

Bounds on the eigenvalue range and on the Field of Values of non-Hermitian and indefinite finite element matrices

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Abstract

In the early seventies Fried formulated bounds on the spectrum of assembled Hermitian Positive (semi-) Definite finite element matrices using the extreme eigenvalues of the element matrices. In this paper we will generalise these results by presenting bounds on the Field of Values, the numerical radius and on the spectrum of general matrices, for both the standard and the generalised problem. The bounds are cheap to compute, involving operations with element matrices only. We illustrate our results with an example from acoustics involving a complex, non-Hermitian matrix. As an application, we show how our estimates can be used to derive an upper bound on the number of iterations needed to achieve a given residual reduction in the GMRES-algorithm for solving linear systems.

Keywords: Eigenvalue bounds, Field of Values, Numerical Radius, Non-Hermitian Finite Element Matrices, Iterative Methods

1 Introduction

For many problems it is sufficient to know a bound on the spectrum of a matrix, without the need to know the actual eigenvalues, which may be expensive to compute. Examples are the determination of stable time steps for explicit time integration and of the iteration parameters for Chebychev-type methods. Several easily computable bounds on the spectrum of a matrix exist, among which

the classical Gerschgorin disks are probably the best known. For a comprehensive overview of these and related bounds we refer to [14].

In the Finite Element method the discrete approximation to a partial differential operator is assembled from element matrices. Each element matrix corresponds to a local discretisation of the continuous operator. Element matrices are small in size and therefore easy to manipulate, whereas the global matrix that results from the assembly process can be very large, in which case operations with this matrix are expensive. It is therefore an attractive idea to relate the characteristics of the global matrix to the properties of the element matrices.

In the early seventies Fried studied in a number of papers [2, 3] the question of how the eigenvalues of the element matrices are related to the spectrum of the global matrix. He derived simple bounds on the spectrum of the standard and generalised Positive Definite eigenproblem that can be computed from element eigenvalues only. Since the size of an element matrix is small the calculation of the element eigenvalues, and hence of the bounds, is a cheap operation.

His results proved to be useful tools for the analysis of the preconditioned Conjugate Gradient method, as exemplified by Wathen in [15, 16]. In [15], Wathen shows the efficiency of a simple diagonal preconditioner for mass-matrix equations, and in [16] he analyses the element-by-element preconditioner introduced by Hughes et al. [7] for a family of Poisson problems. In [13], Van Gijzen generalises these results for nonsymmetric element-by-element preconditioners in combination with GMRES. In his analysis he determines bounds on the condition number of the preconditioned matrix in terms of the norms of element matrices. One of the drawbacks of this approach is that the convergence of GMRES is not well described by the condition number of the matrix alone.

A number of publications use the Field of Values of the (preconditioned) matrix to describe the convergence of GMRES, or more precisely, to give an upperbound on the reduction of the GMRES-residual norm [1, 4, 10, 12]. The Field of Values is a powerful tool to study the characteristics of a (nonnormal) matrix and is for this reason a suitable means to study the convergence of GMRES for nonsymmetric matrices.

In this paper we generalise the results of Fried by providing bounds for the Field of Values and the numerical radius of a general matrix. Moreover, since the extension for matrix-pairs where one of the matrices is Hermitian Positive Definite is both natural and straightforward, we also provide bounds for this case. To illustrate our bounds, we compare them with the actual Field of Values and numerical radius for an example from acoustics.

In the last part of the paper we combine our bounds with an upperbound on the GMRES-residual norm based on the Field of Values. This combination allows us to make a detailed analysis of a symmetric preconditioner for a rather general family of convection-diffusion-reaction problems. Our results are surprisingly strong: we are able to derive an easily computable upperbound on the number of GMRES-iterations that is needed to obtain a given tolerance on the norm of the residual. Moreover, we are able to show for a wide range of parameters that this upperbound is mesh independent.

The structure of this paper is as follows.

- Section 2 provides some (well known) background theory about assembly of Finite Element matrices and about the Field of Values and numerical radius of a matrix.

- Section 3 recalls the bounds of Fried on the spectrum of symmetric Positive Definite matrices and generalises them to bounds on the Field of Values and numerical range of general matrices and matrix-pairs in which one of the matrices is Hermitian Positive Definite.
- Section 4 establishes the quality of the bounds for an example from acoustics involving a complex, non-Hermitian matrix.
- Section 5 uses the bounds on the Field of Values and on the numerical radius to analyse a symmetric preconditioner for a family of convection-diffusion-reaction problems.

Notation

Bold capital characters denote matrices and bold small characters vectors. The superscript T denotes transposition and the superscript H conjugation and transposition. Throughout this paper $\lambda^{\mathbf{A}}$ indicates an eigenvalue of the standard eigenproblem $\mathbf{Ax} = \lambda\mathbf{x}$, and $\lambda^{\mathbf{A},\mathbf{B}}$ indicates an eigenvalue of the generalised eigenproblem $\mathbf{Ax} = \lambda\mathbf{Bx}$. The superscript e is used for element matrices and vectors. As usual, \mathbf{I} is the identity matrix and \mathbf{O} the zero-matrix.

2 Preliminaries

In this Section we recall some well known relations that we will use in the remainder of this paper.

2.1 Assembly of Finite Element matrices

In the Finite Element Method for discretising PDE's the computational domain is subdivided into subdomains, called elements. In each element a set of nodal points is defined, usually in the corners or the midpoints of the elements. Hence, different elements may have nodes in common. A numerical solution is constructed as a linear combination of a set of basis functions. A common choice for the basis functions, also called interpolation or shape functions is the set of piecewise polynomial functions that are one at one nodal point and zero at the others. In order to discretise the PDE plus boundary conditions a (Petrov-)Galerkin approach is used. This procedure yields for each element a so called element matrix that is in element-node ordering small (of order n^e , with n^e the number of variables associated with element e) and dense. Let \mathbf{N}^e be an $n^e \times n$ boolean matrix that maps the global vector of variables into the vector of variables associated with element e . Then the global matrix \mathbf{A} and global vector \mathbf{x} are

$$\mathbf{A} = \sum_{e=1}^{n_e} \mathbf{N}^{eT} \mathbf{A}^e \mathbf{N}^e, \quad \mathbf{x} = \sum_{e=1}^{n_e} \mathbf{N}^{eT} \mathbf{x}^e, \quad (2.1)$$

in which n_e is the number of elements. The above process is called the assembly of the global matrix, respectively global vector. Henceforth we will make frequent use of the above equations, and in particular of

$$\mathbf{x}^H \mathbf{Ax} = \mathbf{x}^H \left(\sum_{e=1}^{n_e} \mathbf{N}^{eT} \mathbf{A}^e \mathbf{N}^e \right) \mathbf{x} = \sum_{e=1}^{n_e} \mathbf{x}^{eH} \mathbf{A}^e \mathbf{x}^e, \quad (2.2)$$

which follows directly from (2.1).

2.2 The Field of Values and numerical radius of a matrix

Let \mathbf{A} be a general square matrix of order n . Then the Field of Values of \mathbf{A} is defined as:

$$FOV(\mathbf{A}) = \left\{ \frac{\mathbf{x}^H \mathbf{A} \mathbf{x}}{\mathbf{x}^H \mathbf{x}}, \quad \mathbf{x} \in \mathbb{C}^n, \mathbf{x} \neq 0 \right\}. \quad (2.3)$$

Like the spectrum (or the set of eigenvalues) $\sigma(\mathbf{A})$ of a matrix \mathbf{A} , the Field of Values $FOV(\mathbf{A})$ can be used to analyse the matrix, and in the case where \mathbf{A} is nonnormal it can give information that the spectrum alone can not give. For a comprehensive overview of the theory of the Field of Values we refer to [6].

The spectrum of a matrix is contained in its Field of Values, which can be seen from the definition 2.3 and by taking \mathbf{x} to be an eigenvector of \mathbf{A} . Hence, a bound on the Field of Values of a matrix is also a bound on its spectrum.

For ease of notation we introduce the following generalised Field of Values for the matrix pair \mathbf{A}, \mathbf{B} , with \mathbf{B} nonsingular:

$$FOV(\mathbf{A}, \mathbf{B}) = \left\{ \frac{\mathbf{x}^H \mathbf{A} \mathbf{x}}{\mathbf{x}^H \mathbf{B} \mathbf{x}}, \quad \mathbf{x} \in \mathbb{C}^n, \mathbf{x} \neq 0 \right\}. \quad (2.4)$$

The set of eigenvalues $\lambda^{\mathbf{A}, \mathbf{B}}$ of the generalised problem is contained in the Field of Values $FOV(\mathbf{A}, \mathbf{B})$, which follows by taking \mathbf{x} to be an eigenvector of $\mathbf{A} \mathbf{x} = \lambda \mathbf{B} \mathbf{x}$. Hence, a bound on the generalised Field of Values of the matrix pair \mathbf{A}, \mathbf{B} is also a bound on the spectrum of the generalised problem $\mathbf{A} \mathbf{x} = \lambda \mathbf{B} \mathbf{x}$.

Let \mathbf{B} be Hermitian Positive Definite, i.e., there exists a matrix \mathbf{C} such that $\mathbf{B} = \mathbf{C} \mathbf{C}^H$. Then

$$FOV(\mathbf{A}, \mathbf{B}) = FOV(\mathbf{C}^{-1} \mathbf{A} \mathbf{C}^{-H}). \quad (2.5)$$

This follows by making the change of variables $\mathbf{y} = \mathbf{C}^H \mathbf{x}$.

Let \mathbf{A} be Hermitian and \mathbf{B} Hermitian Positive Definite. Then the (generalised) Rayleigh quotient $R^{\mathbf{A}, \mathbf{B}}$ is defined as

$$R^{\mathbf{A}, \mathbf{B}}(\mathbf{x}) = \frac{\mathbf{x}^H \mathbf{A} \mathbf{x}}{\mathbf{x}^H \mathbf{B} \mathbf{x}}. \quad (2.6)$$

A well-known property of the Rayleigh quotient is that

$$\lambda_{min}^{\mathbf{A}, \mathbf{B}} \leq R^{\mathbf{A}, \mathbf{B}}(\mathbf{x}) \leq \lambda_{max}^{\mathbf{A}, \mathbf{B}} \quad (2.7)$$

and consequently

$$\lambda_{min}^{\mathbf{A}, \mathbf{B}} \leq FOV(\mathbf{A}, \mathbf{B}) \leq \lambda_{max}^{\mathbf{A}, \mathbf{B}} \quad (2.8)$$

if \mathbf{A} is Hermitian and \mathbf{B} Hermitian Positive Definite.

The Numerical Radius of the matrix \mathbf{A} is defined as

$$r(\mathbf{A}) = \max \{ |z| : z \in FOV(\mathbf{A}) \}.$$

Since the eigenvalues are contained in the Field of Values we have for the spectral radius $\rho(\mathbf{A}) = |\lambda^{\mathbf{A}}|_{max}$ that

$$\rho(\mathbf{A}) \leq r(\mathbf{A}).$$

As before, we introduce for ease of notation the generalised numerical radius for the matrix pair \mathbf{A}, \mathbf{B} as

$$r(\mathbf{A}, \mathbf{B}) = \max \{|z| : z \in FOV(\mathbf{A}, \mathbf{B})\}.$$

3 Bounds on the spectrum, on the Field of Values, and on the Numerical Radius

3.1 Eigenvalue estimates for the Hermitian eigenvalue problem

It is a natural question to ask how the eigenvalues of the element matrices are related to the eigenvalues of the global matrix. This question has been studied by Fried for the symmetric semi-Positive Definite eigenproblem, and for the generalised symmetric eigenproblem with at least one of the matrices Positive Definite [2, 3]. Below we summarise his main results and generalise them for indefinite Hermitian matrices.

Theorem 3.1 *Let $\mathbf{A}^e, e = 1, \dots, n_e$ be Hermitian and $\mathbf{B}^e, e = 1, \dots, n_e$ be Hermitian Positive Definite element matrices and let \mathbf{A} and \mathbf{B} be the global matrices that are assembled from these element matrices. Let ω be the smallest eigenvalue of all element matrix pairs $\mathbf{A}^e, \mathbf{B}^e$, i.e.*

$$\omega = \min_e \lambda_{\min}^{\mathbf{A}^e, \mathbf{B}^e},$$

and let Ω be the largest eigenvalue, i.e.

$$\Omega = \max_e \lambda_{\max}^{\mathbf{A}^e, \mathbf{B}^e}.$$

Then the following bound holds for the eigenvalues $\lambda^{\mathbf{A}, \mathbf{B}}$ of the global eigenproblem $\mathbf{A}\mathbf{x} = \lambda\mathbf{B}\mathbf{x}$:

$$\omega \leq \lambda^{\mathbf{A}, \mathbf{B}} \leq \Omega.$$

Proof: By the Rayleigh quotient (2.7) for the element matrices we have

$$\omega \leq \frac{\mathbf{x}^{eH} \mathbf{A}^e \mathbf{x}^e}{\mathbf{x}^{eH} \mathbf{B}^e \mathbf{x}^e} \leq \Omega \quad \forall e.$$

Multiplying with $\mathbf{x}^{eH} \mathbf{B}^e \mathbf{x}^e$ yields

$$\omega \mathbf{x}^{eH} \mathbf{B}^e \mathbf{x}^e \leq \mathbf{x}^{eH} \mathbf{A}^e \mathbf{x}^e \leq \Omega \mathbf{x}^{eH} \mathbf{B}^e \mathbf{x}^e \quad \forall e.$$

Applying the assembly operation (2.2) gives

$$\omega \mathbf{x}^H \mathbf{B} \mathbf{x} \leq \mathbf{x}^H \mathbf{A} \mathbf{x} \leq \Omega \mathbf{x}^H \mathbf{B} \mathbf{x}.$$

and hence

$$\omega \leq \frac{\mathbf{x}^H \mathbf{A} \mathbf{x}}{\mathbf{x}^H \mathbf{B} \mathbf{x}} \leq \Omega.$$

By the Rayleigh quotient (2.7) for the global matrices we get the desired result. \triangle

The above results hold for the generalised problem, which is the most natural case in the framework of the Finite Element Method. Bounds for the standard problem can be derived by making use of the following inequality

$$\mathbf{x}^H \mathbf{x} \leq \sum_{e=1}^{n_e} \mathbf{x}^{eH} \mathbf{x}^e \leq \mathbf{x}^H \mathbf{x} \eta_{max}. \quad (3.1)$$

Here η_{max} is the maximal number of elements meeting in a nodal point. The following theorem gives the bounds for the standard case.

Theorem 3.2 *Let $\mathbf{A}^e, e = 1, \dots, n_e$ be Hermitian element matrices and let \mathbf{A} be the global matrix that is assembled from these element matrices. Let ω be the smallest eigenvalue of all element matrices \mathbf{A}^e , i.e.*

$$\omega = \min_e \lambda_{min}^{\mathbf{A}^e}$$

and let Ω be the largest eigenvalue, i.e.

$$\Omega = \max_e \lambda_{max}^{\mathbf{A}^e} .$$

Then the following bound holds for the eigenvalues $\lambda^{\mathbf{A}}$ of the global eigenproblem $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$:

$$\begin{aligned} \omega &\leq \lambda^{\mathbf{A}} \leq \eta_{max} \Omega && \text{for } \omega, \Omega \geq 0, \\ \eta_{max} \omega &\leq \lambda^{\mathbf{A}} \leq \eta_{max} \Omega && \text{for } \omega < 0, \Omega \geq 0, \\ \eta_{max} \omega &\leq \lambda^{\mathbf{A}} \leq \Omega && \text{for } \omega, \Omega < 0. \end{aligned} \quad (3.2)$$

Proof: By the Rayleigh quotient (2.7) for the element matrices we have

$$\omega \leq \frac{\mathbf{x}^{eH} \mathbf{A}^e \mathbf{x}^e}{\mathbf{x}^{eH} \mathbf{x}^e} \leq \Omega \quad \forall e.$$

Multiplying with $\mathbf{x}^{eH} \mathbf{x}^e$ and applying the assembly operation (2.2) gives

$$\omega \sum_{e=1}^{n_e} \mathbf{x}^{eH} \mathbf{x}^e \leq \mathbf{x}^H \mathbf{A} \mathbf{x} \leq \Omega \sum_{e=1}^{n_e} \mathbf{x}^{eH} \mathbf{x}^e .$$

The result follows from (3.1) and by using property (2.7) of the Rayleigh quotient. \triangle

3.2 Bounds on the Field of Values of non-Hermitian matrices

We will use the results of the previous Section to derive bounds for the Field of Values and the spectrum of non-Hermitian matrices. In order to derive these bounds we use the fact that any matrix can be split into two Hermitian matrices:

$$\mathbf{A} = \frac{1}{2}(\mathbf{A} + \mathbf{A}^H) + i \frac{1}{2i}(\mathbf{A} - \mathbf{A}^H) = \Re(\mathbf{A}) + i\Im(\mathbf{A}) \quad (3.3)$$

where

$$\Re(\mathbf{A}) = \frac{1}{2}(\mathbf{A} + \mathbf{A}^H) \quad \text{and} \quad \Im(\mathbf{A}) = \frac{1}{2i}(\mathbf{A} - \mathbf{A}^H). \quad (3.4)$$

We therefore have for the Field of Values of \mathbf{A}

$$FOV(\mathbf{A}) = FOV(\Re(\mathbf{A}) + i\Im(\mathbf{A})). \quad (3.5)$$

Since the Field of Values of a Hermitian matrix is real we have the following projection property for the real and imaginary parts of the Field of Values of a non-Hermitian matrix (see [6], property 1.2.5):

$$Re(FOV(\mathbf{A})) = FOV(\Re(\mathbf{A})) \quad \text{and} \quad Im(FOV(\mathbf{A})) = FOV(\Im(\mathbf{A})). \quad (3.6)$$

Hence, bounds on $FOV(\Re(\mathbf{A}))$ and on $FOV(\Im(\mathbf{A}))$ amount to a bounding box in the complex plane for $FOV(\mathbf{A})$. To derive bounds on $FOV(\Re(\mathbf{A}))$ and $FOV(\Im(\mathbf{A}))$ we can apply Theorem 3.2. The result is summarised by:

Theorem 3.3 *Let $\mathbf{A}^e, e = 1, \dots, n_e$ be (possibly non-Hermitian) element matrices and let \mathbf{A} be the global matrix that is assembled from these element matrices. Let ω_R (resp. ω_I) be the smallest eigenvalues of all element matrices $\Re(\mathbf{A}^e)$ (resp. $\Im(\mathbf{A}^e)$), i.e.,*

$$\omega_R = \min_e \lambda_{min}^{\Re(\mathbf{A}^e)} \quad \omega_I = \min_e \lambda_{min}^{\Im(\mathbf{A}^e)},$$

and let Ω_R (resp. Ω_I) be the largest eigenvalue, i.e.,

$$\Omega_R = \max_e \lambda_{max}^{\Re(\mathbf{A}^e)} \quad \Omega_I = \max_e \lambda_{max}^{\Im(\mathbf{A}^e)}.$$

Then the following bounds hold for $FOV(\mathbf{A})$:

$$\begin{aligned} \omega_R &\leq Re(FOV(\mathbf{A})) \leq \eta_{max} \Omega_R \quad \text{for } \omega_R, \Omega_R \geq 0, \\ \eta_{max} \omega_R &\leq Re(FOV(\mathbf{A})) \leq \eta_{max} \Omega_R \quad \text{for } \omega_R < 0, \Omega_R \geq 0, \\ \eta_{max} \omega_R &\leq Re(FOV(\mathbf{A})) \leq \Omega_R \quad \text{for } \omega_R, \Omega_R < 0, \end{aligned} \quad (3.7)$$

$$\begin{aligned} \omega_I &\leq Im(FOV(\mathbf{A})) \leq \eta_{max} \Omega_I \quad \text{for } \omega_I, \Omega_I \geq 0, \\ \eta_{max} \omega_I &\leq Im(FOV(\mathbf{A})) \leq \eta_{max} \Omega_I \quad \text{for } \omega_I < 0, \Omega_I \geq 0, \\ \eta_{max} \omega_I &\leq Im(FOV(\mathbf{A})) \leq \Omega_I \quad \text{for } \omega_I, \Omega_I < 0. \end{aligned} \quad (3.8)$$

Proof: The proof follows from the discussion above. The (Hermitian) matrices $\Re(\mathbf{A})$ and $\Im(\mathbf{A})$ are assembled from the (Hermitian) element matrices $\Re(\mathbf{A}^e), e = 1, \dots, n_e$ and $\Im(\mathbf{A}^e), e = 1, \dots, n_e$. Application of Theorem 3.2 to the matrices $\Re(\mathbf{A})$ and $\Im(\mathbf{A})$ yields the result. \triangle

Remark The above bounds are formulated in terms of $Re(FOV(\mathbf{A}))$ and $Im(FOV(\mathbf{A}))$. Application of (2.8) yields bounds on the eigenvalues of $\Re(\mathbf{A})$ and $\Im(\mathbf{A})$.

The generalised case can be treated analogously if \mathbf{B} is Hermitian Positive Definite. In this case we have for the generalised Field of Values defined by (2.4)

$$FOV(\mathbf{A}, \mathbf{B}) = FOV(\Re(\mathbf{A}) + i\Im(\mathbf{A}), \mathbf{B}). \quad (3.9)$$

Since both $FOV(\Re(\mathbf{A}), \mathbf{B})$ and $FOV(\Im(\mathbf{A}), \mathbf{B})$ are real we have the following projection property (cf. (3.6)):

$$Re(FOV(\mathbf{A}, \mathbf{B})) = FOV(\Re(\mathbf{A}), \mathbf{B}), \quad (3.10)$$

$$Im(FOV(\mathbf{A}, \mathbf{B})) = FOV(\Im(\mathbf{A}), \mathbf{B}).$$

Using the same arguments as above and application of Theorem 3.1 yields the following Theorem:

Theorem 3.4 *Let $\mathbf{A}^e, e = 1, \dots, n_e$ be (possibly non-Hermitian) element matrices and $\mathbf{B}^e, e = 1, \dots, n_e$ be Hermitian Positive Definite element matrices and let \mathbf{A} and \mathbf{B} be the global matrices that are assembled from these element matrices. Let ω_R (resp. ω_I) be the smallest eigenvalues of all element matrix pairs $\Re(\mathbf{A}^e), \mathbf{B}^e$, (resp. $\Im(\mathbf{A}^e), \mathbf{B}^e$), i.e.,*

$$\omega_R = \min_e \lambda_{min}^{\Re(\mathbf{A}^e), \mathbf{B}^e} \quad \omega_I = \min_e \lambda_{min}^{\Im(\mathbf{A}^e), \mathbf{B}^e},$$

and let Ω_R (resp. Ω_I) be the largest eigenvalue

$$\Omega_R = \max_e \lambda_{max}^{\Re(\mathbf{A}^e), \mathbf{B}^e} \quad \Omega_I = \max_e \lambda_{max}^{\Im(\mathbf{A}^e), \mathbf{B}^e}.$$

Then the following bounds hold for $FOV(\mathbf{A}, \mathbf{B})$:

$$\omega_R \leq Re(FOV(\mathbf{A}, \mathbf{B})) \leq \Omega_R, \quad (3.11)$$

$$\omega_I \leq Im(FOV(\mathbf{A}, \mathbf{B})) \leq \Omega_I. \quad (3.12)$$

Proof: Analogous to the proof of Theorem 3.3. \triangle

Remark In this paper we restrict ourselves to the important case where \mathbf{B} is Hermitian Positive Definite. Our results do not hold for the case where \mathbf{B} is general, since then the projection property (3.10) does not hold.

3.3 A bound on the numerical radius

An upperbound on the numerical radius of a general matrix \mathbf{A} is given by:

Theorem 3.5 *Let $\mathbf{A}^e, e = 1, \dots, n_e$ be (possibly non-Hermitian) element matrices and let \mathbf{A} be the global matrix that is assembled from these element matrices. Let ν be defined by*

$$\nu = \max \left\{ |z| : z \in \bigcup_{e=1}^{n_e} FOV(\mathbf{A}^e) \right\}, \quad (3.13)$$

then

$$r(\mathbf{A}) \leq \nu \eta_{max},$$

with η_{max} the maximum number of elements sharing the same node.

Proof: By the definitions (2.3) and (3.13) we have

$$\left| \frac{\mathbf{x}^{eH} \mathbf{A}^e \mathbf{x}^e}{\mathbf{x}^{eH} \mathbf{x}^e} \right| \leq \nu \quad \forall e, \mathbf{x} \in \mathbb{C}^n, \mathbf{x} \neq 0 .$$

Multiplication with $\mathbf{x}^{eH} \mathbf{x}^e$ and assembly yields

$$\sum_{e=1}^{n_e} |\mathbf{x}^{eH} \mathbf{A}^e \mathbf{x}^e| \leq \mathbf{x}^H \mathbf{x} \nu \eta_{max} .$$

The results follows from combining of (3.1) with

$$|\mathbf{x}^H \mathbf{A} \mathbf{x}| = \left| \sum_{e=1}^{n_e} \mathbf{x}^{eH} \mathbf{A}^e \mathbf{x}^e \right| \leq \sum_{e=1}^{n_e} |\mathbf{x}^{eH} \mathbf{A}^e \mathbf{x}^e| . \quad (3.14)$$

△

An upperbound on the numerical radius of the generalised Field of Values $FOV(\mathbf{A}, \mathbf{B})$ with \mathbf{A} general and \mathbf{B} Hermitian Positive Definite is given by:

Theorem 3.6 *Let $\mathbf{A}^e, e = 1, \dots, n_e$ be (possibly non-Hermitian) element matrices and $\mathbf{B}^e, e = 1, \dots, n_e$ be Hermitian Positive Definite element matrices and let \mathbf{A} and \mathbf{B} be the global matrices that are assembled from these element matrices. Let ν be defined by*

$$\nu = \max \left\{ |z| : z \in \bigcup_{e=1}^{n_e} FOV(\mathbf{A}^e, \mathbf{B}^e) \right\}, \quad (3.15)$$

then

$$r(\mathbf{A}, \mathbf{B}) \leq \nu .$$

Proof: By the definitions (2.4) and (3.15) we have

$$\left| \frac{\mathbf{x}^{eH} \mathbf{A}^e \mathbf{x}^e}{\mathbf{x}^{eH} \mathbf{B}^e \mathbf{x}^e} \right| \leq \nu \quad \forall e, \mathbf{x} \in \mathbb{C}^n, \mathbf{x} \neq 0 .$$

Multiplication with $\mathbf{x}^{eH} \mathbf{B}^e \mathbf{x}^e$ and assembly yields

$$\sum_{e=1}^{n_e} |\mathbf{x}^{eH} \mathbf{A}^e \mathbf{x}^e| \leq \mathbf{x}^H \mathbf{B} \mathbf{x} \nu .$$

The results follows from combining this inequality with (3.14). △

4 Example: a quadratic eigenproblem from acoustics

To illustrate the bounds we have derived in the previous section we consider the 2D-version of the example described in [11]. This example models sound propagation in a homogeneous medium in the domain $\Omega = [0, 4] \times [0, 4]$. Three of the boundaries of the domain are reflecting and the fourth boundary is impeding.

The eigensolutions of this problem can be determined from the homogeneous Helmholtz equation

$$\Delta \hat{p} = \hat{\lambda}^2 \hat{p} \quad (4.1)$$

in which \hat{p} is the eigenfunction and $\hat{\lambda}$ the (analytical) eigenvalue. The boundary conditions for the reflecting boundaries are

$$\frac{\partial \hat{p}}{\partial n} = 0 \quad \text{on } \Gamma_1, \quad (4.2)$$

and for the impeding boundary

$$\frac{\partial \hat{p}}{\partial n} = -\frac{\hat{\lambda}}{\zeta} \hat{p} \quad \text{on } \Gamma_2 \quad (4.3)$$

in which ζ is the (possibly complex) impedance.

Straightforward discretisation of the above equations yields a quadratic eigenvalue problem of the form $\lambda^2 \mathbf{M} \mathbf{p} + \lambda \mathbf{C} \mathbf{p} + \mathbf{K} \mathbf{p} = \mathbf{0}$ [11], in which \mathbf{p} is an eigenvector, λ an (algebraic) eigenvalue, and \mathbf{M} , \mathbf{C} , and \mathbf{K} are square matrices of order n , with n the number of grid-points used in the discretisation.

In order to obtain a generalised eigenvalue problem instead of a quadratic eigenproblem one can introduce the additional variable

$$\hat{q} = \hat{\lambda} \hat{p}. \quad (4.4)$$

Substitution of (4.4) into (4.1) and (4.3) yields

$$\hat{\lambda} \hat{q} = \Delta \hat{p} \quad (4.5)$$

and

$$\frac{\partial \hat{p}}{\partial n} = -\frac{1}{\zeta} \hat{q} \quad \text{on } \Gamma_3, \quad (4.6)$$

respectively. Discretisation of the equations (4.2), (4.4), (4.5), and (4.6) yields a $2n \times 2n$ block system of the form

$$\begin{pmatrix} -\mathbf{C} & -\mathbf{K} \\ \mathbf{M} & \mathbf{O} \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{M} & \mathbf{O} \\ \mathbf{O} & \mathbf{M} \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}. \quad (4.7)$$

The element matrices from which the global matrices are assembled have a corresponding block structure. In our example we use triangular elements with linear interpolation functions for both \mathbf{p} and \mathbf{q} on a uniform mesh. Integrals are evaluated numerically using a Newton-Cotes integration rule. The resulting left-hand side element matrices are given by

$$\begin{pmatrix} -\mathbf{C}^e & -\mathbf{K}^e \\ \mathbf{M}^e & \mathbf{O} \end{pmatrix} = \left(\begin{array}{ccc|ccc} -\frac{h}{2\zeta} & 0 & 0 & -1 & \frac{1}{2} & \frac{1}{2} \\ 0 & -\frac{h}{2\zeta} & 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} \\ \hline \frac{h^2}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{h^2}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{h^2}{6} & 0 & 0 & 0 \end{array} \right) \quad (4.8)$$

if the triangular element has a vertex in common with the impeding boundary, and

$$\begin{pmatrix} -\mathbf{C}^e & -\mathbf{K}^e \\ \mathbf{M}^e & \mathbf{O} \end{pmatrix} = \left(\begin{array}{ccc|ccc} 0 & 0 & 0 & -1 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & -\frac{1}{2} \\ \hline \frac{h^2}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{h^2}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{h^2}{6} & 0 & 0 & 0 \end{array} \right) \quad (4.9)$$

elsewhere. The right-hand side element matrices have a very simple structure:

$$\begin{pmatrix} \mathbf{M}^e & \mathbf{O}^e \\ \mathbf{O}^e & \mathbf{M}^e \end{pmatrix} = \frac{h^2}{6} \begin{pmatrix} \mathbf{I}^e & \mathbf{O}^e \\ \mathbf{O}^e & \mathbf{I}^e \end{pmatrix}. \quad (4.10)$$

In our example we have taken $\zeta = 0.2 - 1.5i$ and $h = \frac{4}{10}$. The resulting left-hand side matrix is complex and non-Hermitian. The global right-hand side matrix is obviously diagonal, but unlike the right-hand side element matrices not a scalar times the identity since the assembly process yields diagonal entries for boundary nodes that are different from diagonal entries for nodes in the interior of the domain.

We have applied Theorem 3.4 to derive a bound on the Fields of Values, and Theorem 3.6 to bound the numerical radius. The results are shown in Table 4.1, second column. To assess the quality of these bounds we have calculated the actual minima and maxima of the real and imaginary part of the Field of Values and the spectral radius with the routine `fv` from the Matrix Computation Toolbox of Higham [5]. Since this routine calculates the standard Field of Values we first apply equivalence (2.5) to reduce the generalised problem to a standard problem. The resulting bounds are tabulated in the third column of Table 4.1.

	Bound	Computed
Min Re(FOV)	-27.900	-25.596
Max Re(FOV)	27.625	25.433
Min Im(FOV)	-30.809	-27.871
Max Im(FOV)	28.63	26.402
Numerical Radius	30.820	27.909

Table 4.1: Bounds and computed values for the maximum and minimum of the real and imaginary parts of the Field of Values and the bound and computed value for the numerical radius.

Figure 4.1 shows the spectrum and the actual Field of Values of the matrix, the bounding box that is computed using Theorem 3.4, and a circle around the origin with radius the bound on the numerical radius obtained by applying Theorem 3.6. For comparison we have also included the two outermost Gerschgorin disks. Both Table 4.1 and Figure 4.1 show that our bounds enclose the actual Field of Values tightly. Moreover, Figure 4.1 shows that our bounds are tighter than the bounds provided by the Gerschgorin disks (which are strictly speaking bounds for the eigenvalues and not for the Field of Values).

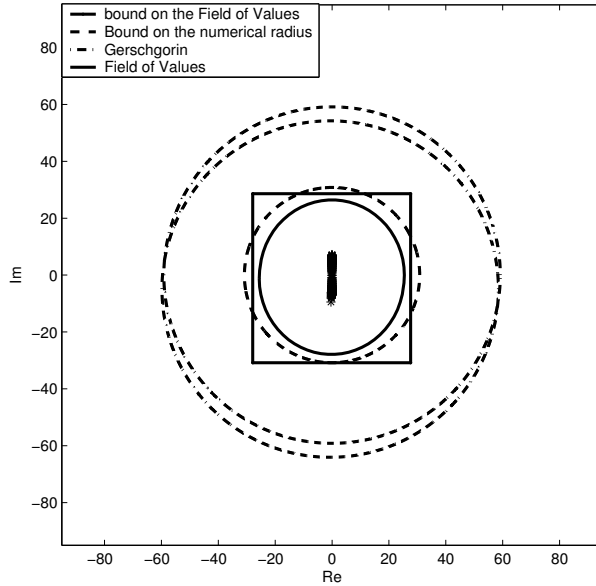


Figure 4.1: Spectrum, Field of Values, bounds on the Field of Values and on the numerical radius, and Gerschgorin disks for the acoustic example.

5 Application: an upperbound on the number of iterations for preconditioned GMRES

5.1 Upperbounds on the norm of the GMRES-residual

GMRES [9] is one of the most popular iterative methods for solving linear system $\mathbf{Ax} = \mathbf{b}$, with a non-symmetric system matrix \mathbf{A} . In order to describe the convergence of the method, various upperbounds on the norm of the GMRES-residual have been proposed. Some of these bounds are based on the Field of Values of \mathbf{A} .

For example, for \mathbf{A} real and Positive Definite (i.e. $\Re(\mathbf{A})$ is symmetric Positive Definite) the following bound holds [1]. Let

$$\theta = \min(\Re(\mathbf{A})) \quad \text{and} \quad \Theta = r(\mathbf{A}).$$

Then the GMRES-residual norm after k iterations satisfies

$$\|\mathbf{r}^k\|/\|\mathbf{r}^0\| \leq \left(1 - \frac{\theta^2}{\Theta^2}\right)^{k/2}. \quad (5.1)$$

A similar bound, involving $\|\mathbf{A}\|$ instead of Θ is given in [10], Theorem 5.3.

Another useful bound is given in [4], page 56. Suppose that $FOV(\mathbf{A})$ is contained in a disk $D = \{z \in \mathbb{C} : |z - c| \leq s\}$ which does not contain the origin. Then the GMRES-residual norm after k iterations satisfies

$$\|\mathbf{r}^k\|/\|\mathbf{r}^0\| \leq 2 \left(\frac{s}{|c|}\right)^k. \quad (5.2)$$

Although the above bounds are often not sharp, they do provide a useful tool for analysing preconditioners, see for example [8]. In the remainder of this Section we show how the above bounds on the norm of the GMRES-residual can be combined with the bounds on the Field of Values and on the numerical radius. This allows us to analyse a symmetric preconditioner for a family of convection-diffusion-reaction equations.

5.2 Application to a class of convection-diffusion-reaction equations

Consider the following family of convection-diffusion-reaction equations

$$-\epsilon\Delta u + \mu u + \beta_x \frac{\partial u}{\partial x} + \beta_y \frac{\partial u}{\partial y} = f \quad . \quad (5.3)$$

We assume that the parameters ϵ (diffusion), μ (reaction), and β_x and β_y (convection) are constant. Furthermore, we assume that $\epsilon > 0$ and $\mu \geq 0$. Discretisation on a uniform mesh with mesh-size h , using linear triangular elements yields element matrices \mathbf{A}^e of the form

$$\mathbf{A}^e = \epsilon \mathbf{L}^e + \mu \mathbf{M}^e + \beta_x \mathbf{B}_x^e + \beta_y \mathbf{B}_y^e \quad .$$

The element matrix \mathbf{A}^e is the sum of four element matrices, each of which corresponds to one of the four terms in (5.3). These element matrices are

$$\begin{aligned} \mathbf{L}^e &= \frac{1}{2} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \quad \mathbf{M}^e = \frac{h^2}{6} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\ \mathbf{B}_x^e &= \frac{h}{6} \begin{pmatrix} 1 & -1 & 0 \\ 1 & -1 & 0 \\ 1 & -1 & 0 \end{pmatrix}, \quad \mathbf{B}_y^e = \frac{h}{6} \begin{pmatrix} 1 & 0 & -1 \\ 1 & 0 & -1 \\ 1 & 0 & -1 \end{pmatrix}. \end{aligned}$$

As a preconditioner we consider the matrix \mathbf{P} that corresponds to the symmetric part of the partial differential operator, i.e., to $-\epsilon\Delta + \mu$. This matrix is assembled from element matrices \mathbf{P}^e given by

$$\mathbf{P}^e = \epsilon \mathbf{L}^e + \mu \mathbf{M}^e, \quad \mathbf{P} = \sum_{e=1}^{n_e} \mathbf{N}^{eT} \mathbf{P}^e \mathbf{N}^e.$$

This preconditioner yields the following matrix splitting

$$\mathbf{A} = \mathbf{P} + \mathbf{B}, \quad (5.4)$$

where the matrix \mathbf{B} is assembled from the element matrices

$$\mathbf{B}^e = \beta_x \mathbf{B}_x^e + \beta_y \mathbf{B}_y^e \quad . \quad (5.5)$$

The element preconditioning matrices \mathbf{P}^e , and consequently also the preconditioner \mathbf{P} , are symmetric and Positive Definite, hence we can make a Cholesky decomposition of \mathbf{P} : $\mathbf{P} = \mathbf{C}\mathbf{C}^T$. We apply the preconditioner symmetrically, that is, we apply GMRES to the system

$$\mathbf{C}^{-1} \mathbf{A} \mathbf{C}^{-T} \mathbf{y} = \mathbf{C}^{-1} \mathbf{f}, \quad \mathbf{x} = \mathbf{C}^{-T} \mathbf{y} \quad .$$

We will derive an upperbound for the GMRES-residual for this system using (5.2). Hence, we have to find a circle in the complex plane that encloses $FOV(\mathbf{C}^{-1}\mathbf{A}\mathbf{C}^{-T})$. Since

$$\mathbf{C}^{-1}\mathbf{A}\mathbf{C}^{-T} = \mathbf{I} + \mathbf{C}^{-1}\mathbf{B}\mathbf{C}^{-T}$$

and therefore

$$FOV(\mathbf{C}^{-1}\mathbf{A}\mathbf{C}^{-T}) = 1 + FOV(\mathbf{C}^{-1}\mathbf{B}\mathbf{C}^{-T}),$$

this amounts to finding a circle around $FOV(\mathbf{C}^{-1}\mathbf{B}\mathbf{C}^{-T})$ which has to be shifted by one to enclose $FOV(\mathbf{C}^{-1}\mathbf{A}\mathbf{C}^{-T})$. We recall that by (2.5) $FOV(\mathbf{C}^{-1}\mathbf{B}\mathbf{C}^{-T}) = FOV(\mathbf{B}, \mathbf{P})$.

5.3 Analysis

We can derive a circle around $FOV(\mathbf{B}, \mathbf{P})$ by enclosing it in a box using Theorem 3.4. To this end, we have to calculate the extreme eigenvalues of the generalised eigenproblems

$$\Re(\mathbf{B}^e)\mathbf{x}^e = \lambda^e\mathbf{P}^e\mathbf{x}^e \quad \text{and} \quad \Im(\mathbf{B}^e)\mathbf{x}^e = \lambda^e\mathbf{P}^e\mathbf{x}^e. \quad (5.6)$$

These eigenvalues can be determined explicitly and are given by

$$\begin{aligned} \lambda_{min}^{\Re(\mathbf{B}^e), \mathbf{P}^e} &= -\gamma \\ \lambda_{max}^{\Re(\mathbf{B}^e), \mathbf{P}^e} &= \gamma \\ \lambda_{min}^{\Im(\mathbf{B}^e), \mathbf{P}^e} &= -\gamma \\ \lambda_{max}^{\Im(\mathbf{B}^e), \mathbf{P}^e} &= \gamma \end{aligned} \quad (5.7)$$

where γ is given by (see appendix A)

$$\gamma = \frac{1}{2} \sqrt{\frac{(\beta_x - \beta_y)^2}{2\epsilon\mu + \frac{2}{3}h^2\mu^2} + \frac{(\beta_x + \beta_y)^2}{2\epsilon\mu + \frac{2}{9}h^2\mu^2}}. \quad (5.8)$$

Application of Theorem 3.4 yields that the Field of Values $FOV(\mathbf{B}, \mathbf{P})$ is enclosed by a square centered at 0 and with corners $(\pm\gamma, \pm i\gamma)$. Hence, the Field of Values $FOV(\mathbf{C}^{-1}\mathbf{A}\mathbf{C}^{-T})$ is enclosed by a circle with center $c = 1$ and radius $s = \sqrt{2}\gamma$.

For this problem we can derive a sharper bound by using Theorem 3.6. Since by definition we have for all $z \in FOV(\mathbf{B}, \mathbf{P}) : |z| \leq r(\mathbf{B}, \mathbf{P})$, we can determine the radius s of a circle around $FOV(\mathbf{B}, \mathbf{P})$ by determining an upperbound on $r(\mathbf{B}, \mathbf{P})$. To this end we apply Theorem 3.6, which implies that we have to determine $r(\mathbf{B}^e, \mathbf{P}^e)$. This value can be computed explicitly (see appendix A) and is given by

$$r(\mathbf{B}^e, \mathbf{P}^e) = \gamma. \quad (5.9)$$

We conclude that the Field of Values $FOV(\mathbf{C}^{-1}\mathbf{A}\mathbf{C}^{-T})$ is enclosed by a circle with center $c = 1$ and radius $s = \gamma$.

If we combine this result with (5.2) we get that for the family of convection-diffusion-reaction problems (5.3), discretised on a regular mesh with the linear

triangular finite elements described above, the residual norm of GMRES, preconditioned with the matrix that corresponds to the reaction-diffusion part of (5.3), satisfies

$$\|\mathbf{r}^k\|/\|\mathbf{r}^0\| \leq 2\gamma^k, \quad (5.10)$$

with γ given by (5.8). This result is quite strong. Since

$$\lim_{h \rightarrow 0} \gamma = \frac{\|\beta\|}{2\sqrt{\epsilon\mu}} \quad (5.11)$$

it implies that we have derived an upperbound on the GMRES-residual norm that is *independent* of the mesh-size h . Moreover, this upperbound is explicitly known and can be easily computed from the convection, diffusion and reaction parameters. However, since (5.2) is only valid if the Field of Values does not contain the origin, the bound (5.10) is only valid for $\gamma < 1$.

In the analysis we have not considered the boundary conditions. Since Neumann boundary conditions do not modify the element matrices but only the right-hand-side vector, the above analysis holds if all boundary conditions are of Neumann type. Application of Dirichlet conditions amounts to removing the rows and columns that correspond to prescribed nodes from the matrix \mathbf{A} . This in general only shrinks the Field of Values, and reduces the number of GMRES-iterations. A rigorous proof that (5.10) also holds if there are Dirichlet conditions can be made by separately considering element matrices in which the columns and rows that correspond to boundary nodes are removed. It is easily verified that for these element matrices the element eigenproblems (5.6) yield extreme eigenvalues that are closer to 0 than for the eigenproblem for elements that have no boundary node. The same is true for the numerical radius. The conclusion is that (5.10) holds, irrespective whether the boundary conditions are Dirichlet or Neumann.

5.4 Comparison with the actual number of GMRES-iterations.

In this Section we validate numerically the above analysis. For this, we will consider equation (5.3) on the unit square with Neumann boundary conditions. For different combinations of parameters we determine the upperbound on the number of iterations and the actual number of iterations needed by GMRES in order to have a residual norm that satisfies the criterion $\|\mathbf{r}^k\|/\|\mathbf{r}^0\| \leq 10^{-8}$. In particular, we investigate the dependence of the number of iterations on the mesh-size. For this, we use discretisations with mesh-sizes that vary from $h = \frac{1}{8}$ to $h = \frac{1}{128}$. As right-hand-side function we take a δ -function with its peak in the middle of the domain.

The first set of experiments studies the effect of an increase in nonsymmetry in the matrix \mathbf{A} by increasing $\|\beta\|$. We use the following parameters $\mu = 1$, $\epsilon = 1$, $\beta_y = 0$ and for β_x we take $\beta_x = 0.01$, $\beta_x = 0.1$, and $\beta_x = 1$, respectively. The results are given in Table 5.1. Columns 2-6 give the upperbound on the number of iterations using (5.10) and columns 7-11 give the actual number of GMRES-iterations. For ϵ not too much smaller than μ , the value of γ as given by (5.8) is virtually independent of the mesh-size h and is well approximated by the upperbound (5.11) on γ . This is confirmed by the results shown in column 2-6. For every choice of β_x the upperbound is independent of the mesh-size. For

Number of iterations:	Upperbound					Actual				
$\beta \setminus h :$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$	$\frac{1}{128}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$	$\frac{1}{128}$
0.01	4	4	4	4	4	3	3	3	3	3
0.1	7	7	7	7	7	4	4	4	4	5
1	28	28	28	28	28	7	7	7	7	8

Table 5.1: Upperbound and actual number of iterations under mesh refinement. $\mu = 1, \epsilon = 1$ and three different values of β_x .

the actual GMRES-computations given in columns 7-11 we observe the same behaviour: the actual number of iterations is virtually constant for all h . By increasing the nonsymmetry in \mathbf{A} the symmetric preconditioner \mathbf{P} becomes less effective. This is confirmed by the fact that both the upperbound and the actual number of iterations grow with β_x . The upperbound becomes rather pessimistic for increasing β_x , but we have to keep in mind that (5.2) is in general not tight.

The second set of experiments studies the effect of changes in the diffusion parameter ϵ . We use the following parameters $\mu = 1, \beta_x = 0.01, \beta_y = 0$ and for ϵ we take $\epsilon = 0.001, \epsilon = 0.01, \text{ and } \epsilon = 0.1$, respectively. Table 5.2 gives the results. Given (5.8) we expect that for ϵ small relative to μ there is a slight

Number of iterations:	Upperbound					Actual				
$\epsilon \setminus h :$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$	$\frac{1}{128}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$	$\frac{1}{128}$
0.001	8	9	10	11	11	6	7	7	8	8
0.01	7	7	7	7	7	5	5	5	5	5
0.1	5	5	5	5	5	4	4	4	4	4

Table 5.2: Upperbound and actual number of iterations under mesh refinement. $\mu = 1, \beta_x = 0.01$ and three different values of ϵ .

initial mesh-dependence of the number of iterations. For h small enough the upperbound on the number of iterations becomes constant. This is illustrated by the results for $\epsilon = 0.001$, columns 2-6. We observe the same behaviour for the actual number of GMRES-iterations which are tabulated in columns 7-11. For the larger values $\epsilon = 0.01$ and $\epsilon = 0.1$, (5.10) gives an upperbound on the number of iterations that is independent of h . This is the same as we observe for the actual number of GMRES-iterations. Moreover, both the bound and the actual number of iterations decreases when ϵ is increased, as is to be expected.

The third set of experiments studies the effect of changes in the reaction parameter μ in the case where there is no diffusion. We use the following parameters $\epsilon = 0, \beta_x = 0.01, \beta_y = 0$ and for μ we take $\mu = 1, \mu = 10, \text{ and } \mu = 100$, respectively. Table 5.3 gives the results. If there is no diffusion, γ tends to infinity when $h \rightarrow 0$. Hence, in this case there is no bound independent of h on the number of GMRES-iterations. This is illustrated by the fact that the upper bounds on the number of iterations given in columns 2-6 grow. For $\mu = 1$ we cannot even determine an upper bound on the finest grid, since in this case $\gamma > 1$. Obviously, the dependence on the mesh-size becomes noticeable later

Number of iterations:	Upperbound					Actual				
$\mu \setminus h :$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$	$\frac{1}{128}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$	$\frac{1}{128}$
1	9	12	21	79	-	7	8	11	17	30
10	5	5	6	8	11	4	4	5	6	8
100	4	4	4	4	5	3	3	3	4	4

Table 5.3: Upperbound and actual number of iterations under mesh refinement. $\epsilon = 0, \beta_x = 0.01$ and three different values for μ .

for larger μ . The actual numbers of GMRES-iterations as tabulated in columns 7-11 show the same behaviour as predicted by the upperbound: the number of iterations grows if the mesh is refined.

In the previous section we argued that the upperbound on the number of GMRES-iterations is valid, irrespective whether the boundary conditions are Dirichlet or Neumann. The experimental results that are given above are obtained for the Neumann problem. In addition, we have also validated the upper bound with the results for the Dirichlet problem. The results for the Dirichlet and the Neumann problem are essentially the same, with only a slightly higher number of iterations for the Neumann problem in some cases.

6 Conclusions

In this paper we have presented bounds on the Field of Values, the numerical radius and on the spectrum of general Finite Element matrices, for both the standard and the generalised problem. For the generalised case we have restricted ourselves to the case where one of the matrices is Hermitian Positive Definite. The bounds are cheap to compute, involving operations with element matrices only.

We have combined bounds on the norm of the GMRES-residual with the bounds on the Field of Values, which allowed us to prove that the number of GMRES iterations to solve a (certain type of) convection-diffusion-reaction problems that is preconditioned with the discrete diffusion-reaction operator is independent of the mesh-size.

We remark that an analysis using the same approach as we have taken in this paper can be performed for any Finite Element system preconditioned with a Hermitian Positive Definite matrix that is assembled from element matrices. This includes for example the important class of diagonal preconditioners.

In the generalised case with one of the matrices Hermitian Positive Definite, our bounds are a natural extension of the bounds for symmetric Positive Definite matrix pairs that have been proposed by Fried. For many important applications, e.g., for the acoustic example we have described, one of the matrices is Hermitian Positive Definite, and hence our bounds can be applied. For certain classes of problems, however, such as the analysis of a nonsymmetric system that is preconditioned by a nonsymmetric matrix, a further generalisation of the bounds is still required.

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A Calculation of a bound for $FOV(\mathbf{B}^e, \mathbf{P}^e)$ and for $r(\mathbf{B}^e, \mathbf{P}^e)$.

The fact that two of the three eigenvectors of \mathbf{P}^e are orthogonal to the column space of \mathbf{B}^e allows us to greatly simplify the calculation of a bound for $FOV(\mathbf{B}^e, \mathbf{P}^e)$.

The eigenvalue decomposition of \mathbf{P}^e is given by

$$\mathbf{P}^e = \mathbf{S}^e \Lambda^e \mathbf{S}^{eT}$$

where

$$\mathbf{S}^e = \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & -\frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \end{pmatrix} \text{ and } \Lambda^e = \begin{pmatrix} \frac{h^2\mu}{6} & 0 & 0 \\ 0 & \frac{\epsilon}{2} + \frac{h^2\mu}{6} & 0 \\ 0 & 0 & \frac{3\epsilon}{2} + \frac{h^2\mu}{6} \end{pmatrix}.$$

Let

$$\mathbf{Q}^e = \mathbf{S}^e \Lambda^{e\frac{1}{2}},$$

then we have using (2.5) that $FOV(\mathbf{B}^e, \mathbf{P}^e) = FOV(\mathbf{Q}^{e-1} \mathbf{B}^e \mathbf{Q}^{e-T})$. The matrix $\mathbf{Q}^{e-1} \mathbf{B}^e \mathbf{Q}^{e-T}$ has the simple form

$$\mathbf{Q}^{e-1} \mathbf{B}^e \mathbf{Q}^{e-T} = \begin{pmatrix} 0 & \frac{\beta_x - \beta_y}{\sqrt{2\epsilon\mu + \frac{2}{3}h^2\mu^2}} & -\frac{\beta_x + \beta_y}{\sqrt{2\epsilon\mu + \frac{2}{3}h^2\mu^2}} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{A.1})$$

Consequently, the matrices $\Re(\mathbf{Q}^{e-1} \mathbf{B}^e \mathbf{Q}^{e-T})$ and $\Im(\mathbf{Q}^{e-1} \mathbf{B}^e \mathbf{Q}^{e-T})$ have only four nonzero entries. It is also easy to verify that they have rank 2, and hence one eigenvalue equal to 0. The other two eigenvalues can be computed from the characteristic polynomial of $\Re(\mathbf{Q}^{e-1} \mathbf{B}^e \mathbf{Q}^{e-T})$, resp. of $\Im(\mathbf{Q}^{e-1} \mathbf{B}^e \mathbf{Q}^{e-T})$, which yields (5.7).

The numerical radius of $\mathbf{Q}^{e-1} \mathbf{B}^e \mathbf{Q}^{e-T}$ can be computed by making use of its special structure. It is known that (see [6], page 17) the numerical radius of a matrix \mathbf{A} of the following form

$$\mathbf{A} = \begin{pmatrix} 0 & \mathbf{U} \\ 0 & 0 \end{pmatrix}$$

equals $\sigma(\mathbf{U})/2$, with $\sigma(\mathbf{U})$ the largest singular value of \mathbf{U} . Since (A.1) has the above structure, we have

$$r(\mathbf{Q}^{e-1} \mathbf{B}^e \mathbf{Q}^{e-T}) = \frac{1}{2} \sqrt{\frac{(\beta_x - \beta_y)^2}{2\epsilon\mu + \frac{2}{3}h^2\mu^2} + \frac{(\beta_x + \beta_y)^2}{2\epsilon\mu + \frac{2}{3}h^2\mu^2}}$$

which is equal to γ .

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