A Mode Selecting Eigensolver for 2D FIT Models of Waveguides

Bastian Bandlow, and Rolf Schuhmann
FG Theoretische Elektrotechnik, EIM-E
University of Paderborn, D-33098 Paderborn, Germany
bandlow@tet.upb.de, schuhmann@tet.upb.de

Abstract ─ For the computation of eigenmodes in multimodal waveguide structures, the Jacobi-Davidson eigenvalue solver is extended by a vector-based weighting function. It allows to generate only modes with a desired field distribution. The performance of this solver is studied by means of an eigenmode computation in a photonic crystal fiber which is discretized by the finite integration technique. The new algorithm is able to separate the modes in the fiber core from a number of non-physical modes which originate from a transversal PML-type boundary condition.

Index Terms─ Jacobi-Davidson, Eigenvalues, Mode Calculation, Photonic Crystal Fiber.

I. INTRODUCTION

The computation of eigenvalues in two- and three-dimensional electromagnetic structures is a challenging task in engineering. Since dielectric waveguides for optical applications (fibers) can be highly multi-modal, the corresponding 2D-eigenvalue problem may include a high number of guided modes, with only little differences in their propagation constants.

For such modes, the power is confined within the core of the fiber, and the field strength in the cross section decays exponentially with increasing radius. With this a-priori knowledge, one may wish to apply an adequate transversal boundary condition, which allows to truncate the mesh close to the core of the fiber. Such an 'open boundary' can be modeled by a perfectly matched layer (PML), which absorbs the evanescent wave parts by real-coordinate stretching [1]. However, the application of the PML changes the discrete eigenvalue problem, and the staggered material layers of the PML themselves can act as a waveguiding structure. This leads to a spoiled spectrum, which consists not only of the desired guided modes within the core, but we observe a lot of additional non-physical modes, which are guided inside the PML.

In order to get rid off of these spurious modes, we use an extended Jacobi-Davidson eigenvalue solver [2] [3] which allows to distinguish between the two classes of eigenvectors *within the solution process* and to produce only the desired core-modes in an efficient way.

Preliminary work has been done by [4], [5] and [6] for microstrip lines and lasing structures. They rely on smart chosen, limited areas of the spectrum in order not to calculate too many of the undesired eigenmodes. However it is unavoidable that some of them occur in their approach since not the eigenvector is analyzed during iteration but only the eigenvalue. Therefore, they identify the desired eigenmodes in an a-posteriori processing step.

II. FORMULATION

The eigenvalue problem for waveguide cross-section is formulated using the finite integration technique (FIT) [7], [7].

The FIT is based on a spatial segmentation of the computational domain by a computational grid pair, the normal grid G and the dual grid $\widetilde{G}$. The degrees of freedom of the method are the so-called integral state variables, defined as integrals of the electric and magnetic field vectors over edges $L_i, \widetilde{L}_i$ and facets $A_j, \widetilde{A}_j$ of the normal grid G and the dual grid $\widetilde{G}$, respectively:

$$\hat{e}_i = \int_{L_i} \vec{E} \cdot d\vec{s} \qquad \hat{\tilde{d}}_i = \int_{\tilde{A}_i} \vec{D} \cdot d\vec{A} \tag{1}$$

$$\hat{\tilde{j}}_i = \int_{\tilde{A}_i} \vec{J} \cdot d\vec{A} \tag{2}$$

$$\hat{h}_j = \int_{\tilde{L}_j} \vec{H} \cdot d\vec{s} \qquad \hat{\tilde{b}}_j = \int_{A_{ji}} \vec{B} \cdot d\vec{A} \tag{3}$$

Using this discrete formulation the fundamental physical properties of Maxwell's equations like energy and charge conservation and also the orthogonality of eigenmodes are maintained. The Maxwell grid equations can be written down as

$$\mathbf{C}\hat{\mathbf{e}} = -\frac{d}{dt}\hat{\hat{\mathbf{b}}} \qquad \tilde{\mathbf{C}}\hat{\mathbf{h}} = \frac{d}{dt}\hat{\hat{\mathbf{d}}} + \hat{\hat{\mathbf{j}}} \tag{4}$$

with the material relations $\hat{\hat{\mathbf{d}}} = \mathbf{M}_\varepsilon \hat{\mathbf{e}}$, $\hat{\hat{\mathbf{j}}} = \mathbf{M}_\kappa \hat{\mathbf{e}}$ and $\hat{\hat{\mathbf{b}}} = \mathbf{M}_\mu \hat{\mathbf{h}}$. $\mathbf{C}$ and $\tilde{\mathbf{C}}$ are the topological curl-operators containing entries with {-1;0;1}. All the FIT matrices of topological operators are sparse and have band structure which allows an efficient processing on computer systems.

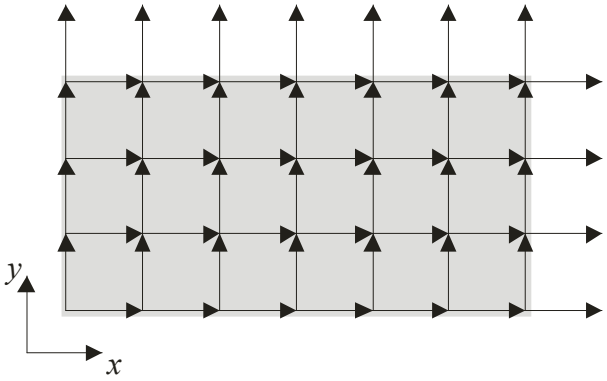

Fig. 1. FIT discretization scheme of the 2D light grey shape. nx components in x-direction and ny components in y-direction: Some components do not exist.

The FIT discretization of a waveguide cross-section is shown in Fig. 1 for the tangential electric grid voltages $\hat{\mathbf{e}}_t$. It has been shown in former work [9] that the eigenvalue problem

$$(\mathbf{A}_1 - k_z^2 \mathbf{A}_2 - \omega^2 \mathbf{I})\hat{\mathbf{e}}_t = 0 \tag{5}$$

can be formulated for unknown k_z or unknown ω. $\mathbf{A}_1$ contains the 2D curl-curl-operator and the inverse permeability. $\mathbf{A}_2$ contains again some material properties cf. [9]. The longitudinal components $\hat{\mathbf{e}}_z$ can be obtained through continuous calculus considerations. The 2D eigenvalue problem for the tangential electric grid voltage $\hat{\mathbf{e}}_t$ (5) leads in the case of a given frequency ω and a PML for evanescent tangential waves to a system matrix $\mathbf{A}_{cc} = \mathbf{A}_2^{-1}(\mathbf{A}_1 - \omega^2\mathbf{I})$, which is in the specific case real and non-symmetric. A symmetrization is in some cases theoretically possible, as long as no complex modes occur. The number of degrees of freedom is $2n_x n_y - (n_x + n_y)$ for n_x, n_y being the number of discretization steps in the particular direction, when no special boundary treatment is applied (cf. Fig. 1).

III. JACOBI-DAVIDSON ALGORITHM

The Jacobi-Davidson algorithm [2], [3] is feasible for the computation of a few interior or exterior eigenvalues of the spectrum. Within the algorithm, the original eigenvalue problem is projected and solved on a low-dimensional subspace $\mathbf{V}$, which is gradually refined by solving a correction equation. We use a Matlab implementation of the JD-algorithm from its original authors which is available from [3]. As so-called target value, an end of the spectrum or an arbitrary value within the spectrum can be specified. According to this target value, the approximate eigenvalues are sorted in different sophisticated ways during the solution process. Moreover, the JD algorithm computes the eigenpairs one after another and not a block of eigenvalues simultaneously.

The solution of the low-dimensional, projected eigenvalue problem, however, does not only yield approximations of the eigenvalues, but of course we also obtain approximations of the corresponding eigenvectors. If we expand them again to full dimension, we can interpret these vectors as approximations of field solutions of the discrete formulation.

To establish a new criterion for the choice of the desired modes, we test these field distributions against a weighting vector $\mathbf{f}$, which describes a scalar spatial distribution for each field component with its maximum at the core and a decay towards the boundaries. The components of these vectors are depicted in Fig. 2. We choose a Gaussian profile, since it is easy to define and it fulfills the requirements of a strong decay toward the boundaries. Moreover, the Gaussian shape is not equal to a solution of the problem and therefore

we do not plug in a pre-known solution into the process.

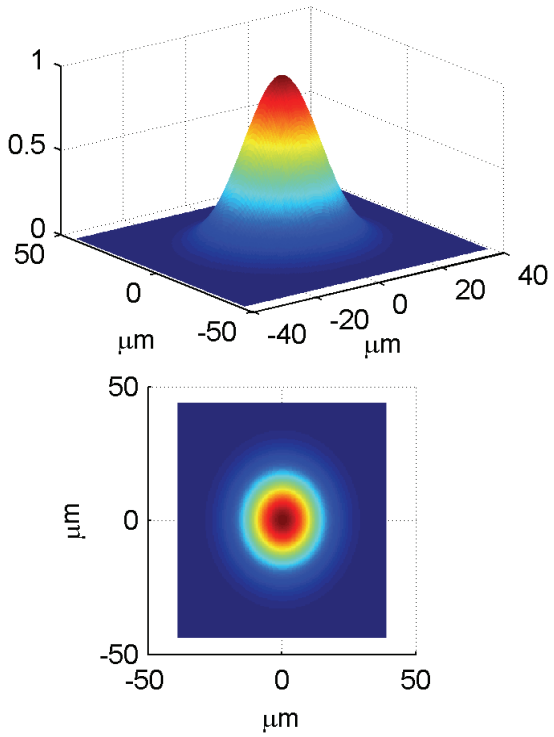

Fig. 2. Weighting vector $\mathbf{f}$ with Gaussian profile for x - and y - components.

Now, we can measure the quality of our approximate eigenvectors u_i within the JD-algorithm very easily. The product

$$\psi = \left\langle \mathbf{f}; |\mathbf{u}_i| \right\rangle \tag{6}$$

with $\|\mathbf{u}_i\|_2 = 1$ and $\|\mathbf{f}\|_\infty = 1$ can be used to decide, whether the field strength is concentrated around the core ($\psi > 1$) or whether it is concentrated inside the boundary ($0 < \psi < 1$). Taking the absolute value of the eigenvector's components $|\mathbf{u}_i|$ ensures that also core guided modes with a null in the center are found. The weighting function does not have to provide necessarily the profile shape of the modal field to be computed. The weighting function only provides information about the spatial distribution of the field to be computed.

Within the original Jacobi-Davidson algorithm the eigenvalue approximations are sorted according to their distance to the target value. In our modification of the algorithm we select only those of the sorted eigenvalue approximations, which fulfill the weighting criterion (6).

IV. NUMERICAL EXAMPLE

We choose a photonic crystal fiber (PCF) [10] as an example, which is operated at 2μm wavelength (Fig. 3). It consists of a glass core ($n_G = 1.45$) with a surrounding hexagonal lattice of air holes. Each hole has a radius of 2.9μm and the lattice constant is 9.4μm. The discrete model is truncated by a PML boundary condition and has the dimensions $74\mu m \times 84\mu m$.

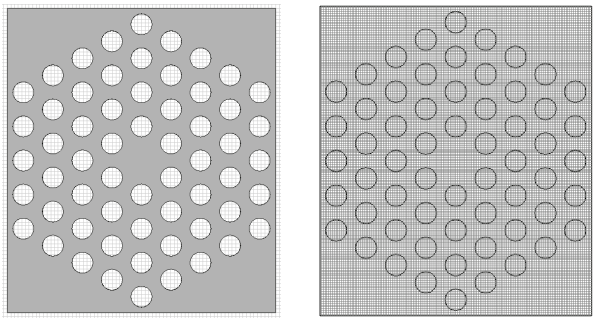

Fig. 3. PCF consisting of glass and air holes ($74\mu m \times 84\mu m$). Mesh settings (155×193 lines).

The cross section of the fiber is discretized by the finite integration technique, using CST MICROWAVE STUDIO [11] for all preprocessing steps. The resulting two-dimensional model has 155×193 grid points, and we add 4 grid lines in each transversal direction for the PML. The eigenvalue problem [9] for the squared propagation constants β^2 is linear, of the type

$$\mathbf{A}_{cc}\mathbf{x} = \lambda \mathbf{x}, \tag{7}$$

and has 64438 degrees of freedom. We are interested in the first two guided modes of the PCF whose distribution of its electrical field strength is depicted in Fig. 4.

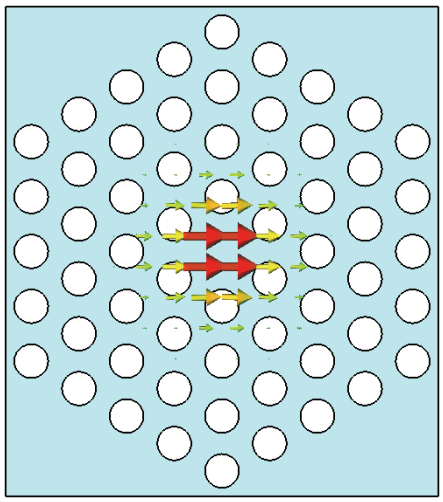

Fig. 4. Electrical field of the first desired mode.

Fig. 6 shows the part of the spectrum with the smallest real part, since the propagation constants β_i are calculated from the eigenvalues λ_i by $\beta_i = \sqrt{-\lambda_i}$. The first 36 modes (marked by diamonds) are guided within the PML according to Fig. 5. Modes 37 and 38 are the ones we are looking for and which fulfill our weighting criterion in equation (6).

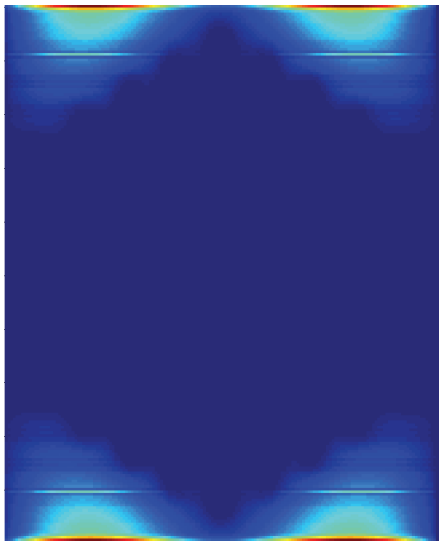

Fig. 5. Magnitude of electrical field of one of the undesired modes: Wave guiding within the PML.

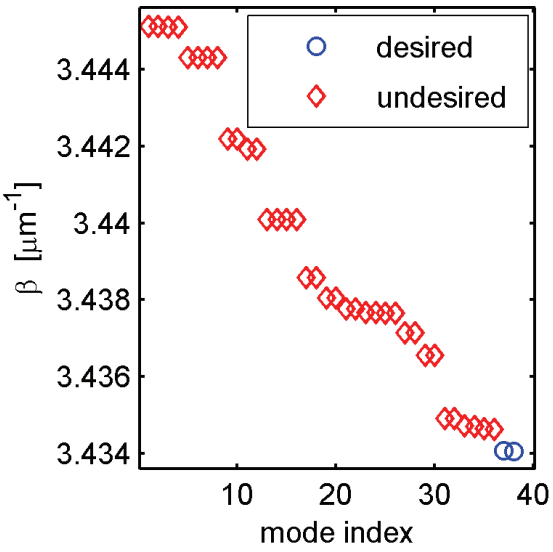

Fig. 6. Propagation constants β of the PCF. The modes with indices 37 and 38 (o) are the desired ones, which are guided by the core.

V. COMPARISON OF JD SOLVERS

The unmodified Jacobi-Davidson solver as well as weighted JD solver are used to compute the first two guided modes of the PCF from the previous section. For all eigensolver computations, the system matrix is preconditioned through a shift of the spectrum before the solver starts, which significantly improves the condition of the eigenvalue problem. The target is chosen to be the smallest real part. The initial subspace is generated randomly and is fed in each of both solvers in order to have equal starting conditions. The correction equation within the JD algorithm is solved by a direct solver in both solvers. This is time-consumptive, but we can expect at least a second order convergence. For the ordinary JD solver the dimension of the search subspace is kept between 7 and 12, while for the weighted JD solver no reduction of the search subspace is done. The eigenvalues are accepted when the residual is below 1e-13.

Table 1: Results of the standard JD and the weighted JD.

Version	Modes	Time	Iterations
standard	38	2678 s	108
weighted	2	165 s	46

The results are given in Table 1. We look for two core guided modes, which are found by both solvers. The weighted JD outperforms the standard JD by a factor of 15 in time. The number of iterations, which are needed to gradually refine the subspace, is reduced by a factor larger than two.

The reason for the disagreement of these two factors can be seen in the convergence history in Fig. 7 and Fig. 8. A lot of iterations are needed at the beginning of both algorithms, in order to improve the quality of the subspace. Once refined, the subspace allows the quick computation of the consecutive eigenvalues.

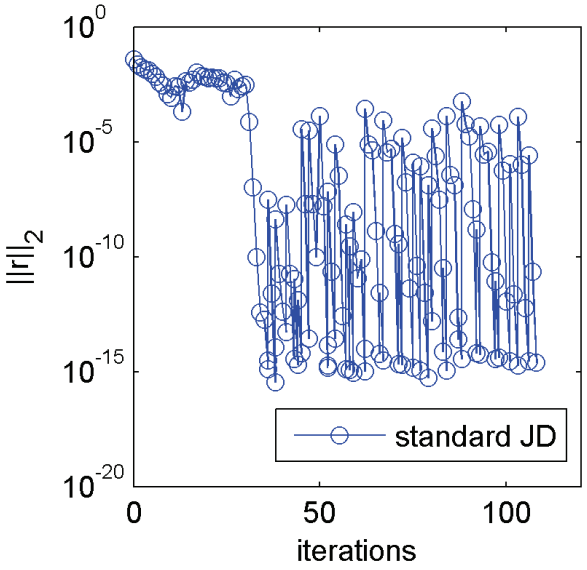

Fig. 7. Convergence history of the standard JD.

VI. SOLVER TUNING

In further investigations we consider the choice of the initial subspace, the correction equation and the maximum dimension of the search subspace. Details to the selection process of the prospective eigenvectors are given.

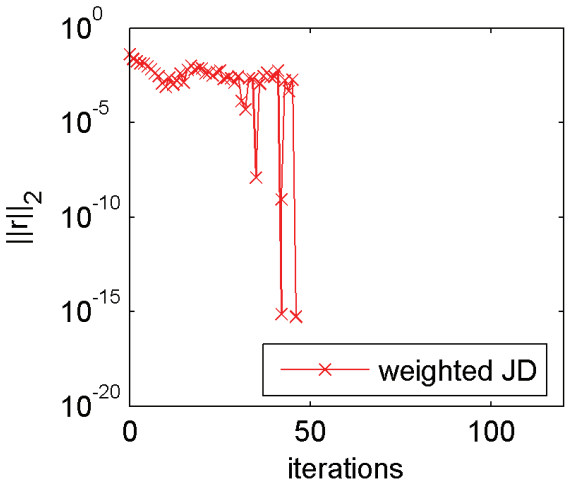

Fig. 8. Convergence history of the weighted-JD.

A. Initial Subspace

Since we are interested in modes, which have a similar spatial field distribution like the weighting function from (6) we use weighting function itself as the start vector for the Jacobi-Davidson process. Fig. 9 shows the convergence history. The number of iterations needed to find both of the desired modes is reduced to 15. This is less than one third of the 46 iterations the weighted JD algorithm without special initial vector treatment needed.

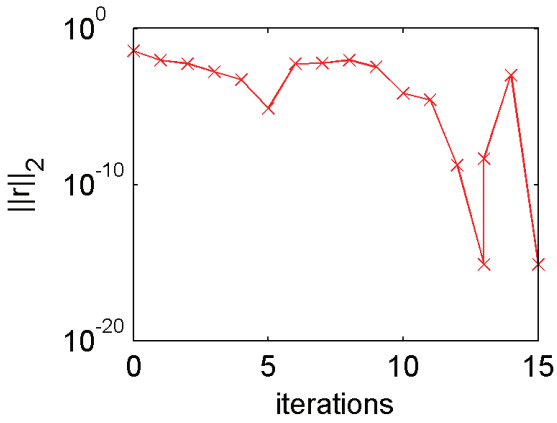

Fig. 9. Convergence history of the weighted-JD with the weighting function applied as start vector.

B. Correction Equation

The correction equation of the Jacobi-Davidson process is used to generate the subsequent extensions for the search subspace. For this, a linear system of equations has to be solved. In the

preceding sections the correction equation has been solved directly, which turns out to be computationally quite expensive. Alternatives are iterative solvers which all need preconditioners in order to perform well. The JD process is supposed to converge even with an inexactly solved correction equation.

We choose exemplarily the bicgstab solver [12] which is included in the jdqr-package from [3]. As a preconditioner we take the LU factorization of $\mathbf{A}-\lambda_{approx}\mathbf{I}$, where λ_{approx} is an approximation of the eigenvalue with the smallest real part. We choose arbitrarily $\lambda_{approx}=3.624e13$, which is not inside the spectrum as the comparison with Fig. 6 shows. As initial subspace we use again the random subspace from section V.

Table 2: Results of the weighted JD solver for different residuals in the solution of the correction equation.

bicgstab Tol	5e-1	1e-1	1e-2
bicgstab MaxIt	200	200	400
JD Iterations	100	48	42
Time / sec	679	773	1566

In Table 2 some results are given and it turns out that indeed the correction equation may be solved with a certain amount of error and the JD process finds the 2 guided modes anyway. Not always is the desired accuracy reached by the bicgstab and the maximum number of iterations aborts the iteration. The number of JD iterations needed is around the same as the result of Table 1. The reason for the increased time, although the number of JD iterations is comparable, is the well-parallel performing direct solver while the iterative bicgstab is more or less single-threaded. An interesting case occurs in the last column where the number of JD iterations is less than in the case where the correction equation is solved exactly. The only reason for that is the rather good preconditioner which is a complete LU factorization at an eigenvalue estimation.

C. Search Subspace Dimension

The reduction of the search subspace after it has reached a specific dimension, limits the maximal dimension of the low-dimensional eigenvalue problem to be solved. We make a study in which we vary the maximum search space dimension. The correction equation is solved exactly. The minimum dimension should not be too small, otherwise it may happen that none of the eigenvector approximations fulfills the weighting criterion.

Table 3: Results of the weighted JD solver for different residuals in the solution of the correction equation.

$\dim_{\min}$	7	7	13
$\dim_{\max}$	12	21	21
JD Iterations	81	59	82

In Table 3 there are the results for different maximum dimensions of the search subspace. It turns out that there is a choice of the maximum dimension, which leads to accelerated convergence.

D. Selection Process

In our first implementation of this algorithm, the eigenvalues of the low-dimensional problem are simply sorted according to their distance to the target. In the second step, only those eigenvalues are retained, whose full-dimension eigenvectors fulfill the weighting criterion (6) with $\psi>1$. It is important to note, that these approximate eigenpairs do not fulfill the eigenvalue problem very well. That means that the residual

$$\|\mathbf{r}\|_2=\|\mathbf{A}\mathbf{u}_i-\theta_i\mathbf{u}_i\|_2 \tag{8}$$

for a specific approximate eigenpair (θ_i,u_i) is not negligible small in general. Especially in the case when the selection process leads to an oscillation between two eigenvalues during the iteration, one of them could be fixed for some iterations, in order to get a better residual and decide afterwards, whether it fulfills the weighting criterion or not. If high-accuracy eigenvectors occur within the process, which do not fulfill the weighting criterion, they can be added to the subspace to prevent the process to regenerate them again.

These circumstances could be considered in an improved implementation.

VII. CONCLUSION AND OUTLOOK

We have shown that a simple extension of the selection process of the approximate eigenpairs within a Jacobi-Davidson algorithm leads to a superior convergence behavior for waveguide models which are surrounded by a PML boundary condition. The number of eigenvalues which have to be computed until we arrive at the desired ones is drastically reduced. The occurrence of degenerated (or nearly degenerated) modes are not unusual in unbounded waveguides. They have also shown up in our examples, and the modified solver obviously has no problems with them. The weighting function should be chosen carefully enough that criterion (6) yields $\psi < 1$ for the external mode (guided within the PML) and $\psi > 1$ for the core guided mode. Then the undesired mode is eliminated by the selection process.

Of course, there are a couple of possible improvements concerning the performance, the computational efficiency, and the range of application of the modified eigensolver:

At first, other weighting functions may be used, e.g. it should be possible to find only modes with a specific polarization, modes with energy transport in specific regions of the cross section, etc. In the current implementation only the values of the electrical grid voltage are taken into account by the weighting function. However, it may also be applied to Poynting's vector or other secondary quantities. Furthermore, the fact that we identify an undesired eigenvector without doing anything against its reoccurrence is not yet satisfactory. Since we also know the corresponding eigenvalue, it should be possible to apply some kind of filter, which is able to suppress the undesired modes. Another idea would be to implement the weighting into other eigensolvers such as the implicitly restarted Arnoldi algorithm, where it should also be possible to eliminate the undesired eigenvectors from the approximate subspace.

Finally, this kind of solver can also be applied to other types of waveguides such as microstrip lines or even three dimensional structures.

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Bastian Bandlow was born in Frankfurt am Main, Germany. He received the Dipl.-Ing. degree in electrical engineering from the Technische Universität Darmstadt, Germany, in 2005, and is currently working toward the Ph.D. degree at the Universität Paderborn, Germany.

Since 2006, he has been with the group of Theoretische Elektrotechnik, Universität Paderborn.

His research is focused on simulation techniques for periodic structures such as metamaterials and photonic crystals at microwave and optical frequencies.

Rolf Schuhmann was born in Osterburken, Germany. He received the Dipl.-Ing. degree and Dr.-Ing. degree in electrical engineering from the Technische Universität Darmstadt, Germany, in 1994 and 1999, respectively.

Since 2005, he has been a Full Professor of Theoretische Elektrotechnik with the Universität Paderborn, Germany. His research interests concern computational electromagnetics with grid-based methods such as finite integration, finite elements, and finite differences. Applications include all types of components in microwave technology and optics and novel material concepts, as well as the characterization of metamaterials.