QUADRATIC EIGENVALUE PROBLEMS IN THE ANALYSIS OF CRACKS IN BRITTLE MATERIALS

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Abstract. In order to analyze the stress distribution at the top of a polyhedral corner or at a crack tip, one typically expands the displacement vector \( U \) in terms of the form \( kr^\alpha u \), where \( r \) is the distance to the tip, \( u \) is a function of the spherical angles and \( k \) is the stress intensity coefficient. The exponent \( \alpha \) and the vector function \( u \) do not depend on the loading but only on the geometry and the material parameters. They form an eigenpair of a quadratic operator eigenvalue problem.

Since the eigenvalue problem can in general not be solved analytically, the finite element method is used to solve it approximately. Locally graded meshes were used to treat the corner singularities in the eigenfunctions. By the finite element approximation, the operator eigenvalue problem is transformed into a quadratic matrix eigenvalue problem with a special structure. It can be reformulated as an eigenvalue problem of a Hamiltonian, a skew-Hamiltonian or a symplectic matrix. We shortly introduce methods which exploit the properties of these matrices and show results of numerical experiments.
1 INTRODUCTION

The study of cracks or, more general, the stress distribution in the vicinity of polyhedral corners or crack tips can be investigated within the linear elasticity framework, as long as the material is brittle, see for example [15, 16, 19]. We give a short two-dimensional example in Section 2; the three-dimensional application is still work in progress. The stress field is derived from the displacement field which can be represented by a regular part and several singular terms of the form \( kr^\alpha u(\varphi, \theta) \) where \( (r, \varphi, \theta) \) are spherical coordinates centered in the point of interest, \( k \) is called stress intensity factor, and \( \alpha \) is the characteristic singular exponent with the associated mode \( u \). These terms are singular when \( \text{Re} \alpha < 1 \) and \( \text{Re} \alpha \neq 0 \).

Mathematically, the pair \((\alpha, u)\) is an eigenpair of a quadratic operator pencil [14, 16]

\[
\alpha(\alpha+1)m(u, v) - (\alpha+1)d(u, v) + \alpha d(v, u) + \frac{1}{4}m(u, v) + \frac{1}{2}d(u, v) + \frac{1}{2}d(v, u) - k(u, v) = 0 \quad (1)
\]

with certain Hermitian sesquilinear forms \( m(\cdot, \cdot) \) and \( k(\cdot, \cdot) \), and a non-Hermitian sesquilinear form \( d(\cdot, \cdot) \), see [3] for details. The eigenvalues of Problem (1) are distributed symmetrically with respect to the line \( \text{Re} \alpha = -1/2 \). In order to shift the spectrum such that the symmetry axis coincides with the imaginary axis \( \text{Re} \alpha = 0 \), we introduce the parameter \( \lambda = \alpha + 1/2 \). Then Problem (1) is equivalent to

\[
\lambda^2m(u, v) + \lambda g(u, v) = k(u, v) \quad (2)
\]

with the skew-Hermitian sesquilinear form \( g(u, v) = d(v, u) - d(u, v) \).

In general, this eigenvalue problem cannot be solved analytically; thus the finite element method is used to solve it approximately. This method is flexible enough, such that also anisotropic or composite materials can be treated. The peculiarity that has to be observed is that the sesquilinear forms are defined on a domain which is part of the unit sphere. Since we introduced spherical coordinates we have to take into account that the transformation \( x_1(\varphi, \theta), x_2(\varphi, \theta), x_3(\varphi, \theta) \), is not a homeomorphism. Optimal approximation results for an \( h \)-version finite element method were derived in [3] on the basis of new local interpolation error estimates. The approximation results are based on the use of graded meshes since the eigenfunctions have singularities themselves. For a further discussion of the discretization of problems on spherical domains, see also [2].

The discretized problem can be written in matrix form

\[
\lambda^2M u + \lambda G u = K u.
\]

The coefficient matrices are large, real and sparse; \( M \) and \( K \) are symmetric, positive definite, \( G \) is skew-symmetric. Typically the coefficients depend on a set of material or geometry parameters. The discretized problem can be reformulated as an eigenvalue problem of a Hamiltonian, a skew-Hamiltonian or a symplectic matrix, see Section 3. In [1], we suggest to solve this problem with the Skew-Hamiltonian Implicitly Restarted
Arnoldi (SHIRA) method, see [23, 12], but we have experience also with the Hamiltonian Implicitly Restarted Lanczos process (HIRL), see [6, 26], and the Implicitly Restarted Symplectic Lanczos process (IRSL), see [26, 5, 11]. In the main section of this paper, Section 3, these methods are shortly introduced and compared with respect to their efficiency.

For further application of quadratic eigenvalue problems we refer to [21, 22, 23] and the references cited therein.

2 PREDICTION OF CRACK FRONTS

Let us consider a brittle, isotropic with a straight crack and apply a pure mode II shear force, see the illustration in Figure 1. The crack kinks under a well-defined angle which can be computed by analytic means. The direction of the crack is assumed to be the one where the ortho-radial component of the stress (hoop stress) attains its maximum. It means that the particles of material undergo the maximum tension in this direction tending to open a new crack starting from the tip of the preexisting one.

The leading term in an expansion of the displacement is characterized by the function

\[ U(r, \varphi) = kr^{1/2} \frac{1}{\lambda + \mu} \left[ (9\mu + 5\lambda) \cos \frac{\varphi}{2} - (\lambda + \mu) \cos \frac{3\varphi}{2} \right] \]

\[ \left( 3\mu - \lambda \right) \sin \frac{\varphi}{2} - \left( \lambda + \mu \right) \sin \frac{3\varphi}{2} \]

with polar coordinates \((r, \varphi)\) centered in the crack tip, compare [25]. This term leads to the hoop stress

\[ \sigma_{\varphi\varphi} = kr^{-1/2} 3\mu \left( \cos \frac{\varphi}{2} - \cos \frac{3\varphi}{2} \right). \]

For fixed \(r\) this function can be plotted, see Figure 2. The maximum value is taken for

\[ \varphi_0 = \arg \max_{\varphi} \sigma_{\varphi\varphi} = 2 \arccos \frac{1}{\sqrt{3}} = 109.47^\circ, \]

which agrees well with practical experience, see also [15, page 25].
The situation is more complex in the three-dimensional case and not yet fully investigated. Leguillon [17] is convinced that a precise knowledge of the 3D singular fields in corners gives information of the very beginning stage of failure in these corners. The initial crack shape is complex but this geometry can be predicted by the singular stress fields prior to failure. Assuming that one can determine the plane undergoing the maximum tension near the singular point, we can plot isolines of the tension component of the stress field within this plane; they are homothetic to each other and define increasing surfaces. Finally, the energy criterion fixes the surface leading to a complete prediction of failure initiation [18].

3 THE QUADRATIC ALGEBRAIC EIGENVALUE PROBLEM

3.1 A special linearization

The finite element discretization of Problem (2) leads to a finite dimensional quadratic eigenvalue problem which reads in matrix notation: Find $\lambda \in \mathbb{C}$, $u \in \mathbb{C}^n$ such that

$$(\lambda^2 M + \lambda G)u = Ku,$$

(3)

where $M, G, K$ are large, real and sparse finite element matrices, $M$ and $K$ are symmetric, positive definite, and $G$ is skew-symmetric.

This problem has a special eigenvalue structure, the so called Hamiltonian eigenvalue symmetry, this means that the spectrum is symmetric with respect to the real and imaginary axes. With

$$J = \begin{bmatrix} O & I \\ -I & O \end{bmatrix}$$

a real $2 \times 2$ block matrix is called Hamiltonian if $JA$ is symmetric; it is called skew-Hamiltonian if $JA$ is skew-symmetric, and symplectic if $A^TJA = J$.

There are several approaches to solve quadratic eigenvalue problems of type (3). A summary of possible linearizations is given in [22]. New research by Zhaojun Bai [4] also suggests to apply a “quadratic Arnoldi”, that is to solve the quadratic eigenvalue problem directly.
We concentrate on a special type of linearization. With
\[ \mathbf{v} = \lambda \mathbf{M} \mathbf{u} + \frac{1}{2} \mathbf{G} \mathbf{u} \]

Problem (3) is equivalent to the 2n-dimensional standard eigenvalue problem: Find \( \lambda \in \mathbb{C} \), \( \mathbf{u}, \mathbf{v} \in \mathbb{C}^n \) such that
\[ H \begin{bmatrix} \mathbf{v} \\ \mathbf{u} \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{v} \\ \mathbf{u} \end{bmatrix} \]

with the Hamiltonian matrix
\[ H = \begin{bmatrix} \mathbf{I} & -\frac{1}{2} \mathbf{G} \\ \mathbf{O} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{O} & \mathbf{K} \\ \mathbf{M}^{-1} & \mathbf{O} \end{bmatrix} \begin{bmatrix} \mathbf{I} & -\frac{1}{2} \mathbf{G} \\ \mathbf{O} & \mathbf{I} \end{bmatrix}. \]

In order to find the eigenvalues of \( H \) nearest a given shift \( \tau \in \mathbb{C} \), we employ the shift-and-invert theory. Since \( (H - \tau \mathbf{I})^{-1} \) has, in general, no special structure, one usually also considers the shift values \( \bar{\tau}, -\tau, \) and \( -\bar{\tau} \). In fact, one can check that

- \( C_2 = (H - \tau \mathbf{I})^{-1}(H + \tau \mathbf{I})^{-1} \) is real and skew-Hamiltonian if \( \tau \) is real or purely imaginary;
- \( C_4 = (H - \tau \mathbf{I})^{-1}(H + \tau \mathbf{I})^{-1}(H - \tau \mathbf{I})^{-1}(H + \tau \mathbf{I})^{-1} \) is real and skew-Hamiltonian for any complex value \( \tau \);
- \( N_0 = H^{-1}, N_2 = H^{-1}C_2, N_4 = H^{-1}C_4 \) are Hamiltonian;
- \( S_2 = (H - \tau \mathbf{I})^{-1}(H + \tau \mathbf{I}) \) is real and symplectic if \( \tau \) is real.

With the help of structured Arnoldi or Lanczos processes, the eigenvalue problems for \( C_i, N_i \), or \( S_2 \) can be solved. The eigenvalues of \( H \) and hence those of Problem (3) can then be extracted from the corresponding results.

For example, consider the skew-Hamiltonian case. In [1] it was suggested to apply the skew-Hamiltonian implicitly restarted Arnoldi process (SHIRA), see [23], to compute the eigenvalues of \( C_2 \) or \( C_4 \). Our experience showed that it is, in general, sufficient to use real shifts, that is to compute the eigenvalues of \( C_2 \). The corresponding eigenvalues of \( H \) are then obtained from the relation \( \lambda_C = (\lambda_H - \tau)^{-1}(\lambda_H + \tau)^{-1} \), this means
\[ \lambda_C^2 = \frac{1}{\lambda_C} + \tau^2. \]

In the Hamiltonian or symplectic cases, structured Lanczos processes, as described in [5, 6, 10, 11, 26], can be applied: the Hamiltonian implicitly restarted Lanczos process (HIRL) or the implicitly restarted symplectic Lanczos process (IRSL). These algorithms allow a cheap extraction of eigenvectors for Problem (3): a simple matrix vector multiplication is sufficient.
The extraction of eigenvectors in the SHIRA process is less efficient. In general, a few steps of time-consuming inverse iteration are necessary. A cheaper algorithm for the extraction of the eigenvectors is described in [12], but still operations like a computation of a Schur decomposition and a square root of a positive definite matrix are used. Therefore this algorithm cannot compete with HIRL or IRSL concerning the eigenvector computation.

3.2 Implementation

With our local program package CoCoS, we are able to compute corner singularities for several domains, for example for the Fichera corner. The singular terms make use of the solutions of a quadratic eigenvalue problem as described in the previous sections. After defining a refinement level for the finite element mesh, the corresponding matrices $M, G, K$ are assembled and the appropriate eigenvalues of Problem (3) are computed. We integrated each of the algorithms SHIRA, HIRL and IRSL in CoCoS and compared their efficiency in a series of tests. The source of CoCoS is partly written in C, but mainly in Fortran. We integrated local libraries of the software developed at Technische Universität Chemnitz, Sonderforschungsbereich 393 (see also [24]).

Since it is necessary to solve a linear system of equations in each iteration, software packages are useful which provide a sparse matrix decomposition. In the SHIRA process, the system matrix is the operator $Q(\tau) = \tau^2 M + \tau G - K$. This operator is not symmetric, hence a sparse LU decomposition is needed. It turned out that the shifted HIRL process is not too efficient, since two decompositions (of the matrices $M$ and $K$) are necessary. For the unshifted HIRL process, one Cholesky decomposition of the matrix $K$ is sufficient. In the IRSL process it is inevitable to perform two decompositions: Cholesky for the matrix $K$ and LU for the operator $Q(\tau) = \tau^2 M + \tau G - K$.

3.3 Software packages providing sparse Cholesky and LU decompositions

In the internet, many software packages are provided that perform matrix decompositions. Table 1 gives a few examples. For our implementation we preferred packages which

<table>
<thead>
<tr>
<th>LU decomposition:</th>
<th>SUPERLU, UMFPack</th>
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<tr>
<td>Cholesky decomposition:</td>
<td>DSCPack, HSL, MUMPS, SPOOLES, TAUCS</td>
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Table 1: A choice of software packages to perform LU or Cholesky decompositions

are freely available and written in C or Fortran. Among others, we tested SUPERLU, UMFPACK, MA27 (HSL library), and TAUCS, see also the manuals [8, 7, 9, 13].

Although the package MA27 performs very well with respect to the average time taken for the solution of one linear system of equations, its factorization time is rather high. This can only be compensated if many systems of equations have to be solved, for instance, if many eigenvalues (probably more than 50) are to be computed. In our practical applications, however, the number of eigenvalues of interest is small, about 3 to 10, pos-
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Problem size n

Time for factorization in s

FICHERA corner

FICHERA

hirl: TAUCS

hirsl: TAUCS/SUPERLU

shira: SUPERLU

Figure 3: Factorization times for the Fic hera corner plotted against matrix dimensions

sibly 15. The amount of storage requested by the package UMFPACK is relatively high. Its factorization and solve times are only average. The packages SUPERLU and TAUCS performed best among the tested packages. In the following section, we present the numerical results, obtained from the comparison of the three eigenvalue algorithms using SUPERLU and UMFPACK for the matrix decompositions.

The package SUPERLU is written in C. It performs a sparse LU decomposition and uses a supernodal approach to sparse partial pivoting. We use SUPERLU for the LU decomposition of the operator \( Q(\tau) = \tau^2 M + \tau G - K \) in the algorithms SHIRA and IRSL.

The package TAUCS is also written in C and performs a multifrontal supernodal Cholesky factorization. We use TAUCS for the Cholesky decomposition of the matrix \( K \) in the algorithms HIRL and IRSL.

3.4 Numerical results

We run the program CoCoS with the Fichera corner as computational domain choosing different refinement levels. Figure 3 displays the times taken for factorization of \( Q(\tau) \) or \( K \) against the problems size. One can see that the time for a Cholesky factorization with TAUCS is much smaller than the time for an LU factorization with SuperLU. Since IRSL needs both a Cholesky and an LU factorization, the time plotted in Figure 3 corresponds to the sum of them. Figure 4 shows that the average time for one solve is comparable for TAUCS and SUPERLU. In order to compare the algorithms SHIRA, HIRL and IRSL,
we have also to consider the number of linear systems which had to be solved. Figure 5 shows that SHIRA beats the other two algorithms in this respect such that, despite of the larger factorization time, SHIRA needs about the same total time as HIRL, see Figure 6. The total times in this figure contain the times needed for the assembly of $M$, $G$ and $K$ and the computation of the eigenvalues, respectively. All tests were run on an Intel Pentium 4 CPU with 1.60 GHz, 1 GB main memory and 256 kB cache.

Due to the large number of linear systems of equations that have to be solved in the IRSL process, we conclude that the symplectic version is not suitable for our purposes. It should be employed in eigenvalue problems where the symplectic structure is not purely artificial. Because of the Hamiltonian structure of our eigenvalue problem, the HIRL and SHIRA processes perform better. The big advantage of the HIRL process is the extremely cheap computation of eigenvectors.

For the Arnoldi process, an adapted version of the software package ARPACK [20] (written in Fortran) was integrated. The stopping criteria used therein are more vigilant than those used in the HIRL process. This is why the number of solves and thus the total computation time for SHIRA beats HIRL. In matlab implementations, however, D. Watkins found that HIRL is much faster than SHIRA. One reason is that there other LU and Cholesky factorization methods are used, provided by the matlab commands lu and chol, such that a Cholesky decomposition is faster in any case. Another reason is that the vigilant stopping criteria implemented in the ARPACK package are not used in the matlab code, such that the number of solves for the SHIRA process is comparable to the

Figure 4: Average times for one solve for the Fichera corner plotted against matrix dimensions

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Figure 5: Number of solves for the Fichera corner plotted against matrix dimensions

Figure 6: Total times for the solution of the eigenvalue problem for the Fichera corner plotted against matrix dimensions
one for the \textit{HIRL} process.

To summarize, we can state that both \textit{SHIRA} and \textit{HIRL} perform well in combination with the solvers \textsc{SUPERLU} and \textsc{TAUCS} whereas the \textit{IRSL} process seems to be not suited for the Hamiltonian eigenvalue problem (3). We draw the conclusion that, if shifts are desired, the \textit{SHIRA} process should be preferred. For the extraction of eigenvectors, however, it is more efficient to apply the \textit{HIRL} process. Furthermore one has to take into account that, although the \textit{HIRL} process performs comparatively well, its parameters have to be tuned more carefully in order to obtain good results in computation time.

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