Computation of Optical Modes inside Axisymmetric Open Cavity Resonators

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Abstract

The computation of optical modes inside axisymmetric cavity resonators with a general spatial permittivity profile is a formidable computational task. In order to avoid spurious modes the vector Helmholtz equations are discretised by a mixed finite element approach. We formulate the method for first and second order Nédélec edge and Lagrange nodal elements. We discuss how to accurately compute the element matrices and to solve the resulting large sparse complex symmetric eigenvalue problems. We validate our approach by three numerical examples that contain varying material parameters and absorbing boundary conditions (ABC).

Key words: optical mode computation, numerical device simulation, axisymmetric cavity, body of revolution, semiconductor laser, finite element method, large sparse complex symmetric eigenproblem, Jacobi–Davidson algorithm, Nédélec edge elements

1 Introduction

In this paper we discuss the comprehensive computation of optical modes inside axisymmetric cavity resonators. If optical gain, radiation and absorption

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losses are taken into account the numerical solution of complex symmetric eigenproblems is required. In this work the latter result from a finite element method (FEM) discretisation of the vector Helmholtz eigenproblem (VHEP) for open cavities. Typical resonators, the optical modes of which are of interest, are semiconductor lasers [32,34], lossy waveguides [16], circular–grating resonators [23], photonic band gap structures [20].

Until recently, new resonator designs and changes to the design of existing devices had to be investigated purely experimentally, by changing the cavity structure, fabricating and characterising the device. Due to the savings in design time and cost comprehensive simulators are becoming essential tools to explore the design parameter space for an optimal solution. The foundations of such a simulator will be discussed in this article.

From the point of view of computing optical modes, a resonator structure is described in terms of a spatially non–uniform complex symmetric permittivity function $\varepsilon(x)$, see Figure 1. As mentioned earlier, we restrict our attention to axisymmetric structures.

In order to simulate radiation leakage from the cavity one has to make sure that outside the cavity electro-magnetic waves are only outgoing. If it is possible to extinguish the electro-magnetic waves outside the cavity without causing any back-scattering the computational domain can be truncated and made finite without changing the wave inside the cavity. This can be accomplished by an absorbing layer.
A method that has been used for open region scattering problems [13], is to model the absorber as lossy perfectly matched layer (PML) [5,29]. The characteristics of the PML are first, waves propagating though the PML are attenuated and second, the reflection coefficient is zero. Such a PML is available for cylindrical coordinates [33] and is used here to compute the optical modes of open cavities.

A simulation tool has to be capable of handling very general spatial permittivity profiles $\varepsilon(x)$ to be of practical use. Various methods to compute optical modes of resonant cavities were proposed in the past, yet only some of them [30,22,28,6,32] are suited to treat a general form of a non–uniform dielectric function.

The paper is organized as follows. In Section 2 we give a weak formulation of the problem. The frequency domain FEM formulation of the dielectric optical resonator problem employed in this work is related to [17,27,28,32]. With this approach, in principle, optical modes for arbitrary cavities can be computed. Typically, using a 2D body of revolution (BOR) expansion for an axisymmetric device, leads to large sparse generalised complex symmetric eigenvalue problems of the order of approximately 500’000 which have to be solved. The present article assesses the value of higher order finite element functions for this approach. In Section 3 we discuss a finite element discretisation of the problem that avoids spurious modes. We deal with the accurate computation of the finite element matrices and the numerical solution of the resulting eigenvalue problem. In Section 4 we present three experiments with the purpose to demonstrate the superiority of the quadratic over the linear elements and the flexibility of our approach in dealing with different media, including absorbing ones. Both of these features constitute the important building blocks for the investigation of realistic optical resonators as shown in Figure 1. We draw our conclusions in Section 5.

2 Formulation of the Problem

As mentioned earlier, we want to investigate the resonance behaviour of axisymmetric cavities by approximatively solving the corresponding VHEPs. The latter arise (implicitly) whenever the Maxwell equations are used to express vector fields, which, by virtue of the aforementioned resonance behaviour, are assumed to be time–harmonic. In that case the sinusoidal ansatz is chosen to be $F(x, t) = \text{Re}[F(x)e^{i\omega t}]$, where $F$ is any of the considered vector fields. In this paper only work with the electric field $E$.

If we assume that the cavity $\Omega$ is non driven ($J = 0$), charge free ($\rho = 0$) and perfectly electrically conducting (PEC) on the boundary $\Gamma = \partial\Omega$, Maxwell’s
frequency domain equations [15] can be combined in order to lead to the following

**Problem 1 (VHEP)** Find a vector field $E$ and $\lambda \in \mathbb{C}$, such that

\[
\begin{align*}
\nabla \times \mu^{-1} \nabla \times E &= \lambda \varepsilon E, & \forall x \in \Omega, \\
\nabla \cdot \varepsilon E &= 0, & \forall x \in \Omega, \\
\mathbf{n} \times E &= 0, & \forall x \in \Gamma,
\end{align*}
\]

(2.1) \hspace{1cm} (2.2) \hspace{1cm} (2.3)

hold, where $\mathbf{n}$ denotes the outer surface normal on $\Gamma = \partial \Omega$ and $\lambda = \omega^2/c^2$.

Recall, that according to the constitutive relations, the complex symmetric tensors $\varepsilon(x)$ and $\mu(x)$ describe the materials’ permittivity and permeability, respectively.

The divergence free condition (2.2) serves as a filter, in that it discards all scalar potential field solutions, i.e. the fields constituting the infinite dimensional nulls pace of the curl–curl operator. Conversely, any divergence free solution $E$ is guaranteed to be associated with a non–zero eigenvalue $\lambda$, see [11].

Solving these problems exactly is not possible except for a few particular geometries and media combinations, see [19]. It is therefore reasonable to compute approximate solutions, e.g. by applying the FEM approach. To this end, Problem 1 needs to be recast into its weak form.

**Problem 2 (Weak VHEP)** Find $E \in H_0(\text{curl}; \Omega)$ and $\lambda \in \mathbb{C}$, such that for all $V \in H_0(\text{curl}; \Omega)$ and $\psi \in H^1_0(\Omega)$

\[
\begin{align*}
\int_{\Omega} \langle \nabla \times V, \nabla \times E \rangle_{\mu^{-1}} d\Omega &= \lambda \int_{\Omega} \langle V, E \rangle_{\varepsilon} d\Omega, \\
\int_{\Omega} \langle \nabla \psi, E \rangle_{\varepsilon} d\Omega &= 0,
\end{align*}
\]

(2.4) \hspace{1cm} (2.5)

hold, where $\langle u, v \rangle = u^T v = \sum_k u_kv_k$ is a complex symmetric bilinear form and $\langle u, v \rangle_A = \langle u, Av \rangle$.

For the definition of these function spaces we refer to [11]. Resonator cavities, such as semiconductor lasers, are often axisymmetric, in which case the problem above can best be described by means of cylinder coordinates

\[
E(x) = U(\phi) \hat{E}(r) = U(\phi)[\hat{E}_r(r), \hat{E}_\phi(r), \hat{E}_z(r)]^T \quad \text{and} \quad \psi(x) = \hat{\psi}(r),
\]

where $U(\phi)$ contains the cylindrical unit vectors and $\hat{E}(r)$ represents the corresponding coordinates. The advantages of this transform become evident, if the material tensors $\mu$ and $\varepsilon$ have no angular dependency. In this case a Fourier series expansion of the fields and potentials involved in Problem 2
\[
\hat{\textbf{E}}(r) = \sum_{m=0}^{\infty} \hat{\textbf{E}}^{(c)}_m(r, z) \cos(m\phi) + \hat{\textbf{E}}^{(s)}_m(r, z) \sin(m\phi),
\]
\[
\hat{\psi}(r) = \sum_{m=0}^{\infty} \hat{\psi}^{(c)}_m(r, z) \cos(m\phi) + \hat{\psi}^{(s)}_m(r, z) \sin(m\phi),
\]
nicely isolates all azimuthal influences. We define \(\hat{\textbf{E}}^{(c)}_{m,p} = [\hat{E}^{(c)}_{m,r}, \hat{E}^{(c)}_{m,z}]^T\) and \(\hat{\textbf{E}}^{(s)}_{m,p} = [\hat{E}^{(s)}_{m,r}, \hat{E}^{(s)}_{m,z}]^T\), replace the Cartesian curl and gradient operators in Problem 2 with their cylindrical counterparts and finally apply the above Fourier expansions. The original problem then splits into a sequence of two dimensional eigenvalue problems, one for each angular wave number \(m\). In order to keep formulations compact, let us introduce the bilinear forms \(a_i(\cdot, \cdot)\) and \(b_j(\cdot, \cdot)\),

\[
\begin{align*}
a_1(v, u) &= \int_{\Omega_p} r(\nabla_p \times \hat{v}, \nabla_p \times \hat{u})_{\hat{\mu}_{p^{-1}}} \, d\Omega_p, \\
a_2(v, u) &= \int_{\Omega_p} r^{-1}(\hat{v}, \hat{u})_{\hat{\mu}_{p^{-1}}} \, d\Omega_p, \\
a_3(v, u) &= \int_{\Omega_p} r^{-1}(<\nabla_p(rv), \nabla_p(ru)>_{\hat{\mu}_{p^{-1}}} \, d\Omega_p, \\
a_4(v, u) &= \int_{\Omega_p} r^{-1}(<\nabla_p(rv), \nabla_p(ru)>_{\hat{\mu}_{p^{-1}}} \, d\Omega_p, \\
b_1(v, u) &= \int_{\Omega_p} r(<\hat{v}, \hat{u})_{\hat{z}_{p^{-1}}} \, d\Omega_p, \\
b_2(v, u) &= \int_{\Omega_p} r(<v, u)_{\hat{z}_{p^{-1}}} \, d\Omega_p.
\end{align*}
\]

Here, \(\nabla_p\) denotes the Cartesian operator with respect to the coordinates \((r, z)\).

Problem 2 can now be recast into its cylindrical counterpart. Thereby, we neglect the divergence condition, since according to the aforementioned filter property it is sufficient to consider only non–zero eigenvalues. For the sake of brevity the subscript \(m\) will be omitted in the following.

**Problem 3 (Weak Axisymmetric VHEP)** *Let \(m \in \mathbb{N}_0\) be a given angular wave number and \(\Omega = [0, 2\pi] \times \Omega_p\) an axisymmetric cavity. Find \(\hat{\textbf{E}}^{(c)}, \hat{\textbf{E}}^{(s)} \in \hat{H}_0(\text{curl}; \Omega_p)\) and \(\lambda \in \mathbb{C}\), such that for all \(\hat{\textbf{V}}^{(c)}, \hat{\textbf{V}}^{(s)} \in \hat{H}_0(\text{curl}; \Omega_p)\)

\[
\begin{align*}
a_1(\hat{\textbf{V}}^{(c)}, \hat{\textbf{E}}^{(c)}) + a_4(\hat{\textbf{V}}^{(s)}, \hat{\textbf{E}}^{(s)}) \\
+ m^2a_2(\hat{\textbf{V}}^{(c)}, \hat{\textbf{E}}^{(c)}) + ma_3(\hat{\textbf{V}}^{(c)}, \hat{\textbf{E}}^{(s)}) + ma_3(\hat{\textbf{E}}^{(c)}, \hat{\textbf{V}}^{(s)}) \quad (2.7)
\end{align*}
\]

\[
\begin{align*}
= \lambda b_1(\hat{\textbf{V}}^{(c)}, \hat{\textbf{E}}^{(c)}) + \lambda b_2(\hat{\textbf{V}}^{(s)}, \hat{\textbf{E}}^{(s)}), \\
a_1(\hat{\textbf{V}}^{(s)}, \hat{\textbf{E}}^{(c)}) + a_4(\hat{\textbf{V}}^{(s)}, \hat{\textbf{E}}^{(s)}) \\
+ m^2a_2(\hat{\textbf{V}}^{(s)}, \hat{\textbf{E}}^{(c)}) - ma_3(\hat{\textbf{V}}^{(s)}, \hat{\textbf{E}}^{(s)}) - ma_3(\hat{\textbf{E}}^{(c)}, \hat{\textbf{V}}^{(s)}) \quad (2.8)
\end{align*}
\]

\[
\begin{align*}
= \lambda b_1(\hat{\textbf{V}}^{(s)}, \hat{\textbf{E}}^{(c)}) + \lambda b_2(\hat{\textbf{V}}^{(c)}, \hat{\textbf{E}}^{(s)}),
\]

hold.*
Notice that the new function spaces \( \hat{H}_0(\text{curl}; \Omega_p) \) and \( \hat{H}_1^0(\Omega_p) \) are derived from \( H_0(\text{curl}; \Omega) \) and \( H_0^1(\Omega) \) by applying the above transformations, see [24]. The bilinear form require that the radial component of \( \hat{E} \in \hat{H}_0(\text{curl}; \Omega_p) \) satisfies \( \hat{E}_r \in O(r^{1/2}) \) while \( \hat{E}_z \in O(1) \) for \( m = 0 \) and \( \hat{E}_z \in O(r) \) for \( m > 0 \). Similarly, \( \hat{E}_\phi \in O(r^{3/2}) \) for \( \hat{E}_\phi \in \hat{H}_1^0(\Omega_p) \).

In addition, the formerly mentioned angular independence of the material tensors implies that \( \hat{\mu} = U^T\mu U = \text{diag}(\hat{\mu}_r, \hat{\mu}_\phi, \hat{\mu}_z) \) and \( \hat{\varepsilon} = U^T\varepsilon U = \text{diag}(\hat{\varepsilon}_r, \hat{\varepsilon}_\phi, \hat{\varepsilon}_z) \) from which we derive the matrices \( \hat{\mu}_p = \text{diag}(\hat{\mu}_r, \hat{\mu}_z) \) and \( \hat{\varepsilon}_p = \text{diag}(\hat{\varepsilon}_r, \hat{\varepsilon}_z) \), in accordance with the definitions of the planar subcomponents \( \hat{E}_p^c \) and \( \hat{E}_p^s \).

We conclude this section by pointing out that any solution of subproblem (2.7) can be transformed into a solution of (2.8) by a simple sign change in the azimuthal component, i.e. \( \hat{E}_p^s = \hat{E}_p^c \) and \( \hat{E}_\phi^c = -\hat{E}_\phi^s \). Therefore it suffices to compute solutions of one subproblem — we opt for (2.7).

### 3 Finite Element Discretisation

In this section we discuss how to obtain approximate solutions of subproblem (2.7) using the FEM. We assume, that the cross-section \( \Omega_p \) has been discretised by means of a mixed regular mesh consisting of a set of triangles \( T \) and paraxial rectangles \( R \).

The next step in the FEM process consists in defining piecewise polynomial basis functions whose supports are spatially confined and whose span forms a subset of the spaces \( \hat{H}_0(\text{curl}; \Omega_p) \) and \( \hat{H}_1^0(\Omega_p) \). The application of the weak form (2.7) to these finite element functions will then lead to a finite dimensional approximation of the operator (2.7).

Unfortunately the choice of appropriate finite element functions is very delicate, mainly because of the continuous operator having infinitely many zero eigenvalues. The degenerate null space has to be reflected by the discrete operator as well, in order to obtain reasonable approximations, see [14,7,8,21] and [9], to name a few. If this is not done properly, so-called spurious modes are likely to arise, i.e. eigenvalues with no physical meaning.

A possible choice that avoids this spectral pollution consists in modelling the field components \( \hat{E}_p^c \) and \( \hat{E}_\phi^s \) by Nédélec edge and modified Lagrange nodal element functions, as described in [25]. These so called hybrid element functions are guaranteed to reproduce a portion of the nulls pace correctly and thus lead to spurious free approximations.
It is well known, that the quality of FEM approximations depends on the mesh width as well as on the order of the element functions. In this article we will use both, first and second order hybrid element functions defined over both, triangles and paraxial rectangles.

To be more precise, we define $T_0$ to be the reference triangle with vertices $(0, 0), (1, 0)$ and $(0, 1)$. Additionally, we introduce the simplex coordinates $\zeta_1 = 1 - r - z$, $\zeta_2 = r$ and $\zeta_3 = z$. The element functions whose support intersect $T_0$ (see Figure 2) are then defined as (see [18])

$$
\begin{align*}
N^T_0(r, z) &= \zeta_i \\
N^T_{i+3}(r, z) &= 4 \zeta_{i+1} \zeta_i \\
N^T_{i+6}(r, z) &= \zeta_{i+2} (\zeta_i \nabla_p \zeta_{i+1} - \zeta_{i+1} \nabla_p \zeta_i)
\end{align*}
$$

where the indices of the $\zeta$ functions wrap in modulo arithmetic fashion and $i = 1, 2, 3$. See Figure 3 in order to understand how to interpret the degrees of freedom (DOF). In analogy to $T_0$, let $R_0$ be the reference rectangle with vertices $(0, 0), (1, 0), (1, 1)$ and $(0, 1)$. Again, we introduce new coordinates $\zeta_1 = \ldots$.

Fig. 2. Vector element functions $N^T_1, N^T_4$ and $N^T_7$ related to the bottom edge of an arbitrary triangle $T_i$. The other vector functions can be obtained by “cyclic rotation”.

Fig. 3. DOF placement for triangles. The positions of the nodal functions are marked as white numbered dots, whereas vector functions are represented by means of white numbered arrows. (left) First order functions. (right) Second order functions including interior ones.
Fig. 4. Vector element functions $N_{R_j}^1$, $N_{R_j}^5$ and $N_{R_j}^9$ related to the bottom edge of an arbitrary paraxial rectangle $R_j$. The other vector functions can be obtained by “cyclic rotation”.

$1 - r$, $\zeta_2 = 1 - z$, $\zeta_3 = r$ and $\zeta_4 = z$. The element functions whose support intersect with $R_0$ (see Figure 4) are then defined to be (see [18])

\[
\begin{align*}
N_{iR_0}^1(r, z) &= \zeta_i\zeta_{i+1} & N_{iR_0}^1(r, z) &= -\zeta_{i+1} \nabla_p \zeta_i \\
N_{i+4R_0}^1(r, z) &= 4 \zeta_i\zeta_{i+1}\zeta_{i+2} & N_{i+4R_0}^1(r, z) &= (1 - 2\zeta_i)\zeta_{i+1} \nabla_p \zeta_i \\
N_{9R_0}^1(r, z) &= 16 \zeta_1\zeta_2\zeta_3\zeta_4 & N_{i+8R_0}^1(r, z) &= \zeta_i\zeta_{i+1}\zeta_{i+2} \nabla_p \zeta_{i+1}
\end{align*}
\]

where the indices of the $\zeta$ wrap in modulo arithmetic fashion and $i = 1, 2, 3, 4$.

Figure 5 in order to understand how to interpret the DOF.

Note that in both cases, the left columns represent the nodal element functions whereas the right columns denote the vector element functions. Moreover, if the approximation is of first order, only the first row of functions is used, in each case. For second order approximations, the remaining functions are incorporated into the discrete spaces as well. However, before these functions can be used, they must be (affinely) mapped onto each of the triangles $T_i$ and rectangles $R_j$.

The finite element functions, whose restriction to a single polygon has been described above, constitute the discrete function space, in which the desired

Fig. 5. DOF placement for rectangles. The positions of the nodal functions are marked as white numbered dots, whereas vector functions are represented by means of white numbered arrows. (left) First order functions. (right) Second order functions including interior ones.
approximations reside. In order to compute these approximations, it is necessary to construct the discrete operators described by the weak form (2.7). To this end we expand the field components used in Problem 3 by means of the finite element functions given above, i.e.

\[
\begin{align*}
\hat{E}^{(c)}_p = & \sum_k \left\{ \bar{x}_k \right\} N_k(r, z) \\
\hat{V}^{(c)}_p = & \sum_k \left\{ \bar{y}_k \right\} r^{-1} N_k(r, z), \\
\hat{E}^{(s)} = & \sum_k \left\{ \bar{x}_k \right\} N_k(r, z) \\
\hat{V}^{(s)} = & \sum_k \left\{ \bar{y}_k \right\} r^{-1} N_k(r, z),
\end{align*}
\]

where the element functions are now globally numbered. Note, that the \( r^{-1} \) factor in front of \( N_k(r, z) \) is the modification which guarantees spurious free approximations. Unfortunately, the price for this modification is a change in the set of boundary conditions prescribed by \( \hat{H}_0(\text{curl}; \Omega_p) \) and \( \hat{H}_0^1(\Omega_p) \).

Inserting the finite element expansions (3.1) into (2.7) of Problem 3 and considering that the latter must hold for all functions \( \hat{V}^{(s)} \), leads to a system of equations

\[
Az = \begin{bmatrix} A_1 + m^2 A_2 & mA_3 \\ mA_3^T & A_4 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda Bz
\]

where the sub–blocks \( A_i \) and \( B_j \) are associated with the corresponding bilinear forms \( a_i(\cdot, \cdot) \) and \( b_j(\cdot, \cdot) \) in (2.6).

An important point to note is that both, the inner products and the tensors, are symmetric. Since the latter may be complex, the resulting general eigenvalue problem (3.2) turns out to be complex symmetric, as well. In addition, both matrices \( A \) and \( B \) will be sparse, due to the locally confined supports of the finite element functions.

### 3.1 Accurate Evaluation of Bilinear Forms

Despite the formal simplicity of the matrix assembling process, care has to be taken when numerically evaluating the bilinear forms. Recall, that even though the element functions are mere polynomials \( q(r, z) \), some of the integrals possess a weighting term \( r^{-1} \). Explicit evaluation of these integrals leads to very large expressions which suffer from cancellation. But the alternative application of standard numerical integration techniques, such as Gaussian quadrature, requires many function evaluations in order to obtain accurate results, which becomes even worse, if tensor product rules are used. Also, this straightforward numerical quadrature leads to cancellation.

To avoid these problems, we transform integrals over triangles into integrals over triangle boundaries, i.e. sums of one dimensional integrals. By applying
Green’s theorem we get
\[ \int_T x^{-1} q(x, y) \, dT = \sum_k u_k \int_0^1 (x_k + u_k t)^{-1} Q(x_k + u_k t, y_k + v_k t) \, dt, \]
where \( Q(x, y) = \int q(x, y) \, dy \). The parameters \( u_k = x_{k+1} - x_k \) and \( v_k = y_{k+1} - y_k \) denote the differences between the \( x \) and \( y \) coordinates of the counterclockwise oriented triangle vertices \((x_k, y_k)\) with \( k = 1, 2, 3 \).

Integrals over paraxial rectangles are recast into product form and lead to integrals of the form
\[ \int_R x^{-1} q(x, y) \, dR = u_0 \int_0^1 (x_0 + u_0 t)^{-1} [Q(x_0 + u_0 t, y_0 + v_0) - Q(x_0 + u_0 t, y_0)] \, dt, \]
where again, the parameters depend on the underlying rectangle, i.e. \((x_0, y_0)\) denotes its lower left corner and \( u_0 \) and \( v_0 \) its width and height, respectively.

Hence, the original integration problem can be reduced to a set of line integrals with weight function \((\alpha + \beta t)^{-1}\), for which the construction of appropriate Gauss quadrature rules is feasible. Notice, that each element requires its own quadrature rule! Nevertheless, these quadrature rules can be constructed cheaply [12], whence the bilinear forms can be evaluated efficiently and accurately.

4 Numerical Experiments

This section is devoted to the validation of the previously described modelling process. To this end we investigate cavities whose geometries and material arrangements admit solving (2.1) in closed form. The analytical solutions can then be compared to the approximate ones, obtained from solving the FEM models. Note that throughout this section we assume that \( \mu = I \).

In order to compute a few of the eigenvalues of the generalised complex symmetric eigenvalue problem (3.2) close to a target value \( \tau \) it is advisable to transform it into the form
\[ (A - \sigma B)^{-1} B z = \nu z, \quad \nu = (\lambda - \sigma)^{-1}, \quad (4.1) \]
where \( \sigma \) is a shift equal or close to the target. The latter is usually found by means of a related simplified problem. (4.1) is called a shift–and–invert spectral transformation [4] with shift \( \sigma \). By means of the spectral transformation the eigenvalues of the matrix pencil \((A; B)\) that are close to the shift become the largest in modulus of (4.1). The eigenvectors remain unchanged.
The Arnoldi algorithm is a well-known method for calculating a few of the extremal eigenvalues of a large matrix. We use the implicitly restarted Arnoldi algorithm as it is implemented in the MATLAB function \texttt{eigs}. \texttt{eigs} actually is an interface to a compiled routine of ARPACK [26]. The implicit restarts make it possible to control the memory requirements without losing the favourable convergence properties of the Arnoldi algorithm.

The shift–and–invert spectral transformation exposes the interior eigenvalues close to the shift. But the transformation entails that a system of equations of the form

\[(A - \sigma B)x = By\] 

must be solved in every step of the Arnoldi iteration. As our problems are not too large we use a direct solver to this end. Notice that it is important to permute the matrix $A - \sigma B$ to reduce fill–in, e.g. by minimum degree reordering. By suppressing pivoting we can save the symmetry of the problem, however at the expense of stability! When $A - \sigma B$ will become too large to be factored we will employ a variant of the Jacobi–Davidson algorithm, JDCS, that has been adapted to the complex symmetric eigenvalue problem [3].

\[4.1\] A hollow cylinder cavity

The first cavity we investigate is a hollow cylindrical resonator. We assume the cylinder is empty ($\varepsilon = 1$) with unit radius and height ($R = H = 1$) and surrounded by a PEC layer. The exact solutions can be constructed by separation of variables, see [19]. Thus, the eigenvalues can be expressed in the form

\[
\begin{align*}
\lambda^{(\text{TM})}_{m,n,l} & = b_{m,n} R^{-2} + l^2 \pi^2 H^{-2} \\
\lambda^{(\text{TE})}_{m,n,l+1} & = b'_{m,n} \\
\end{align*}
\]

Here $b_{m,n}$ denotes the $n$th root of the Bessel function $J_m(x)$ and $b'_{m,n}$ denotes the $n$th root of its first derivative $J'_m(x)$. Some of the roots $b_{m,n}$ and $b'_{m,n}$ are listed in [2].

This is a real eigenvalue problem. The desired eigenvalues are the lowest ones. In Figures 6 and 7 the convergence of a few of these eigenvalues are plotted in log–log scale. The plots nicely show the theoretically predicted convergence behaviour. The linear elements have linear convergence rate, the quadratic elements display a quadratic convergence rate.

In Table 4.1, another point of view of the same data is given. There, $DpD$ (DOF–per–Digit) denotes the factor with which the number of the degrees of freedom have to be multiplied to gain a decimal digit in accuracy. The
Fig. 6. Comparison of first and second order functions over triangular elements. The plots show the relative errors w.r.t. the mesh width, using first order (thin) and second order (thick) elements. The random triangular meshes were generated using MATLAB’s PDE Toolbox. (left) Angular wavenumber $m = 0$. Relative error of $\lambda_{010}^{(TM)}$ (solid), $\lambda_{011}^{(TM)}$ (dashed) and $\lambda_{011}^{(TE)}$ (dotted). (right) Angular wavenumber $m = 1$. Relative error of $\lambda_{111}^{(TE)}$ (solid), $\lambda_{110}^{(TM)}$ (dashed) and $\lambda_{111}^{(TM)}$ (dotted).

lower this factor the better. Again, it is clear that for a given accuracy many fewer degrees of freedom are required with the quadratic than with the linear elements. The factors for the rectangles are better than those for the triangles. The difference, at least for the 2nd order elements, is small.

### 4.2 Two concentric dielectric spheres

In this second example we consider a cavity consisting of two concentric dielectric spheres with radii $a = 1$ and $b = 2$, respectively. Moreover, the permittivity

Fig. 7. Comparison of first and second order functions over rectangular elements. The plots show the relative errors w.r.t. the mesh width, using first order (thin) and second order (thick) elements. The meshes consisted of equidistant squares and were generated by the commercially available mesh generator of ISE. (left) Angular wavenumber $m = 0$. Relative error of $\lambda_{010}^{(TM)}$ (solid), $\lambda_{011}^{(TM)}$ (dashed) and $\lambda_{011}^{(TE)}$ (dotted). (right) Angular wavenumber $m = 1$. Relative error of $\lambda_{111}^{(TE)}$ (solid), $\lambda_{110}^{(TM)}$ (dashed) and $\lambda_{111}^{(TM)}$ (dotted).
The equations for the eigenvalues can be expressed by means of the determinants $k$ of (1). Let

$$\lambda_{010}^{(TM)} = 10.4 \quad \lambda_{010}^{(TM)} = 3.17$$

$$\lambda_{011}^{(TM)} = 10.8 \quad \lambda_{011}^{(TM)} = 3.19$$

$$\lambda_{101}^{(TM)} = 12.3 \quad \lambda_{101}^{(TM)} = 3.47$$

The computation of the exact solution can be carried out following the lines incorporated into our model.

The fact that the second order approximations no longer converge quadratically, see Figure 8, can be ascribed to the geometrical discretisation of the domain. The two concentric semi-discs that are used to model the cavity are approximated by regular triangular meshes. Consequently, their perimeter are discretised as polygons which reduces the approximation power of the quadratic elements. Strang and Fix [31] state that the convergence rate should be $O(h^{3/2})$. We observed a strong reduction of the convergence rate to almost linear, see Table 4.2. We believe that we can rectify this problem by introducing curvilinear elements.
Fig. 8. Comparison of first and second order element functions. The plots show the relative errors w.r.t. the mesh width, using first order (thin) and second order (thick) elements. The meshes consisted of triangles and were generated using MATLAB’s PDE toolbox. (left) Angular wavenumber $m = 0$. Relative error of $\lambda_{010}^{(TM)}$ (solid), $\lambda_{011}^{(TM)}$ (dashed) and $\lambda_{011}^{(TE)}$. (right) Angular wavenumber $m = 1$. Relative error of $\lambda_{111}^{(TM)}$ (solid), $\lambda_{110}^{(TM)}$ (dashed) and $\lambda_{111}^{(TM)}$ (dotted).

Table 2
Comparison of the DOF–per–Digit ratio between first and second order element approximations.

<table>
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<tr>
<th></th>
<th>1st order</th>
<th>DpD[Δ]</th>
<th>2nd order</th>
<th>DpD[Δ]</th>
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<td></td>
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<td>11.2</td>
<td></td>
<td>$\lambda_{111}^{(TM)}$</td>
<td>9.64</td>
</tr>
</tbody>
</table>

4.3 A free dielectric sphere

To show the generality of our approach, we conclude this section with an open resonator cavity example. We consider a dielectric sphere of radius $a = 1$ and $\varepsilon_a = 10$ immersed in free space ($\varepsilon = 1$) and are interested in its fundamental mode, i.e. the lowest TE mode corresponding to the angular wave number $m = 1$. A characteristic equation for this problem can be found in [10,1] and reads

$$
\frac{J_{l-1/2}(k\sqrt{\varepsilon_a}a)}{J_{l+1/2}(k\sqrt{\varepsilon_a}a)} - \frac{1}{\sqrt{\varepsilon_a}} \frac{H_{l-1/2}^{(2)}(k\sqrt{\varepsilon_a})}{H_{l+1/2}^{(2)}(k\sqrt{\varepsilon_a})} = 0,
$$

(4.6)

where again $k = \sqrt{\lambda}$ and $l \geq m$. Note the use of Hankel functions of second kind which are necessary to enforce the so–called Sommerfeld radiation condition, i.e. a condition requiring that no waves are incoming from infinity.
Fig. 9. An open cavity resonator problem with truncated simulation domain. The PML layer (light) absorbs and extinguishes outgoing waves and thence inhibits reflections on the outermost PEC boundary. (left) For the PML to be effective it must not be placed too close to the actual cavity. This layer is constructed such as to absorb planar waves and hence has to be put in the so–called far–field. (right) Comparison of the relative error of first (thin) and second order (thick) approximations on a mixed mesh.

As explained in Section 1, the computational domain is truncated by means of an absorbing PML layer enclosed by a PEC boundary. The inner boundary of the 3 unit thick absorber is positioned 15 units from the origin and modelled according to [13]. Thus, our computational domain consists of different materials, some of which are complex. A sketch of the geometry is given in Figure 9.

We were not able to solve larger problems with the quadratic elements because of the memory limitations given in MATLAB. Clearly, the quadratic elements give a much higher accuracy for a given mesh than the linear ones. Due to the inhomogeneous grid refinement the plots in Figure 9 do not clearly reflect the theoretic expectations as they were observed in Experiment 1. There the problem was real and the grid refinement manageable.

5 Conclusions

We have given weak formulations for the axisymmetric vector Helmholtz problem and have discussed its finite element discretisation. We have shown how the corresponding FE matrices can be computed accurately and how the resulting eigenvalue problems can be solved. We then carried out three numerical experiments to show that our approach is suitable for the simulation of general optical resonators.

We are still limited by our experimental environment. MATLAB’s memory restrictions do not permit us to deal with the matrix sizes that are typical
for real world problems. These large problems will also require factorisation–
free eigenvalue solvers like the Jacobi–Davidson algorithm. This issues will be
addressed in future work.

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