

Preconditioned Jacobi-Davidson Algorithm for Nonsymmetric, Complex Eigenvalue Problems Arising with Gyrotropic Materials in Resonator Cavities

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Abstract

For the numerical solution of complex eigenvalue problems, arising with gyrotropic materials in resonators, the Jacobi-Davidson method is considered. In this paper the correction equation, which has to be solved within the Jacobi-Davidson method, is simplified and several preconditioning strategies, including also a multigrid scheme, are compared for the approximate solution of this correction equation. Comparisons between this multigrid-solver and standard solvers regarding computation time are performed.

1 INTRODUCTION

Gyrotropic materials such as ferrites are used in modern cavity design for tuning and vacuum isolation purposes [1]. For most practical cavities the geometry is sufficiently complicated that analytical solutions for the eigenmodes supported by the cavity do not exist. The geometry of the test problem which is used for the further analysis of our numerical eigenvalue solver is sketched in Fig. 1. The



Figure 1: Cylindrical resonator including a dielectric ring covered with a gyrotropic material

simulation of electromagnetic fields in gyrotropic materials is not straightforward, since their material tensor typically is non-symmetric and complex-valued. Using the Finite Integration Technique (FIT) [2] for the simulation of electromagnetic waves in structures including gyrotropic materials lead to complex-valued, non-symmetric algebraic eigenvalue problems. The Jacobi-Davidson subspace iteration method is used to solve these eigenvalue problems involving large, sparse, complex and non-symmetric matrices.

2 GYROTROPIC MATERIALS

Gyrotropic materials represent a subgroup of anisotropic materials with a second order material tensor. Those magnetic and electric tensor material characteristics are central to a broad class of complex materials such as plasmas and ferrites. The gyrotropic material properties are due to an

electric or magnetic material tensor and thus such a material is either referred to as gyroelectric or gyromagnetic, respectively.

Since the most important gyromagnetic materials in accelerator technique are the ferrites, the material tensor of those is presented here only. The magnetic tensor for ferrites with gyrotropic coupling of x- and y- components is given in reference [3]:

$$\vec{\mu} = \begin{pmatrix} \mu_1(\omega) & i\mu_2(\omega) & 0 \\ -i\mu_2(\omega) & \mu_1(\omega) & 0 \\ 0 & 0 & \mu_3(\omega) \end{pmatrix}, \quad (1)$$

with the complex diagonal and non-diagonal elements

$$\mu_1(\omega) = \mu_0 \left(\mu_\infty + \frac{\omega_m(\omega_l + i\omega\alpha)}{(\omega_l + i\omega\alpha)^2 - \omega^2} \right),$$

$$\mu_2 = \mu_0 \frac{\omega\omega_m}{(\omega_l + i\omega\alpha)^2 - \omega^2}, \quad \mu_3 = \mu_0,$$

where ω_m is the gyrotropic frequency, ω_l is the Lamor frequency and α is a damping constant. The dielectric tensor of ferrite is diagonal. For the further analysis it is of importance, that $\vec{\mu}$ is complex and non-symmetric if $\alpha \neq 0$.

3 NUMERICAL MODELING

Using the FIT for the numerical modeling the analytical eigenvalue equation $(\nabla \times \vec{\mu}^{-1} \nabla \times - \omega^2 \vec{\epsilon}) \vec{e} = 0$ results in the discrete algebraic eigenvalue equation:

$$(\tilde{\mathbf{C}} \mathbf{M}_{\mu^{-1}}(\omega) \mathbf{C} - \omega^2 \mathbf{M}_\epsilon(\omega)) \vec{e} = 0. \quad (2)$$

Where \mathbf{C} and $\tilde{\mathbf{C}}$ are symmetric matrices and represent the discrete curl operators. The operators $\mathbf{M}_{\mu^{-1}}$, \mathbf{M}_κ and \mathbf{M}_ϵ are the material-matrices and in case of gyrotropic materials they are non-diagonal, non-symmetric, complex and frequency dependent [4]. These matrices are obtained by introducing a grid on which the primary field components are allocated. The material distribution is discretized with respect to this grid and represented in the material matrices. Neglecting the frequency dependence of $\mathbf{M}_\epsilon(\omega)$ and $\mathbf{M}_{\mu^{-1}}(\omega)$ (2) yields a linear generalized eigenvalue problem.

$$(\tilde{\mathbf{C}} \mathbf{M}_{\mu^{-1}} \mathbf{C} - \omega^2 \mathbf{M}_\epsilon) \vec{e} = 0 \quad (3)$$

An estimation of the eigenvalue ω can be used to determine \mathbf{M}_ϵ and $\mathbf{M}_{\mu^{-1}}$. For gyromagnetic materials \mathbf{M}_ϵ is diagonal and can be inverted easily. In this case a standard eigenvalue problem

$$\mathbf{A} \vec{e} = \omega^2 \vec{e} \quad (4)$$

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with the system-matrix $\mathbf{A} = \mathbf{M}_\varepsilon^{-1} \tilde{\mathbf{C}} \mathbf{M}_{\mu-1} \mathbf{C}$ has to be solved. For most applications in accelerator technology only the smallest dynamical eigenvalues are of interest. The solutions of (4) also include the static solutions with $\omega = 0$. Since these static solutions will be a problem when trying to find the lowest dynamical eigenvalues a gauging using a grad-div augmentation of (2) can be performed [5].

4 JACOBI-DAVIDSON METHOD

The Jacobi-Davidson (JD) subspace iteration method is applicable for non-symmetric and complex matrices \mathbf{A} and can also be extended to solve generalized eigenvalue problems [6]. In this approach a search subspace is generated onto which the given eigenvalue problem is projected. The projected eigenvalue problem is solved and this leads to an approximation for the original much larger eigenvalue problem. In each iteration step the search subspace is expanded by a correction vector \mathbf{v} which is computed by approximately solving the correction equation

$$(\mathbf{I} - \mathbf{q}\mathbf{q}^T)(\mathbf{A} - \lambda\mathbf{I})(\mathbf{I} - \mathbf{q}\mathbf{q}^T)\mathbf{v} = -\mathbf{r}, \quad (5)$$

where \mathbf{q} is the estimated eigenvector, \mathbf{q}^T is the transposed vector of \mathbf{q} , λ is the approximated eigenvalue and \mathbf{r} is the residual vector of the eigenvalue problem

$$\mathbf{r} = (\mathbf{A} - \lambda\mathbf{I})\mathbf{q}. \quad (6)$$

The correction equation (5) has to be solved only approximately. However, for large matrices the computation of (5) is the most time consuming part in this algorithm. For the test problems it was found, that even a solution $\mathbf{v} = -\mathbf{r}$ instead of (5) will result in a convergence of the JD method, but then the convergence is rather slow. A better approximation to (5) lies in the solution of

$$\mathbf{A}\mathbf{v} = -\mathbf{r}. \quad (7)$$

For the test problem the convergence history computing the 5 lowest eigenvalues is plotted in Fig. 2 using (5) and (7). The solution of the exact correction equation (5) shows a faster convergence in terms of the required number of iterations. The more important criterion, namely the time consumption, will be discussed in the next section.

5 INTERIOR SOLVERS

For the solution of (5) and (7) in the JD algorithm the iterative BICGSTAB method was used. It was found that a relative residual of 10^{-2} resulted in the fastest convergence of the JD algorithm. Solutions with a smaller residual do not result in sufficiently smaller numbers of iterations, whereas more unprecise solutions will increase the number of iterations or may lead to a stagnation of the exterior JD method.

The number of iterations and the computation time for the JD method computing the lowest eigenvalue using (5) and (7) (solved with BICGSTAB) are stated in Table 1.a

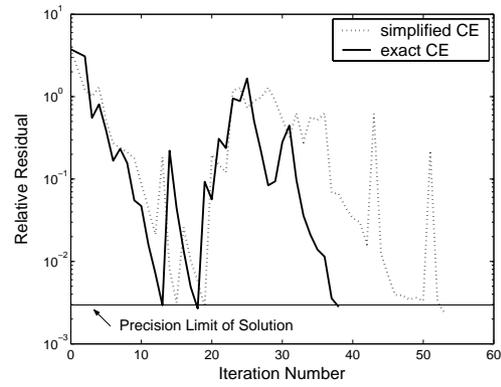


Figure 2: Relative residual versus iteration step for the solution of the exact and simplified correction equation (CE), computing the 3 lowest eigenvalues of the test problem.

and Table 1.b respectively. Different preconditioners such as the incomplete LU factorization, Jacobi and SSOR were applied to the BICGSTAB-solver. As Table 1 shows, the best results can be obtained using the incomplete LU factorization. However, for large systems the ILU factorization itself is extremely time consuming and therefore not suitable for our problems. A different possibility solving

Correction Equation $\mathbf{M}\mathbf{v} = -\mathbf{r}$	Iter.	Time
a.) $\mathbf{M} = (\mathbf{I} - \mathbf{q}\mathbf{q}^T)(\mathbf{A} - \lambda\mathbf{I})(\mathbf{I} - \mathbf{q}\mathbf{q}^T)$ - BICGSTAB(tol= 10^{-2})	16	65s
b.) $\mathbf{M} = \mathbf{A}$ - BICGSTAB(tol= 10^{-2}) - BICGSTAB(tol= 10^{-2} , ILU(0)) - BICGSTAB(tol= 10^{-2} , JACOBI) - BICGSTAB(tol= 10^{-2} , SSOR)	21 10 20 19	31s 20s 38s 36s
c.) $\mathbf{M} = \mathbf{I}$ - exact	542	212s
d.) $\mathbf{M} = \tilde{\mathbf{L}}\tilde{\mathbf{U}} + \mathbf{R}$ - exact: $\mathbf{v} = \tilde{\mathbf{U}}^{-1}\tilde{\mathbf{L}}^{-1}(-\mathbf{r})$	114	48s
e.) $\mathbf{M} = (\mathbf{D} + \mathbf{L})\mathbf{D}^{-1}(\mathbf{D} + \mathbf{U})$ - exact	143	70s
f.) Multigrid-solver $\mathbf{M} = \mathbf{A}$	21	25s

Table 1: Computation time and number of inner iteration steps, calculating the lowest eigenvalue of the test problem (10^4 gridpoints), for different correction equations and solvers on a 1.8GHz PC. The first argument of the BICGSTAB solver refers to the tolerance of the solution (relative residuum) and the second argument refers to the used preconditioner. The matrix \mathbf{L} represent the lower triangular part respectively \mathbf{U} the upper triangular part of the matrix \mathbf{A} . \mathbf{D} is the diagonal of \mathbf{A} .

(7) approximately is to replace \mathbf{A} itself with an easy to invert approximation to \mathbf{A} , such as the incomplete LU factorization (Table 1.d) and the Gauss-Seidel decomposition (Table 1.e) of \mathbf{A} . Once \mathbf{A} is substituted in this way, an ex-

act solution of the obtained approximation can be derived. Even the approximation $\mathbf{A}=\mathbf{I}$ leads to convergence of the JD method (Table 1.c), but the convergence is rather slow.

A new promising method to solve the algebraic system $\mathbf{A}\mathbf{x} = -\mathbf{r}$ approximately involves a multigrid scheme [7]. A geometrical multigrid method solving $\mathbf{A}\mathbf{x} = -\mathbf{r}$ was developed and implemented in MATLAB. This multigrid method uses the ω -Jacobi-relaxation iteration [7] as a smoother on each grid level. For a couple of test problems it was observed, that $\omega = 0.5$ showed the best convergence behavior. Using this multigrid solver in the JD method a competitive computation time was achieved (Table 1.f).

To test the convergence behavior and the asymptotic complexity of the multigrid method, the system $\mathbf{A}\mathbf{x} = \mathbf{b}$ with random right hand side vector \mathbf{b} was solved with our multigrid method and compared with standard MATLAB-solvers for real-valued and for non-symmetric, complex matrices \mathbf{A} . The relative residual norm of the solution was chosen to be 10^{-6} for all solvers. The matrix \mathbf{A} was obtained from the test problem without gyrotropic materials for the symmetric case or with gyrotropic materials for the non-symmetric and complex case respectively. The slope in Fig. 3 for the multigrid method, corresponding to the exponent of the asymptotic complexity, is measured to be 1.1 and is thus smaller than that of the other standard solvers in the observed range of problem sizes ($10^3 < \dim(\mathbf{A}) < 2 \cdot 10^5$).

For the complex and non-symmetric case the multigrid method shows an even better convergence behavior compared with the standard solvers as for a symmetric matrix \mathbf{A} . If the test problem contains materials with big

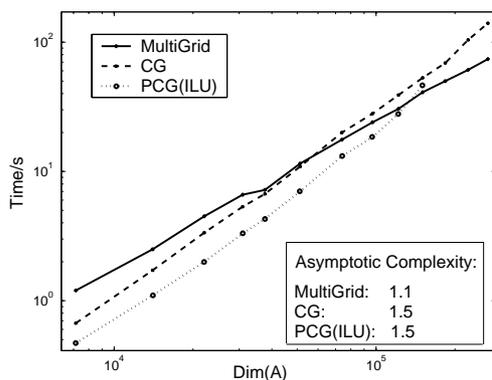


Figure 3: Computation time versus matrix size for the solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$ with different solvers, for a symmetric and real system-matrix \mathbf{A}

local jumps in the material properties ($\Delta\epsilon, \Delta\mu > 5$) the present multigrid method, however, does not converge. Furthermore, the method will show no convergence for gyrotropic materials with large nondiagonal elements ($\Im(\mu_2), \Re(\mu_2) \geq |\mu_1|$). In all other cases, the multigrid-solver could compute the solutions to a residual of 10^{-12} without further problems.

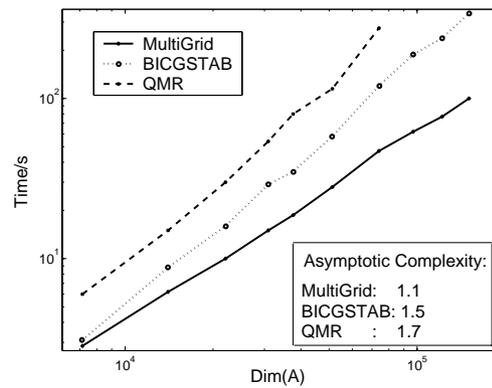


Figure 4: Computation time versus matrix size for the solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$ with different solvers, for a non-symmetric and complex system-matrix \mathbf{A}

6 CONCLUSIONS

The JD method was used to solve large, complex-valued and non-symmetric eigenvalue problems arising with gyrotropic materials in resonator cavities. Since the solution of the correction equation within the JD method represents the most time consuming part, different solution strategies were studied. It was found that it is efficient to solve the simplified correction equation to compute the lowest eigenvalues. Different solvers to compute the approximate solution of this simplified correction equation were compared. A multigrid-solver specially developed for this task showed the best asymptotic complexity compared to solvers such as BICGSTAB, QMR (for non-symmetric and complex problems) or PCG(ILU) (for symmetric problems) and thus appears best suited for large scale simulations.

7 REFERENCES

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