COMPARISON OF EIGENVALUE SOLVERS FOR LARGE SPARSE MATRIX PENCILS *

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Abstract

Efficient and accurate computation of eigenvalues and eigenvectors is of fundamental importance in the accelerator physics community. Moreover, the eigensystem analysis is generally used for the identifications of many physical phenomena connected to vibrations. Therefore, various types of algorithms such that Arnoldi, Lanczos, Krylov-Schur, Jacobi-Davidson etc. were implemented to solve the eigenvalue problem efficiently. In this direction, we investigate the performance of selected commercial and freely available software tools for the solution of a generalized eigenvalue problem. We choose characteristic setups by considering spherical and billiard resonators next to a TESLA nine-cell cavity in order to test the robustness, accuracy, and computational speed as well as memory consumption issues of the recent versions of CST, Matlab, Pysparse, SLEPc and CEM3D. Simulations were performed on a standard personal computer and on a cluster computer to enable the handling of large sparse matrices in the order of hundreds of thousands up to several millions degrees of freedom (DOF). We obtain interesting comparison results with the examined solvers which is useful for choosing the appropriate solvers for a given practical application.

INTRODUCTION

In this paper, we consider the numerical solution of the generalized eigenvalue problem

$$A\,x = \lambda\,B\,x \quad \text{for} \quad B > 0 \tag{1}$$

for a given symmetric, real valued, large and diagonally dominant sparse matrix pencils A and B. The problem can be derived from Maxwell's equations for a source free bounded domain having perfectly conducting boundary condition on its surface. In principle, such a mathematical model coincides with a superconducting cavity which enclosures excited electromagnetic fields. Therefore, accurate calculation of eigenvalues λ has a critical importance and it leads to find the eigenfrequencies of several modes which are of fundamental importance for the acceleration of charged particles. In this context, performance of eigensolvers are always of interest in industry and scientific communities which constitutes the main motivation of our study.

Jacobi-Davidson method [1] which is based on iterative expansions of subspaces is recommended to solve eigenvalue problems dealing with diagonally dominant large matrices in the literature [2, 3, 4]. Therefore, we select CEM3D, Pysparse and SLEPc solvers which all can employ Jacobi-Davidson implementation in their simulations. Here, we just mention the idea behind of the method shortly. Let $V_k = \text{span}\{v_1, \cdots, v_k\}$ be a subspace where $v_k^T B v_j = \delta_{kj}$. Then a Ritz pair $(\theta_j,\ u_j)$ in V_k, can be obtained from the projected eigenvalue problem choosing the closest value to a given target τ. In the next step, a convergence criteria

$$\| r \|_2 := \| (A - \theta B)u \|_2 < \epsilon\,. \tag{2}$$

is checked for θ if it could be an eigenvalue for a selected ϵ. Afterwards, the so-called correction equation

$$(I - Buu^T)(A - \theta B)(I - uu^T B)z = -r \tag{3}$$

is solved iteratively with *tfqmrs* in CEM3D, with *bcgsl* in SLEPc and with *qmrs* in Pysparse for the unknown z where $z \perp u$ and u^T is the transpose of u. Then we expand the subspace $V_{k+1} = \text{span}\{v_1, \cdots, v_{k+1}\}$ for the next iteration which starts finding approximate Ritz pairs for the updated subspace [5].

NUMERICAL EXPERIMENTS

In the numerical tests, spherical and billiard resonators and a 9-cell TESLA cavity are considered. Structures are drawn and meshed with tetrahedrons having planar elements. Corresponding meshes are imported to CEM3D [6] in order to generate input sparse matrices for the eigenvalue solvers Pysparse [4], SLEPc [7] and Matlab [8]. Here, CEM3D is a parallel and a higher order FEM code which was implemented in our institute for the accurate calculations of eigenfrequencies for a given structure. Furthermore the same structures are used for the eigenvalue simulations in CST [9]. It is also noted that among these solvers only CEM3D and SLEPc have the capability to run on a distributed memory machine with multiprocessors in parallel.

For the comparison of different solver results, we first compute the eigenvalues of a spherical resonator from analytical expressions given in [10] by employing a root-finding algorithm which is simply explained in [11]. Eigenvalues are also calculated with SLEPc for different DOF and a relative error is calculated as,

$$\text{relative error} = \max_{i \in \text{DOF}} \frac{|\,\lambda^{\text{analytical}} - \lambda_i^{\text{numerical}}\,|}{\lambda^{\text{analytical}}} \tag{4}$$

by considering the worst computed degenerated mode eigenfrequency, see Figure 1.

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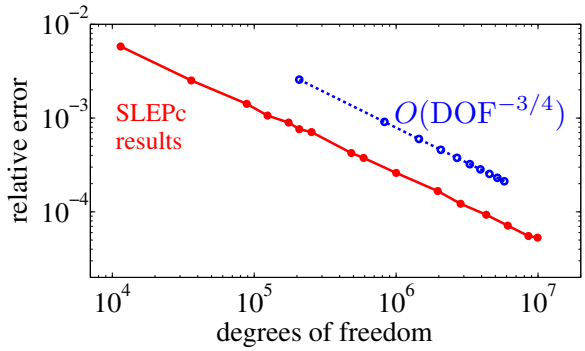

Figure 1: Convergence rate of SLEPc eigencomputations.

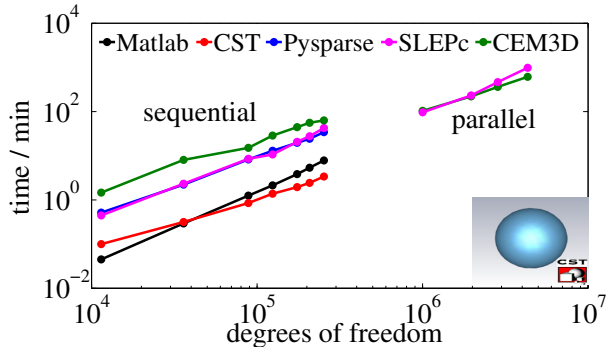

Figure 2: Time Consumption for a Spherical Resonator.

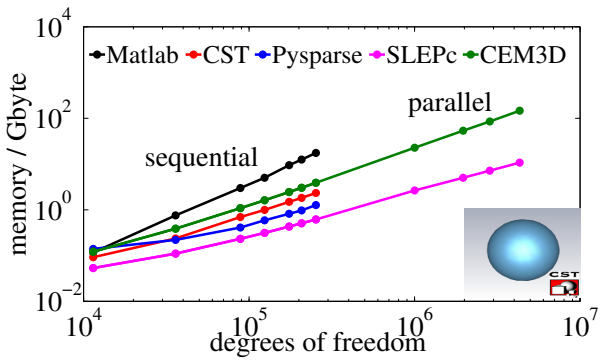

Figure 3: Memory Consumption for a Spherical Resonator.

In our simulation studies, we experienced that it is sufficient to use a single personal computer e.g. 2.27 GHz (2 processors) having 24 GB memory to compute 20 eigenvalues with the same accuracy for all solvers up to 10^5 degrees of freedoms but for the larger amount of DOF it is necessary to run solvers in parallel. Along this line results presented in this paper for approximately DOF $\geq 2.5 \times 10^5$ are obtained using parallel run on a cluster with SLEPc / CEM3D and this issue is indicated in time consumption illustrations in Figures 2, 4, 6 with two seperated regions by disconnected line plots.

In all simulations, we first mesh related geometries in CST with tetrahedrons and extract first 20 eigenvalues of the spectrum choosing accuracy 10^{-9} for different DOF with different solvers. Basically, structures have different eigenvalue spectrum's depending on their geometries and this phenomena may effect the performance of the solvers. Therefore we also test solvers with a chaotic billiard resonator which has a clustered eigenvalue distribution [12].

Spherical Resonator

As a first experiment, we consider a spherical resonator with a radius 1m. We run several simulations to obtain time and memory consumption results which are shown in Figure 2 and Figure 3, respectively. It can be concluded from the simulation results that iterative solvers needs long time but less memory as to be expected. Therefore, CST or Matlab can be recommended for the applications having DOF up to 10^5 in the case of providing enough computation sources. However, it should be noted that Matlab requires more memory as compared to the other solvers, so that SLEPc and Pysparse can also be considered a very good option in this DOF region. Especially, SLEPc has a very good characteristic from memory usage point of view for the very large DOF. On the other hand, a desired portion of the eigenvalues in the spectrum or the electromagnetic field distribution can be computed with CEM3D or CST straightforwardly. It should be noted that these tools are robust in nature even to unproperly chosen target values.

Nine-cell TESLA Cavity

For the second experiment, a 9-cell TESLA cavity with approximately 1m length is chosen. Here, Matlab and CST are clearly separated from the other solvers in time consuming, see Figure 4. On the other hand, as an important difference from the previous experiment now except SLEPc, all solvers memory consumption plots are more close to each other which actually emphasizes Matlab's good perfomance for this case. Furthermore, a linear $O(\mathrm{DOF})$ behavior is observed for DOF $\geq 10^6$ in the memory consumption of SLEPc, see Figure 5.

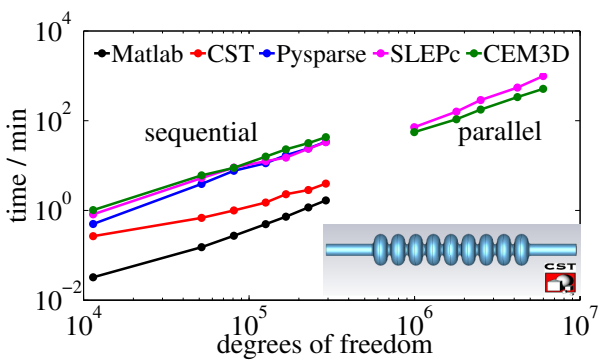

Figure 4: Time Consumption for a Tesla Cavity.

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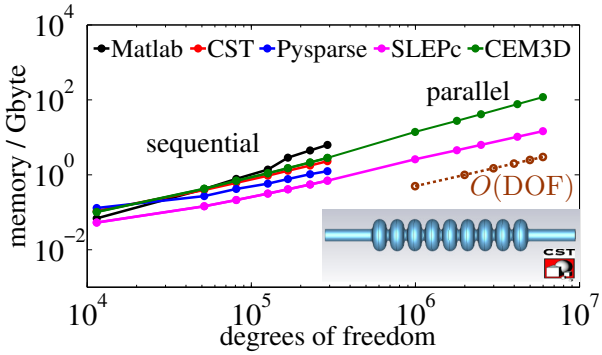

Figure 5: Memory Consumption for a Tesla Cavity.

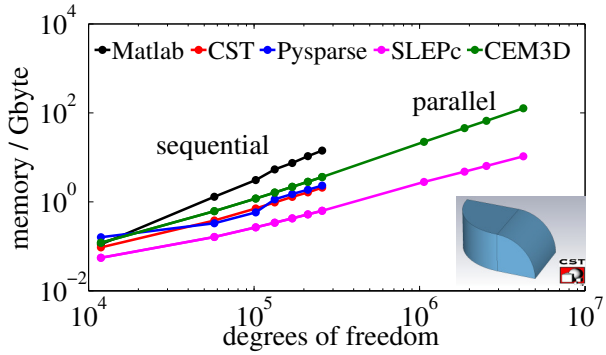

Figure 7: Memory Consumption for a Billiard Resonator.

Billiard Resonator

In the billiard resonator experiment, it is initially observed that the time and memory consumption behaviors of solvers for billiard resonator is more close to spherical resonator than a TESLA cavity. This may be a consequence of the similarity of the shapes. On the other hand, it should be emphasized that the nature of the solvers change only slightly even for a very different eigenvalue spectrum. It is shown in Figure 6 that time consumption of Matlab and CST are very similar in a region $10^5 \leq \text{DOF} \leq 2.5 \times 10^5$. However, curve of best fit of Matlab is more steep than CST for larger DOF. Moreover Pysparse and SLEPc have a similar time consumption characteristics but as it is similar in the previous simulations SLEPc requires the least memory source for billiard resonator calculations.

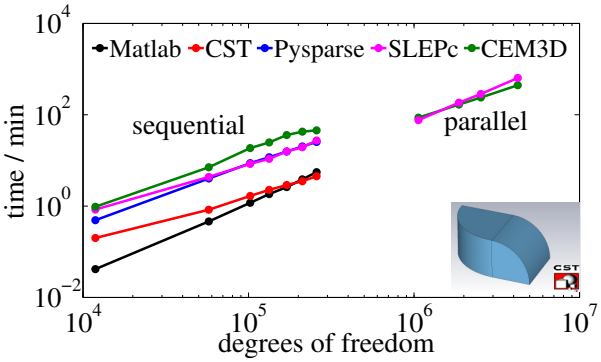

Figure 6: Time Consumption for a Billiard Resonator.

CONCLUSIONS

As a result of all experiments, we immediately conclude that solvers change their behavior only slightly depending on the geometry of the problem or the type of the eigenvalue spectrum. From time consuming point of view, Matlab and CST can be considered as one group and SLEPc, Pysparse, CEM3D can be considered as a second group according to their similar values. The flexibility of choosing target value in CST and CEM3D increases the applicability of these solvers. In the case of knowing the target value for single personal computer applications Matlab has an impressive performance in time. Free tools Pysparse and SLEPc has similar characteristics in time consuming but SLEPc uses the least memory in all three experiments and it can be used either on a single computer or on a cluster for very large amount of DOF.

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