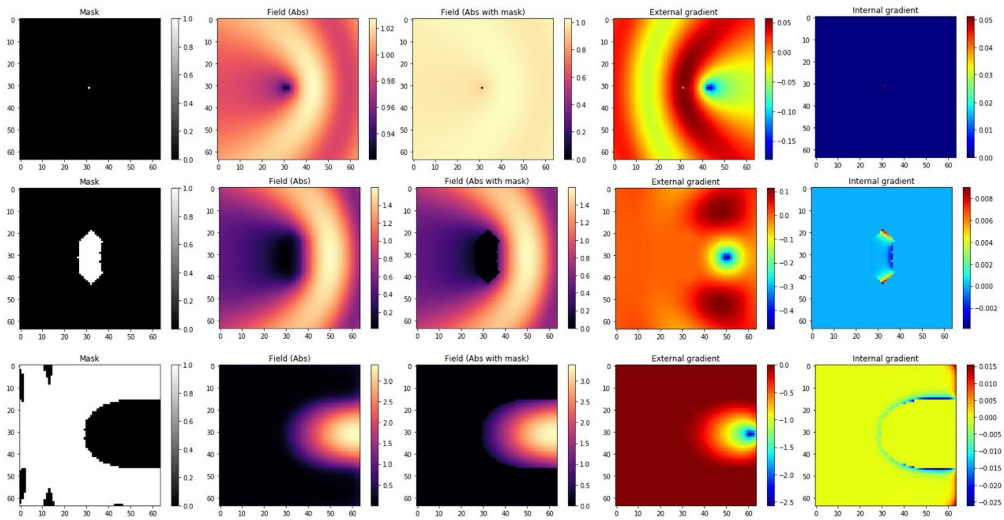


FIGURE 11.

12.3.3. *One wavelength. Discrete greedy multy-buliding neighbours optimizer with gradient extended by subtraction of mask*

12.3.4. *One wavelength. Discrete greedy multy buliding neighbours optimizer with gradient*

12.3.5. *One wavelength. Discrete greedy multy buliding neighbours optimizer with gradient*

12.3.6. *Two wavelengths. Discrete greedy multy buliding neighbours optimizer with gradient*

[h]

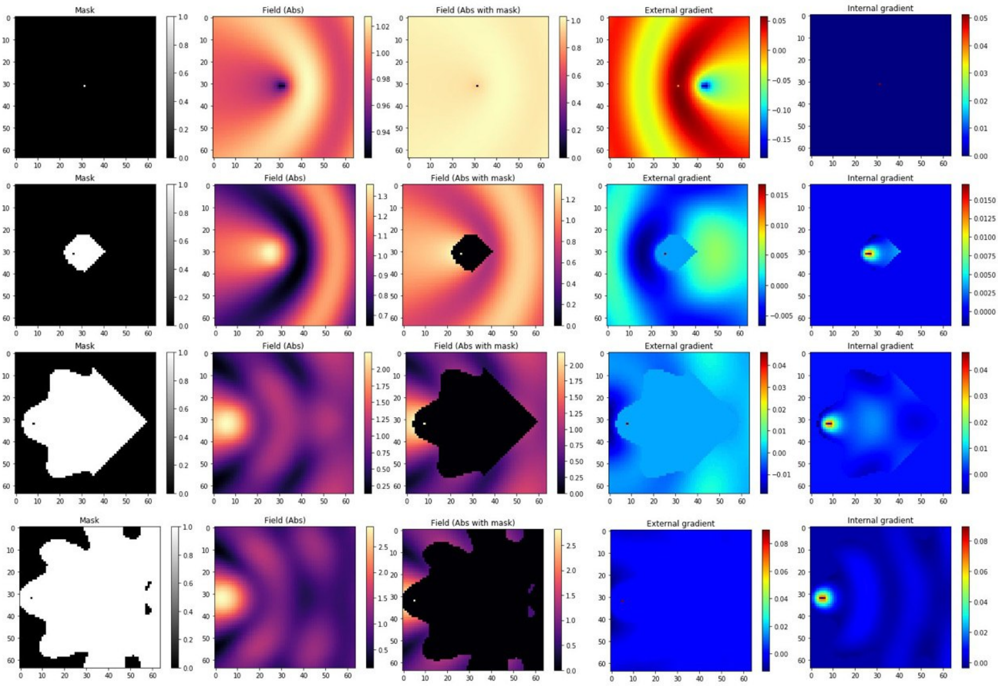
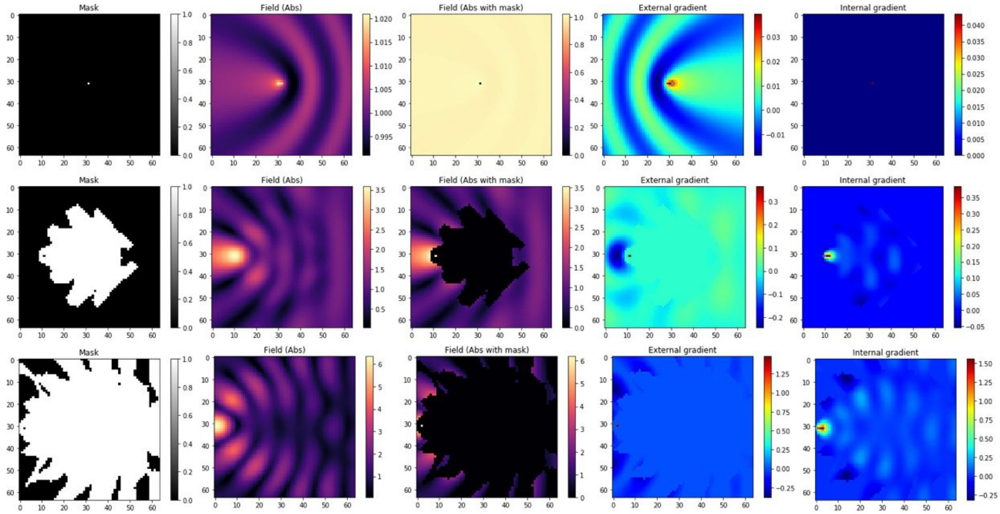

Mask
Field (Abs)
Field (Abs with mask)
External gradient
Internal gradient

Figure 12.


Mask
Field (Abs)
Field (Abs with mask)
External gradient
Internal gradient

[h]

FIGURE 13.

13. Production of formulas:

$$
\begin{gathered}
Ax = f \\
\text{where: } A = I - Gdiag[k^2(\varepsilon - 1)(M_{stationar} + M_{changed})] \\
\frac{\partial}{\partial M_{changed}} [Ax] = \frac{\partial f}{\partial M_{changed}} = \\
= Gk^2(\varepsilon - 1)diag(\varepsilon) + \big(I - Gdiag(k^2(\varepsilon - 1)M_{changed}\big) \frac{\partial x(M_{changed})}{\partial M_{changed}} = \frac{\partial f(M_{changed})}{\partial M_{changed}} = 0 \\
\textbf{Thus, } Ax = B, \\
\text{where: } A = I - Gdiag[k^2(\varepsilon - 1)(M_{stationar} + M_{changed})] \\
B = -k^2(\varepsilon - 1)diag(x(M_{changed}))
\end{gathered} \tag{13.1}
$$

$$
\begin{gathered}
\frac{\partial}{\partial m}\|x\|^2 = \frac{\partial}{\partial m}(x^* \cdot x) \underbrace{=}_{v=x^*} = \frac{\partial}{\partial m}(v \cdot x) = x^T \frac{\partial v}{\partial m} + v^T \frac{\partial x}{\partial m} \underbrace{=}_{v=u^*} x^T \frac{\partial x^*}{\partial m} + \\
+ x^{*T} \frac{\partial x}{\partial m} \underbrace{=}_{\frac{\partial x^*}{\partial m} = J^{*T}} = x^T J^{*T} + x^{*T} J = \\
= u\overline{J(u)}u + \overline{u}J(u) = u\overline{J(u)} + \overline{u\overline{J(u)}} = f + \overline{f} = 2\mathbf{Re}\ (x^{*T} J)
\end{gathered} \tag{13.2}
$$

$$
\begin{gathered}
J^T A^T = B^T \\
J^T = B^T A^{-T} \\
J^T x = B^T A^{-T} x = B^T Y, \\
\text{where: } Y = A^{-T} x \\
x = A^T Y
\end{gathered} \tag{13.3}
$$

REFERENCES

Jensen, J. S. and Sigmund, O., "Topology optimization for nano-photonics," *Laser & Photon.*, vol. 5 (2011), pp. 308–321. doi:10.1002/lpor.201000014.

Alexander, Y., Piggott, et al, *Inverse design and implementation of a wavelength demultiplexing grating coupler*, pp all.