Accurate Determination of Thousands of Eigenvalues for Large-Scale Eigenvalue Problems

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***Abstract*—In this paper we address a fast approach for an accurate eigenfrequency determination. The major challenges posed by our work are: first, the ability of the approach to tackle the large-scale eigenvalue problem and second, the capability to extract many, i.e. order of thousands of eigenfrequencies for the considered problem. At this point, we demonstrate that the proposed approach is able to extract many eigenfrequencies of a closed resonator in a relatively short time. In addition to the need to ensure a high precision of the calculated eigenfrequencies, we compare them side by side with the reference data available from analytical expressions and CEM3D eigenmode solver. Furthermore, the simulations have shown high accuracy of this technique and good agreement with the reference data. Finally, all of the results indicate that the suggested technique can be used for precise determination of many eigenfrequencies.**

***Index Terms*—Finite element methods, eigenvalues and eigenvectors.**

I. Introduction

Within this work, we investigate quantum billiards with its statistical eigenvalue properties, which reveal the periodic orbits in the quantum spectra and give the quantum chaotic scattering. Specifically, we simulate superconducting microwave resonators with chaotic characteristics (consisted of two quarter cylinders with radii $r_1 = 200.0$ mm and $r_2 = 141.4$ mm) and we compute the eigenfrequencies that are needed for the level spacing analysis [1]. Accordingly, the eigenfrequency analysis requires many (in order of thousands) eigenfrequencies to be calculated and the accurate determination of the eigenfrequencies has a crucial significance.

As a result, the main aim of our study coincides with solving the electromagnetic problem for a superconducting cavity, which enclosures excited electromagnetic fields. For this purpose, the finite element method based on curvilinear tetrahedrons is utilized [2]. Hereby, we consider the numerical solution of the generalized large-scale eigenvalue problem. It is the task of finding the real scalars λ_k and the corresponding real-valued vectors $\vec{x_k} \neq 0$ such that

$$A\vec{x_k} = \lambda_k B\vec{x_k}, \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$ and $B \in \mathbb{R}^{n\times n}$ are symmetric matrices, B is positive definite, $k = 1, 2, ..., n$, and n is several thousands. Despite the fact that many algorithms for eigenvalue determination (Jacobi-Davidson, Arnoldi, Krylov-Schur, etc) exist, not as many are specifically adapted for computing a large number of eigen pairs, located in a specified range, for matrices with dimension in excess of several millions.

The Lanczos method with its variations is very attractive for our project necessities. The major practical advantage of this method is the tridiagonal reduction of the eigenvalue problem that yields minimal storage requirements. Also, the required arithmetic operations are small, allowing work with very large tridiagonal, as well as, real symmetric matrices. Consequently, our investigations comprise efficient, robust, and accurate computations of many wanted eigenfrequencies by employing the Lanczos method.

II. B-Lanczos Algorithm

The main idea of the B-Lanczos procedure [3] is to replace the eigenvalue problem for the given matrix pair (A, B) by an eigenvalue problem of a simpler Lanczos matrix. It is an orthogonal projection technique onto a Krylov subspace $K_m(B^{-1}A, \vec{v_1})$ and can be viewed as a simplification of the Arnoldi's method for the particular case when the matrices are Hermitian.

1) B-Lanczos with Shift-and-invert: Along the line of our requirements, the eigenvalue solver must deal with a very wide requested frequency range of interest. To overcome this issue, it is naturally desirable to access the matrix only in parts. Applying the spectral transformation to the original problem $A\vec{x} = \lambda B\vec{x}$, we get

$$(A - \sigma B)^{-1} B\vec{x} = \theta\vec{x}, \tag{2}$$

where the matrix $(A - \sigma B)^{-1}$ is never explicitly formed. This transformation enables one to find closely spaced eigenvalues in the neighborhood of σ in a well-separated form.

2) Filtered B-Lanczos: This method is based on spectral transformation using polynomials in order to extract eigenvalues in a given interval and their associated eigenvectors.

III. Simulation Results

A. Implementation Details

The B-Lanczos and B-Lanczos with shift-and-invert (SI) solvers are implemented in C / C++ and built on the commonly used libraries: Intel Math Kernel Library (MKL) 10.2

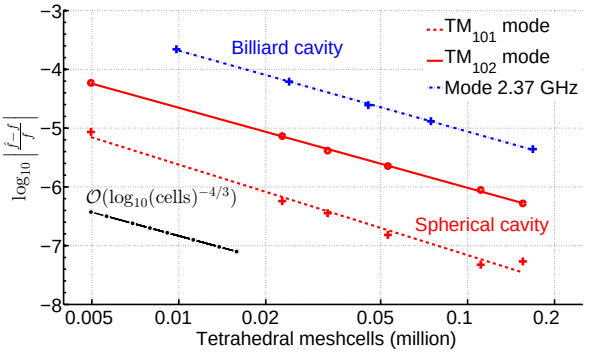

Figure 1: Relative deviation of the numerically obtained values $\hat{f}$ to the reference results f as a function of the degrees of freedom for a spherical and billiard resonator. The first two worst computed degenerated mode eigenfrequencies are considered for the spherical cavity, whereas for the billiard cavity the 2.37 GHz mode eigenfrequency is determined.

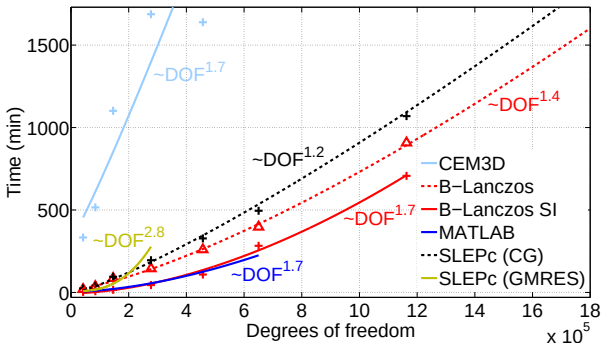

Figure 2: Time consumption for a billiard cavity. Different number of curvilinear tetrahedrons is used within the solvers.

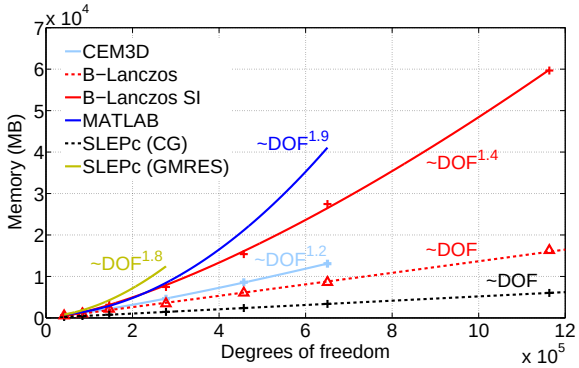

Figure 3: Memory consumption for a billiard cavity. Different number of curvilinear tetrahedrons is used within the solvers.

with BLAS and LAPACK, SuperLU, and PETSc [1]. The matrices A and B are generated from an external program CEM3D [2]. Additionally, the implementation exploits a partial reorthogonalization [4], which is favored over the full reorthogonalization [5]. In case that extreme eigenvalues are sought, at each B-Lanczos iteration step, an iterative conjugate gradient (CG) method (implemented in PETSc) along with Jacobi preconditioner is used for the solution of the resulting linear system of equations. However, for the interior eigenvalue determination an LU factorization, followed by a forward-backward substitution, is performed using the SuperLU direct solver.

B. Accuracy

The accuracy of the approach for eigenfrequency determination is tested for both analytically and non-analytically resolvable electromagnetic problems (see Fig. 1). Namely, due to verification purposes, a spherical cavity with radius $R = 1$ m is analyzed, whose exact solution can be analytically evaluated. It has perfectly conducting walls and contains a perfect vacuum. Besides the analytically resolvable resonator, the relative error is also measured for the chaotic billiard resonator. In order to verify the results extremely accurate reference data from CEM3D eigenmode solver are used. As the number of discretization mesh cells increases, a relative deviation in the order of 10^{-6} is present, next to the clearly observable 4^{th} order convergence.

C. Comparison with other Eigenvalue Solvers

We choose the recent versions of Matlab, SLEPc, and CEM3D to compare the computational speed as well as the memory consumption issues of the B-Lanczos solvers (see Fig. 2 and Fig. 3). Each simulation run computes the largest 100 eigenvalues of the billiard cavity. The eigenvalues in MATLAB are obtained employing the Arnoldi's method implementation, while in SLEPc the Krylov-Schur method was used in combination with Jacobi preconditioner of the CG and GMRES method. The CEM3D solver implements the Jacobi-Davidson method. As observed in Fig. 2 and Fig. 3, the iterative solvers need long time, but less memory, as to be expected. Here, the B-Lanczos solver next to SLEPc with CG can be considered as one group. On another side, B-Lanczos SI and Matlab are clearly separated from the other solvers in time consuming sense. However, it should be noted that these solvers require more memory than the CEM3D, B-Lanczos, and SLEPc with CG solvers. In the full paper more details on the accurate and memory-efficient eigenvalue determination will be given.

[1] The used software libraries will be referenced in the full paper.

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