

Studies on methods for verifying the accuracy
of numerical solutions
of symmetric saddle point linear systems
対称な鞍点行列を係数に持つ連立一次方程式の解に対する
精度保証付き数値計算法に関する研究

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CONTENTS

ACKNOWLEDGMENTS	iii
CHAPTER 1. INTRODUCTION	1
1.1. Background	2
1.2. Purpose	4
1.3. Organization	5
CHAPTER 2. PRELIMINARIES	7
2.1. Notations and Definitions	8
2.2. Previous works	9
CHAPTER 3. NEW VERIFICATION METHODS	13
3.1. Regularization of A	14
3.2. Eigenvalues of the preconditioned matrix	17
3.3. New error bound	20
3.4. Error bounds for preconditioned problem	22
3.5. Verification Methods	24
CHAPTER 4. NUMERICAL EXPERIMENTS	27
4.1. Example 1	29
4.2. Example 2	32
4.3. Example 3 (Stokes equation [4, §6])	34
4.4. Example 4 (the Brinkman problem [12])	37
CHAPTER 5. CONCLUSION	41
BIBLIOGRAPHY	43

CHAPTER 1

INTRODUCTION

Let \mathbb{R} be the set of real numbers. Let m and n be positive integers. Throughout this thesis, let $A \in \mathbb{R}^{n \times n}$ and $C \in \mathbb{R}^{m \times m}$ be symmetric positive semidefinite matrices with $m \leq n$, and $B \in \mathbb{R}^{n \times m}$ be a full rank matrix. Let $x, f \in \mathbb{R}^n$ and $y, g \in \mathbb{R}^m$. In this thesis, we put $l = n + m$. We consider a numerical method for verifying the accuracy of numerical solutions of the following symmetric saddle point linear systems:

$$\mathcal{H}u = b, \tag{1}$$

where

$$\mathcal{H} = \begin{pmatrix} A & B \\ B^T & -C \end{pmatrix}, \quad u = \begin{pmatrix} x \\ y \end{pmatrix}, \quad b = \begin{pmatrix} f \\ g \end{pmatrix}.$$

We treat the case where \mathcal{H} is nonsingular.

Purposes of this study are to verify the existence and the uniqueness of an exact solution of (1) and to compute an error bound between an approximate solution and the exact solution of (1) such that

$$\|u^* - u\|_2 \leq \kappa, \quad \text{for } u \in \mathbb{R}^l,$$

where u^* is the exact solution of (1). In this thesis, such a method is called a verification method.

1.1. BACKGROUND

In a scientific computation, when we consider a natural or a social phenomenon and compute its numerical solution, the obtained numerical solution include various errors as Figure 1.1. In many case, when we compute an error bound between the approximation and the exact solution using the verification method, we take into account approximation errors and numerical errors (Error 2 and Error 3 in Figure 1.1). In this thesis, especially we focus on numerical errors (Error 3 in Figure 1.1).

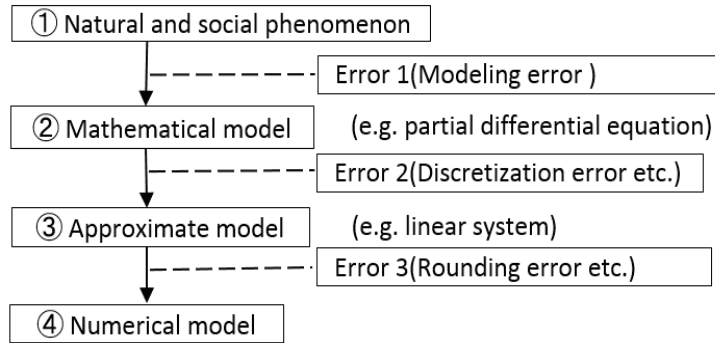


FIGURE 1.1. Numerical computing models and errors.

Here, we show an easy example of numerical errors. We consider the following system:

$$\begin{pmatrix} 64919121 & -159018721 \\ 41869520.5 & -102558961 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

In this problem, the exact solution is

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 205117922 \\ 83739041 \end{pmatrix}.$$

However, when we compute it using Gaussian elimination with IEEE 754 double-precision floating point numbers, we get the following solution:

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 106018308.0071325 \\ 43281793.0017831 \end{pmatrix}.$$

This may be an artificial example. However, even such simple linear systems will cause trouble. So, it is important to verify the accuracy of obtained solutions.

On the other hand, saddle point linear systems described by (1) arise from the various problems [3, 4, 6, 12]. For example, we apply a mixed finite element method to partial differential equations, then we get a discretized equation having saddle point form. Moreover, when we solve a convex optimization problem using an interior point

algorithm, we need to solve saddle point linear systems. According to the ubiquity of saddle point systems, methods and results on their numerical solution have appeared in many books and papers. Therefore, to verify the accuracy of an approximation of linear systems in saddle point form is very important.

1.2. PURPOSE

A large amount of work has been devoted to developing efficient algorithms for solving (1) (see [3]). For example, as a method for solving (1) with the positive definiteness of A , there is a method using Schur complement. Here, Schur complement of A in \mathcal{H} is defined as $S = C + B^T A^{-1} B$. Using Schur complement, we can obtain a solution as follows:

$$\begin{aligned} Sy &= B^T A^{-1} f - g, \\ Ax &= f - By. \end{aligned} \tag{2}$$

In optimization, structural analysis, and electrical engineering, this method is called the range-space method, the displacement method, and the nodal analysis method, respectively [13]. Another method is the method that is based on the null space for the matrix B^T . In optimization, this method is popular and is called the reduced Hessian methods [8, 14]. However, this method requires $C = O$. There methods solve two reduced systems whose size is smaller than the size of original one. Also, some iterative methods like the Arrow-Hurwicz method and the Uzawa method [1] have been developed. Moreover, when A is singular, the augmented Lagrangian method can be used. The idea of this method is to replace the original systems with the singularity of A with the ones with the nonsingularity of A . In this thesis, we mainly consider the verification method using Schur complement.

In general, the verification method for solving linear systems uses an approximation of the inverse of the coefficient matrix. However, in [5, 6], authors have proposed the verification methods using the special structure of saddle point matrix without

using an approximation of \mathcal{H}^{-1} . In [5], Chen and Hashimoto have studied the verification methods for an approximate solution of (1) with A is symmetric positive definite. These methods are based on the system (2). In [6], Kimura and Chen have studied the verification methods for approximate solutions of (1) with $C = O$. These methods use the preconditioner with Schur complement. These methods are efficient compared to methods using an approximation of \mathcal{H}^{-1} for saddle point linear systems. However, a verification method for a solution of (1) with both A and C are symmetric positive semidefinite was not developed yet. Therefore, in this thesis, we consider the case where both A and C are symmetric positive semidefinite matrices.

We propose fast verification methods using results of an algebraic analysis of a block diagonal preconditioner. These method are based on the extension of theorem studied by Kimura and Chen [6]. These method can be used alternatively to the methods developed by Kimura and Chen [6], or to the ones by Chen and Hashimoto [5]. All quantities required to compute in the proposed verification method are also required to compute in executing Chen-Hashimoto's method. Thus, once all quantities needed in Chen-Hashimoto's methods are computed, then all quantities needed to execute the proposed verification methods are provided.

1.3. ORGANIZATION

In Chapter 2, we denote some notations and definitions. And we review some previous works. In Chapter 3, we propose new verification methods for approximate solutions of (1). First, we show a method of regularizing A of (1). Next, we define a preconditioner and propose a theorem for all eigenvalues of the preconditioned matrix. And, we propose a new error bound for (1) using the above theorem. In Chapter 4, we compare our verification methods with Chen-Hashimoto's methods and the verification methods for an approximate solution of general linear systems. We show numerical results to illustrate the effectiveness of the proposed methods. Finally, we conclude results of our studies in Chapter 5.

CHAPTER 2

PRELIMINARIES

2.1. NOTATIONS AND DEFINITIONS

Let \mathbb{R} be the set of real numbers. Let m and n be positive integers ($n \geq m$). We set $l = m + n$. The superscript T is the transpose. I is an identity matrix and O is a zero matrix. A positive definite or semidefinite matrix is defined as follows:

DEFINITION 2.1.

Let $M \in \mathbb{R}^{n \times n}$ and $z \in \mathbb{R}^n$.

M is positive definite if $z^T M z > 0$ for all $z \neq 0$.

M is positive semidefinite if $z^T M z \geq 0$ for all $z \neq 0$.

Moreover, $M \succ O$ ($M \succeq O$) denote that M is positive (semi-)definite. Throughout this thesis, let $A \in \mathbb{R}^{n \times n}$ be a symmetric positive semidefinite matrix and $\tilde{A} \in \mathbb{R}^{n \times n}$ be a symmetric positive definite matrix. Let $B, \tilde{B} \in \mathbb{R}^{n \times m}$ be full rank matrices and $C, \tilde{C} \in \mathbb{R}^{m \times m}$ be symmetric positive semidefinite matrices. For the matrix

$$\mathcal{H} = \begin{pmatrix} A & B \\ B^T & -C \end{pmatrix},$$

Schur complement of A in \mathcal{H} is defined as $S := C + B^T A^{-1} B$.

The comparison matrix $\langle M \rangle$ is defined as follows:

$$\langle M \rangle_{ij} := \begin{cases} |M_{ij}| & \text{if } i = j \\ -|M_{ij}| & \text{if } i \neq j \end{cases}.$$

Let $N \in \mathbb{R}^{n \times m}$. The infinity norm of a matrix N is defined as follows:

$$\|N\|_\infty := \max_{1 \leq i \leq n} \sum_{j=1}^m |N_{ij}|.$$

The 2-norm of N is defined as follows:

$$\|N\|_2 := \sqrt{\lambda_{\max}(N^T N)}.$$

where $\lambda_{\max}(N)$ is a maximum eigenvalue of N .

2.2. PREVIOUS WORKS

Here, we briefly review some previous works.

Theorem 2.1 is studied by Kimura and Chen [6, Theorem 2.1]. This theorem can be applied to the following equation:

$$\mathcal{H}u = b, \quad \mathcal{H} = \begin{pmatrix} A & B \\ B^T & O \end{pmatrix}, b = \begin{pmatrix} f \\ g \end{pmatrix}, \quad (3)$$

where $A \in \mathbb{R}^{n \times n}$ is symmetric positive semidefinite and $B \in \mathbb{R}^{n \times m}$ has full rank.

THEOREM 2.1 ([6, Theorem 2.1]). *Assume that $A \in \mathbb{R}^{n \times n}$ is symmetric positive semidefinite and $B \in \mathbb{R}^{n \times m}$ has full rank. Let W be an $m \times m$ symmetric positive semidefinite matrix such that*

$$\tilde{A} = A + BWB^T,$$

is symmetric positive definite. Let u^ be a rigorous solution of (3). For any $u \in \mathbb{R}^l$, we have*

$$\|u^* - u\|_2 \leq \frac{2}{\sqrt{5} - 1} \max \left(\|\tilde{A}^{-1}\|_2, \|\tilde{A}\|_2 \|(B^T B)^{-1}\|_2 \right) \|b - \mathcal{H}u\|_2.$$

Theorem 2.2 is studied by Chen and Hashimoto [5, Theorem 1]. The authors consider the following equation:

$$\tilde{\mathcal{H}}u = \tilde{b}, \quad \tilde{\mathcal{H}} = \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{B}^T & -\tilde{C} \end{pmatrix}, \tilde{b} = \begin{pmatrix} \tilde{f} \\ \tilde{g} \end{pmatrix}, \quad (4)$$

where $\tilde{A} \in \mathbb{R}^{n \times n}$ and $\tilde{C} \in \mathbb{R}^{m \times m}$ are symmetric positive definite and semidefinite respectively, $\tilde{B} \in \mathbb{R}^{n \times m}$ has full rank.

THEOREM 2.2 ([5, Theorem 1]). *Assume that $\tilde{A} \in \mathbb{R}^{n \times n}$ and $\tilde{C} \in \mathbb{R}^{m \times m}$ are symmetric positive definite and semidefinite respectively, $\tilde{B} \in \mathbb{R}^{n \times m}$ has full rank,*

and $\tilde{S} := \tilde{C} + \tilde{B}^T \tilde{A}^{-1} \tilde{B}$. Let $u^* = (x^{*T}, y^{*T})^T$ be a rigorous solution of (4). For any $u = (x^T, y^T)^T \in \mathbb{R}^l$, we have the following inequalities:

$$\begin{aligned} \|x^* - x\|_2 &\leq \|\tilde{A}^{-1}\|_2 \left(\|r_1\|_2 + \|\tilde{B}\|_2 \|y^* - y\|_2 \right), \\ \|y^* - y\|_2 &\leq \|\tilde{S}^{-1}\|_2 \left(\|r_2\|_2 + \|\tilde{B}^T \tilde{A}^{-1}\|_2 \|r_1\|_2 \right), \end{aligned}$$

and

$$\|\tilde{S}^{-1}\|_2 \leq \frac{\|\tilde{A}\|_2 \left\| \left(\tilde{B}^T \tilde{B} \right)^{-1} \right\|_2}{1 + \|\tilde{A}\|_2 \left\| \left(\tilde{B}^T \tilde{B} \right)^{-1} \right\|_2 \lambda_{\min}(\tilde{C})}, \quad (5)$$

where the residual vectors r_1, r_2 is defined as

$$\begin{pmatrix} r_1 \\ r_2 \end{pmatrix} = \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{B}^T & -\tilde{C} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} - \begin{pmatrix} \tilde{f} \\ \tilde{g} \end{pmatrix},$$

and $\lambda_{\min}(\tilde{C})$ is a minimum eigenvalue of \tilde{C} .

Theorem 2.3 is studied by Chen and Hashimoto [5, estimation (15) and (16)]. The authors treat the following equation:

$$\begin{pmatrix} \tilde{A} & \tilde{B}L^{-T} \\ (\tilde{B}L^{-T})^T & -L^{-1}\tilde{C}L^{-T} \end{pmatrix} \begin{pmatrix} x \\ L^T y \end{pmatrix} = \begin{pmatrix} \tilde{f} \\ L^{-1}\tilde{g} \end{pmatrix}. \quad (6)$$

where $\tilde{A} \in \mathbb{R}^{n \times n}$ and $\tilde{C} \in \mathbb{R}^{m \times m}$ are symmetric positive definite and semidefinite respectively, $\tilde{B} \in \mathbb{R}^{n \times m}$ has full rank, and $L \in \mathbb{R}^{m \times m}$ is a nonsingular matrix.

THEOREM 2.3 ([5, estimation (15) and (16)]). *Assume that $\tilde{A} \in \mathbb{R}^{n \times n}$ and $\tilde{C} \in \mathbb{R}^{m \times m}$ are symmetric positive definite and semidefinite respectively, $\tilde{B} \in \mathbb{R}^{n \times m}$ has full rank, and $L \in \mathbb{R}^{m \times m}$ is nonsingular. Let $u^* = (x^{*T}, y^{*T})^T$ be a rigorous solution of (6). Let $S_l = L^{-1}\tilde{C}L^{-T} + (\tilde{B}L^{-T})^T \tilde{A}^{-1} \tilde{B}L^{-T}$ be Schur complement of \tilde{A} in the*

coefficient matrix of (6). The Residual vectors r_1, r_2 are defined as in Theorem 2.2.

For any $u = (x^T, y^T)^T \in \mathbb{R}^l$, we have the following inequality:

$$\begin{aligned}\|x^* - x\|_2 &\leq \|\tilde{A}^{-1}\|_2 \left(\|r_1\|_2 + \|\tilde{B}L^{-T}\|_2 \|L^T(y^* - y)\|_2 \right), \\ \|L^T(y^* - y)\|_2 &\leq \|S_t^{-1}\|_2 \left(\|L^{-1}r_2\|_2 + \left\| \left(\tilde{B}L^{-T} \right)^T \tilde{A}^{-1} \right\|_2 \|r_1\|_2 \right),\end{aligned}$$

and

$$\|S_t^{-1}\|_2 \leq \frac{\|\tilde{A}\|_2 \left\| L^T \left(\tilde{B}^T \tilde{B} \right)^{-1} L \right\|_2}{1 + \|\tilde{A}\|_2 \left\| L^T \left(\tilde{B}^T \tilde{B} \right)^{-1} L \right\|_2 \lambda_{\min}(L^{-1}\tilde{C}L^{-T})}.$$

CHAPTER 3

NEW VERIFICATION METHODS

3.1. REGULARIZATION OF A

In this thesis, we will propose methods based on Schur complement. However, since A of (1) is symmetric positive semidefinite, that may be singular, we can't directly apply those methods to (1). So, in this section, we show a method that regularize A of (1).

First, we show the following proposition and prove it.

PROPOSITION 3.1. *Let $A \in \mathbb{R}^{n \times n}$ and $C \in \mathbb{R}^{m \times m}$ be symmetric positive semidefinite, and $B \in \mathbb{R}^{n \times m}$ has full rank. Assume that $W \in \mathbb{R}^{m \times m}$ is symmetric positive definite. Under the conditions that \mathcal{H} of (1) is nonsingular, there exists a matrix W satisfying the following conditions:*

- (a) $\tilde{A} := A + BWB^T$ is a symmetric positive definite matrix,
- (b) $\tilde{B} := B - BWC$ has full rank,
- (c) $\tilde{C} := C - CWC$ is a symmetric positive semidefinite matrix.

PROOF. We use the method of proof by contradiction to prove that the condition (a) is satisfied. We assume that $\bar{x} \neq 0$ is a solution of $\tilde{A}\bar{x} = 0$, then we have

$$\bar{x}^T \tilde{A} \bar{x} = \bar{x}^T A \bar{x} + \bar{x}^T B W B^T \bar{x} = 0.$$

Since A and BWB^T are positive semidefinite, we obtain

$$\bar{x}^T A \bar{x} = 0 \quad \text{and} \quad \bar{x}^T B W B^T \bar{x} = 0.$$

By the positive definiteness of W , we have

$$B^T \bar{x} = 0.$$

Moreover, since A is symmetric positive semidefinite, we can factorize as $A = L_A L_A^T$ ($L_A \in \mathbb{R}^{n \times n}$) and the following equations are satisfied

$$\bar{x}^T A \bar{x} = \bar{x}^T L_A L_A^T \bar{x} = 0.$$

Then

$$\|L_A^T \bar{x}\| = 0.$$

Thus, we have

$$A \bar{x} = 0.$$

Let $z = (\bar{x}, 0)^T$, then $\mathcal{H}z = 0$. However, this contradicts to the fact that \mathcal{H} is nonsingular. Thus, \tilde{A} is symmetric positive definite.

It remains to prove that conditions (b) and (c) are satisfied. In the case of $C = O$, it is clear to satisfy conditions (b) and (c). In this case, W can be chosen as follows:

$$W = \frac{\alpha}{\|BB^T\|_2} I,$$

where α satisfies $0 < \alpha < 1$ (See [6]).

Next, we consider the case $C \neq O$. For example, we can take

$$W = \frac{\alpha}{\|C\|_2} I, \tag{7}$$

where α satisfies $0 < \alpha < 1$. Denote λ_i ($i = 1, \dots, m$) as the nonnegative eigenvalues of C . Since C is symmetric positive semidefinite, C can be factorized as

$$C = Q^T D Q, \tag{8}$$

where D is a diagonal matrix whose diagonal elements are λ_i ($i = 1, \dots, m$) and Q is an orthogonal matrix.

By (7), (8), and $\tilde{B} := B - BWC$, we have

$$\begin{aligned}\tilde{B} &= B(I - WC), \\ &= B(Q^T Q - \frac{\alpha}{\|C\|_2} Q^T D Q), \\ &= BQ^T(I - \frac{\alpha}{\|C\|_2} D)Q.\end{aligned}$$

Since B has full rank, Q is an orthogonal matrix, $\|C\|_2 = \max(\lambda_i)$, $D = \text{diag}(\lambda_i)$, and $0 < \alpha < 1$, then \tilde{B} has full rank.

Similarly, by (7), (8), and $\tilde{C} := C - CWC$, we have

$$\begin{aligned}\tilde{C} &= C - CWC, \\ &= Q^T D Q - (Q^T D Q) \frac{\alpha}{\|C\|_2} I (Q^T D Q), \\ &= Q^T D Q - \frac{\alpha}{\|C\|_2} Q^T D (Q Q^T) D Q, \\ &= Q^T D^{1/2} (I - \frac{\alpha}{\|C\|_2} D) D^{1/2} Q,\end{aligned}$$

where $D^{1/2} = \text{diag}(\sqrt{\lambda_i})$. Since $\|C\|_2 = \max(\lambda_i)$, $D = \text{diag}(\lambda_i)$, $0 < \alpha < 1$, and Q is an orthogonal matrix, for $x \neq 0$, we have

$$x^T \tilde{C} x = x Q^T D^{1/2} (I - \frac{\alpha}{\|C\|_2} D) D^{1/2} Q x \geq 0. \quad (9)$$

Thus \tilde{C} is symmetric positive semidefinite. \square

Next, using the W in Proposition 3.1, we define a preconditioner as follows:

$$\mathcal{P}_w = \begin{pmatrix} I & BW \\ O & (I - WC)^T \end{pmatrix}. \quad (10)$$

Multiplying both sides of (1) by \mathcal{P}_w , equation (1) can be rewritten as

$$\tilde{\mathcal{H}}u = \tilde{b}, \quad \tilde{\mathcal{H}} := \mathcal{P}_w \mathcal{H} = \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{B}^T & -\tilde{C} \end{pmatrix}, \quad \tilde{b} := \mathcal{P}_w b = \begin{pmatrix} \tilde{f} \\ \tilde{g} \end{pmatrix}, \quad (11)$$

where \tilde{A} , \tilde{B} , and \tilde{C} are defined as in Proposition 3.1, $\tilde{f} := f + BWg$, and $\tilde{g} := g - CWg$. Since \tilde{A} of (11) is nonsingular, we can apply the methods based on Schur complement to (11).

The preconditioner \mathcal{P}_w is nonsingular, because it is upper triangular block matrix and its diagonal block matrices I and $(I - WC)^T$ are nonsingular. So, (11) is equivalent to (1) and the coefficient $\tilde{\mathcal{H}}$ becomes nonsingular. It is known that when \tilde{A} is nonsingular, $\tilde{\mathcal{H}}$ is nonsingular if and only if \tilde{S} is nonsingular (see [3]). Because $\tilde{\mathcal{H}}$ can be factorized as follows:

$$\tilde{\mathcal{H}} = \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{B}^T & -\tilde{C} \end{pmatrix} = \begin{pmatrix} I & O \\ \tilde{B}^T \tilde{A}^{-1} & I \end{pmatrix} \begin{pmatrix} \tilde{A} & O \\ O & \tilde{S} \end{pmatrix} \begin{pmatrix} I & \tilde{B} \tilde{A}^{-1} \\ O & I \end{pmatrix},$$

where

$$\tilde{S} := \tilde{C} + \tilde{B}^T \tilde{A}^{-1} \tilde{B}. \quad (12)$$

Since $\tilde{\mathcal{H}}$ is nonsingular, \tilde{S} becomes nonsingular.

3.2. EIGENVALUES OF THE PRECONDITIONED MATRIX

In next section, we will propose a new error bound for an approximate solution of (11). This method is based on results of an algebraic analysis of a preconditioner. First, we consider an inclusion of all eigenvalues of the preconditioned matrix. For (11), we define the following preconditioner:

$$\mathcal{P} = \begin{pmatrix} \tilde{A} & O \\ O & \tilde{S} \end{pmatrix}, \quad (13)$$

where $\tilde{S} := \tilde{C} + \tilde{B}^T \tilde{A}^{-1} \tilde{B}$.

In [2], Axelsson and Neytcheva have proved that all eigenvalues of the preconditioned matrix $\mathcal{P}^{-1} \tilde{\mathcal{H}}$ are included in

$$\left[-1, -\frac{1}{2} \right] \cup [1, 2].$$

We improve this inclusion of all eigenvalues of the preconditioned matrix as follows:

THEOREM 3.1. *A preconditioner \mathcal{P} is defined as (13). All eigenvalues of the preconditioned matrix $\mathcal{P}^{-1}\tilde{\mathcal{H}}$ are included in*

$$\left(-1, \frac{1-\sqrt{5}}{2}\right] \cup \left[1, \frac{1+\sqrt{5}}{2}\right).$$

PROOF. Let $\mu \neq 0$ be an eigenvalue of $\mathcal{P}^{-1}\tilde{\mathcal{H}}$ with an eigenvector $(u^T, v^T)^T \neq 0$, i.e.,

$$\begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{B}^T & -\tilde{C} \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \mu \begin{pmatrix} \tilde{A} & O \\ O & \tilde{S} \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}. \quad (14)$$

We show that $\mu = 1$ if and only if v is a zero vector. If $\mu = 1$, the first equation of (14) can be rewritten as

$$\tilde{A}u + \tilde{B}v = \tilde{A}u.$$

Since \tilde{B} is full rank, $v = 0$. If $v = 0$, the first equation of (14) can be rewritten as

$$\tilde{A}u = \mu\tilde{A}u. \quad (15)$$

By $(u^T, v^T)^T \neq 0$ and A is nonsingular, we have $\tilde{A}u \neq 0$. Thus $\mu = 1$.

If $\mu \neq 1$, then v is a nonzero vector. In this case, (14) can be rewritten as

$$\tilde{A}u + \tilde{B}v = \mu\tilde{A}u, \quad (16a)$$

$$\tilde{B}^T u - \tilde{C}v = \mu\tilde{S}v. \quad (16b)$$

From (16a), we have

$$u = \frac{1}{(\mu-1)}\tilde{A}^{-1}\tilde{B}v. \quad (17)$$

Substituting (17) to (16b), we get the following equation:

$$(\mu^2 \tilde{S} - \mu(\tilde{B}^T \tilde{A}^{-1} \tilde{B}) - \tilde{S})v = 0. \quad (18)$$

Equation (18) can be rewritten as

$$\tilde{B}^T \tilde{A}^{-1} \tilde{B}v = \lambda \tilde{S}v, \quad (19)$$

where

$$\lambda = \frac{\mu^2 - 1}{\mu}. \quad (20)$$

Now, we try to include the eigenvalues of (19). First, we show $0 < \lambda \leq 1$.

If $v \neq 0$ and $\tilde{C}v = 0$, then from the nonsingularity of \tilde{S} , it follows that $\tilde{B}^T \tilde{A}^{-1} \tilde{B}v \neq 0$ and $\lambda = 1$. Conversely, if $\lambda = 1$, then $\tilde{C}v = 0$.

If $\lambda \neq 1$, then (19) can be rewritten as

$$\tilde{B}^T \tilde{A}^{-1} \tilde{B}v = \frac{\lambda}{1 - \lambda} \tilde{C}v.$$

Since $\tilde{B}^T \tilde{A}^{-1} \tilde{B}$ and \tilde{C} are positive definite and semidefinite respectively and $\tilde{C}v \neq 0$, the generalized eigenvalues $\lambda/(1 - \lambda)$ must be positive. Hence $0 < \lambda < 1$. We showed $0 < \lambda \leq 1$ for (19).

Since (20) and $0 < \lambda \leq 1$, we have

$$1 < \frac{1}{2} \left(\lambda + \sqrt{\lambda^2 + 4} \right) \leq \frac{1}{2} (1 + \sqrt{5}),$$

and

$$-1 < \frac{1}{2} \left(\lambda - \sqrt{\lambda^2 + 4} \right) \leq \frac{1}{2} (1 - \sqrt{5}).$$

Consequently, all eigenvalues of the preconditioned matrix $\mathcal{P}^{-1} \tilde{\mathcal{H}}$ are included in

$$\left(-1, \frac{1 - \sqrt{5}}{2} \right] \cup \left[1, \frac{1 + \sqrt{5}}{2} \right).$$

□

3.3. NEW ERROR BOUND

From Theorem 3.1, we obtain the following rigorous error bound for (11).

THEOREM 3.2. *Assume that $\tilde{A} \in \mathbb{R}^{n \times n}$ and $\tilde{C} \in \mathbb{R}^{m \times m}$ are symmetric positive definite and semidefinite respectively, $\tilde{B} \in \mathbb{R}^{n \times m}$ has full rank, and $\tilde{S} := \tilde{C} + \tilde{B}^T \tilde{A}^{-1} \tilde{B}$. $\tilde{\mathcal{H}}$ and \tilde{b} are defined by (11). Let u^* be a rigorous solution of (11). For any $u \in \mathbb{R}^l$, we have*

$$\|u^* - u\|_2 \leq \frac{2}{\sqrt{5} - 1} \max\left(\|\tilde{A}^{-1}\|_2, \|\tilde{S}^{-1}\|_2\right) \|\tilde{b} - \tilde{\mathcal{H}}u\|_2.$$

PROOF. Obviously, we have

$$\|u^* - u\|_2 \leq \|\tilde{\mathcal{H}}^{-1}\|_2 \|\tilde{b} - \tilde{\mathcal{H}}u\|_2.$$

Let \mathcal{L} be a nonsingular matrix such that $\mathcal{L}\mathcal{L}^T = \mathcal{P}$. We define

$$\mathcal{G} = \mathcal{L}^{-1} \tilde{\mathcal{H}} \mathcal{L}^{-T}. \quad (21)$$

Then, the inverse of $\tilde{\mathcal{H}}$ can be given as

$$\tilde{\mathcal{H}}^{-1} = \mathcal{L}^{-T} \mathcal{G}^{-1} \mathcal{L}^{-1}.$$

Since $\tilde{\mathcal{H}}$ and \mathcal{G} are symmetric, we have

$$\begin{aligned} \|\tilde{\mathcal{H}}^{-1}\|_2 &= \max_{v \in \mathbb{R}^l, v \neq 0} \left| \frac{v^T \mathcal{L}^{-T} \mathcal{G}^{-1} \mathcal{L}^{-1} v}{v^T v} \right|, \\ &= \max_{v \in \mathbb{R}^l, v \neq 0} \left| \frac{v^T \mathcal{L}^{-T} \mathcal{G}^{-1} \mathcal{L}^{-1} v}{v^T \mathcal{L}^{-T} \mathcal{L}^{-1} v} \frac{v^T \mathcal{L}^{-T} \mathcal{L}^{-1} v}{v^T v} \right|, \\ &\leq \max_{w \in \mathbb{R}^l, w \neq 0} \left| \frac{w^T \mathcal{G}^{-1} w}{w^T w} \right| \max_{v \in \mathbb{R}^l, v \neq 0} \left| \frac{v^T \mathcal{P}^{-1} v}{v^T v} \right|, \\ &= \|\mathcal{G}^{-1}\|_2 \|\mathcal{P}^{-1}\|_2. \end{aligned}$$

From (21) and $\mathcal{L}\mathcal{L}^T = \mathcal{P}$, we have

$$\mathcal{G} = \mathcal{L}^T \mathcal{P}^{-1} \tilde{\mathcal{H}} \mathcal{L}^{-T}.$$

Hence, \mathcal{G} and $\mathcal{P}^{-1} \tilde{\mathcal{H}}$ have the same eigenvalues.

By Theorem 3.1, all eigenvalues of $\mathcal{P}^{-1} \tilde{\mathcal{H}}$ are included in

$$\left(-1, \frac{1 - \sqrt{5}}{2}\right] \cup \left[1, \frac{1 + \sqrt{5}}{2}\right).$$

Hence the norm of the matrix \mathcal{G}^{-1} satisfies

$$\|\mathcal{G}^{-1}\|_2 \leq \frac{2}{\sqrt{5} - 1},$$

then we obtain

$$\|\tilde{\mathcal{H}}^{-1}\|_2 \leq \frac{2}{\sqrt{5} - 1} \|\mathcal{P}^{-1}\|_2.$$

Moreover, from (13), we have

$$\|\mathcal{P}^{-1}\|_2 \leq \max\left(\|\tilde{A}^{-1}\|_2, \|\tilde{S}^{-1}\|_2\right).$$

□

In this thesis, when we compute the matrix norm $\|\tilde{S}^{-1}\|_2$, we use the following inequality:

$$\|\tilde{S}^{-1}\|_2 \leq \frac{\|\tilde{A}\|_2 \left\| \left(\tilde{B}^T \tilde{B} \right)^{-1} \right\|_2}{1 + \|\tilde{A}\|_2 \left\| \left(\tilde{B}^T \tilde{B} \right)^{-1} \right\|_2 \lambda_{\min}(\tilde{C})}. \quad (22)$$

The proof of this inequality can be found in [5]. Usually, when we compute $\|(\tilde{C} + \tilde{B}^T \tilde{A}^{-1} \tilde{B})^{-1}\|_2$ using the verification method, the main computing cost is $\frac{1}{3}m^3 + 4mn^2 + 4m^2n + \frac{1}{3}n^3$. The details are as follows:

$$\text{the inverse of } \tilde{A} : \quad \frac{1}{3}m^3,$$

the inclusion of $\tilde{B}^T \tilde{A}^{-1} \tilde{B}$: $4mn^2 + 4m^2n$,

the norm of $(\tilde{C} + \tilde{B}^T \tilde{A}^{-1} \tilde{B})^{-1}$: $\frac{1}{3}n^3$.

However, when we compute the right hand side of the inequality (22), the main computing cost is $\frac{2}{3}m^3 + 4m^2n + \frac{1}{3}n^3$. The details are as follows:

the norm of \tilde{A} : $\frac{1}{3}n^3$,

the inclusion of $\tilde{B}^T \tilde{B}$: $4m^2n$,

the norm of $(\tilde{B}^T \tilde{B})^{-1}$: $\frac{1}{3}m^3$,

the minimum eigenvalue of \tilde{C} : $\frac{1}{3}m^3$.

REMARK 3.1. *Theorem 3.2 is the extension of Theorem 2.1 in [6]. If $C = O$, then Theorem 3.2 reduces to Theorem 2.1 in [6].*

REMARK 3.2. *By computing the matrix norms $\|\tilde{A}^{-1}\|_2$, $\|\tilde{S}^{-1}\|_2$, and the residual $\|\tilde{b} - \tilde{\mathcal{H}}u\|_2 = (\|r_1\|_2^2 + \|r_2\|_2^2)^{1/2}$, one can obtain two bounds for $\|u^* - u\|_2$ from Theorems 3.2 and 2.2. Comparing the two bounds, we can choose smaller one.*

3.4. ERROR BOUNDS FOR PRECONDITIONED PROBLEM

In [5, 6], a useful preconditioner is proposed for (11). A method used the preconditioner is efficient when $\|(\tilde{B}^T \tilde{B})^{-1}\|_2$ is large. The error bound of Theorem 3.2 depends on $\|\tilde{S}^{-1}\|_2$ that includes $\|(\tilde{B}^T \tilde{B})^{-1}\|_2$. Therefore, the error bound may become large when $\|(\tilde{B}^T \tilde{B})^{-1}\|_2$ is large. However, when this method is used, the error bound may be improved. To improve the error bound of Theorem 3.2, we apply the preconditioning method to Theorem 3.2.

Let $L \in \mathbb{R}^{m \times m}$ be a nonsingular matrix. We define a preconditioner

$$\mathcal{P}_l = \begin{pmatrix} I & O \\ O & L^{-1} \end{pmatrix}. \quad (23)$$

In this thesis, we use an approximation of the Cholesky factor of $\tilde{B}^T \tilde{B}$ as L . Multiplying both side of (11) by (23), then we have

$$\mathcal{P}_l \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{B}^T & -\tilde{C} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \mathcal{P}_l \begin{pmatrix} \tilde{f} \\ \tilde{g} \end{pmatrix}.$$

This can be rewritten as

$$\begin{pmatrix} \tilde{A} & \tilde{B}L^{-T} \\ (\tilde{B}L^{-T})^T & -L^{-1}\tilde{C}L^{-T} \end{pmatrix} \begin{pmatrix} x \\ L^T y \end{pmatrix} = \begin{pmatrix} \tilde{f} \\ L^{-1}\tilde{g} \end{pmatrix}. \quad (24)$$

Moreover, the residual (r_1, r_2) of the approximate solution (x, y) satisfies

$$\begin{pmatrix} r_1 \\ L^{-1}r_2 \end{pmatrix} = \begin{pmatrix} \tilde{A} & \tilde{B}L^{-T} \\ (\tilde{B}L^{-T})^T & -L^{-1}\tilde{C}L^{-T} \end{pmatrix} \begin{pmatrix} x \\ L^T y \end{pmatrix} - \begin{pmatrix} \tilde{f} \\ L^{-1}\tilde{g} \end{pmatrix}.$$

Applying Theorem 2.2 to (24), we immediately obtain Theorem 2.3. Similarly, by applying Theorem 3.2 to (24), we have the following theorem:

THEOREM 3.3. *Assume that $\tilde{A} \in \mathbb{R}^{n \times n}$ and $\tilde{C} \in \mathbb{R}^{m \times m}$ are symmetric positive definite and semidefinite respectively, $\tilde{B} \in \mathbb{R}^{n \times m}$ has full rank, and $L \in \mathbb{R}^{m \times m}$ is nonsingular. \mathcal{P}_l is defined by (23). $\tilde{\mathcal{H}}$ and \tilde{b} are defined by (11). Let $S_l = L^{-1}\tilde{C}L^{-T} + (\tilde{B}L^{-T})^T \tilde{A}^{-1} \tilde{B}L^{-T}$ be Schur complement of \tilde{A} in the coefficient matrix of (24). Let u^* be a rigorous solution of (24). For any $u \in \mathbb{R}^l$, we have*

$$\|u^* - u\|_2 \leq \frac{2}{\sqrt{5} - 1} \max \left(\|\tilde{A}^{-1}\|_2, \|S_l^{-1}\|_2 \right) \|\mathcal{P}_l^T\|_2 \left\| \mathcal{P}_l \begin{pmatrix} \tilde{b} - \tilde{\mathcal{H}}u \end{pmatrix} \right\|_2,$$

where

$$\|\mathcal{P}_l^T\|_2 \leq \max(1, \|L^{-1}\|_2).$$

PROOF. We have

$$\begin{aligned}\|u^* - u\|_2 &= \left\| \mathcal{P}_l^T \mathcal{P}_l^{-T} \tilde{H}^{-1} \mathcal{P}_l^{-1} \mathcal{P}_l (\tilde{b} - \tilde{H}u) \right\|_2 \\ &\leq \|\mathcal{P}_l^T\|_2 \left\| (\mathcal{P}_l \tilde{H} \mathcal{P}_l^T)^{-1} \right\|_2 \left\| \mathcal{P}_l (\tilde{b} - \tilde{H}u) \right\|_2.\end{aligned}$$

Since $\mathcal{P}_l \tilde{H} \mathcal{P}_l^T$ is symmetric, we have

$$\left\| (\mathcal{P}_l \tilde{H} \mathcal{P}_l^T)^{-1} \right\|_2 \leq \frac{2}{\sqrt{5} - 1} \max \left(\left\| \tilde{A}^{-1} \right\|_2, \left\| S_l^{-1} \right\|_2 \right).$$

Moreover, from (23), we have

$$\|\mathcal{P}_l^T\|_2 \leq \max(1, \|L^{-1}\|_2).$$

□

In this thesis, when we compute the matrix norm $\|S_l^{-1}\|_2$, we use the following inequality:

$$\|S_l^{-1}\|_2 \leq \frac{\left\| \tilde{A} \right\|_2 \left\| L^T (\tilde{B}^T \tilde{B})^{-1} L \right\|_2}{1 + \left\| \tilde{A} \right\|_2 \left\| L^T (\tilde{B}^T \tilde{B})^{-1} L \right\|_2 \lambda_{\min}(L^{-1} \tilde{C} L^{-T})}.$$

The proof is similar to the proof of (22).

3.5. VERIFICATION METHODS

We have to further consider rounding errors to compute the rigorous error bounds based on Theorems 3.2 and 3.3. We use interval arithmetic to take care of rounding errors.

For obtaining the rigorous error bounds based on Theorems 3.2 and 3.3, we need to compute the upper bound of the 2-norms of a symmetric matrix and its inverse. To compute these upper bounds, we use two methods which are pointed out in Rump [9, Eq.(3.19), (5.10-12)]. First, we show a method of computing the error bound of the 2-norm of a matrix.

METHOD 3.1 (Verification method for the 2-norm of a matrix). *Assume that M is symmetric. Let \tilde{p} be an approximation of $\|M\|_2$, for any $M \in \mathbb{R}^{n \times n}$. We define $p = (1 + e)\tilde{p}$ for any $e > 0$. If*

$$M^T = M, \quad pI - M \succeq 0 \quad \text{and} \quad pI + M \succeq 0$$

is satisfied, then

$$\|M\|_2 \leq p.$$

A method of computing the error bound of the 2-norm of an inverse matrix is studied by Rump [9, p12].

METHOD 3.2 (Verification method of the 2-norm of an inverse matrix). *We define*

$$p = \|L_D^T G^{-1} L_D\|_2,$$

where $G \in \mathbb{R}^{n \times n}$ is symmetric, $D \in \mathbb{R}^{n \times n}$ is symmetric positive definite, and L_D is the Cholesky factor of D such that $L_D L_D^T = D$. And we define \tilde{q} is an approximation of the minimum eigenvalue of a generalized eigenvalue problem $Gx = \lambda Dx$ and $q = (1 - e)\tilde{q}$ for any $0 < e < 1$. If

$$q > 0 \quad \text{and} \quad G - qD \succeq 0$$

is satisfied, then

$$p \leq q^{-1}.$$

In the actual computing, we use the function `isspd` of INTLAB [11] to verify the positive definiteness. INTLAB is a toolbox of MATLAB for using interval arithmetic. This function uses the Cholesky decomposition when the matrix is symmetric, so the computational cost is $\mathcal{O}(n^3/3)$. If a matrix is sparse, then the computational cost

is smaller. Note that when we compute $\|C\|_2$, $\|L^{-1}\|_2$, and other norms using the function `isspd`, we set $e = 10^{-6}$, 10^{-4} , and 10^{-2} , respectively.

Obviously, an error bound of Theorem 3.2 depends on the choice of W . In this thesis, if A is singular, we consider the following choice:

$$W = \frac{\alpha}{\|BB^T\|_2}I \quad (C = O) \quad \text{or} \quad W = \frac{\alpha}{\|C\|_2}I \quad (C \neq O),$$

where α satisfies $0 < \alpha < 1$. We set $W = O$ if A is nonsingular.

When we compute the rigorous error bounds using a preconditioned method (Theorem 3.3), we use the technique in [5, 6]. Let \hat{L} be an approximation of the Cholesky factor of $\tilde{B}^T \tilde{B}$ such that $\hat{L}\hat{L}^T \approx \tilde{B}^T \tilde{B}$. Let R_l be an approximation of the inverse of \hat{L} such that $\hat{L}R_l \approx I$. Define the error matrices by $E_1 := \hat{L}\hat{L}^T - \tilde{B}^T \tilde{B}$ and $E_2 := R_l \hat{L} - I$. Moreover, let $E_3 := E_2 + E_2^T + E_2 E_2^T - R_l E_1 R_l^T$ be.

If $\|E_3\|_2 < 1$ is satisfied, then, by [5], we have the following inequalities:

$$\left\| R_l^{-T} \left(\tilde{B}^T \tilde{B} \right)^{-1} R_l^{-1} \right\|_2 \leq \frac{1}{1 - \|E_3\|_\infty},$$

and

$$\left\| R_l \tilde{B}^T \right\|_2^2 \leq \left\| \left(R_l \tilde{B}^T \right)^T \right\|_2^2 \leq 1 + \|E_3\|_\infty.$$

CHAPTER 4

NUMERICAL EXPERIMENTS

To illustrate the usefulness of the proposed methods, we carried out some numerical examples and compared the proposed verification methods based on Theorems 3.2 and 3.3 with the methods based on Theorems 2.2 and 2.3, the method studied by Rump [10], and the method studied by Minamihata, Sekine, Ogita, Rump, and Oishi [7, Theorem 3.3]. Here, Rump's method and Minamihata-Sekine-Ogita-Rump-Oishi's method are the verification methods for an approximate solution of general linear systems. We briefly show these methods.

THEOREM 4.1 (Rump's method[10]). *Let $H \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$ be given. Let $\tilde{x} \in \mathbb{R}^n$ be an approximation of $Hx = b$ and $R \in \mathbb{R}^{n \times n}$ be an approximation of H^{-1} . Assume that $v > 0 \in \mathbb{R}^n$ satisfies $u := \langle RH \rangle v > 0$. Let $D \in \mathbb{R}^{n \times n}$ be the diagonal part of $\langle RH \rangle$. $w \in \mathbb{R}^n$ is defined as:*

$$w_k := \max_{1 \leq i \leq n} \frac{G_{ik}}{u_i} \quad \text{for } 1 \leq k \leq n.$$

where $G := I - \langle RH \rangle D^{-1} \geq O$. Then RH is nonsingular and

$$|H^{-1}b - \tilde{x}| \leq (D^{-1} + vw^T)|c|, \quad c := R(b - H\tilde{x}).$$

THEOREM 4.2 (Minamihata et al. method[7]). *Let $H, R \in \mathbb{R}^{n \times n}$ and $b, \tilde{x} \in \mathbb{R}^n$ be given. c, u, v, w , and D are defined as in Theorem 4.1. We define $D_s := \text{diag}(s_1, \dots, s_n) \in \mathbb{R}^{n \times n}$ with*

$$s_k := u_k w_k \geq 0 \quad (1 \leq k \leq n).$$

Then RH is nonsingular and

$$|H^{-1}b - \tilde{x}| \leq (D^{-1} + vw^T)(I + Ds)^{-1}|c|.$$

Numerical experiments were carried out on the following environment:

- OS : CentOS 6.6
- CPU : 2.6GHz × 24 Intel(R) Xeon(R) CPU E5-2690

- memory: 252.2GB
- tool : MATLAB R2016a, INTLAB V9 [11]

We use INTLAB [11] to take care of rounding errors.

4.1. EXAMPLE 1

We consider linear systems as follows:

$$\mathcal{H}u = \begin{pmatrix} A & B \\ B^T & -C \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}, \quad (25)$$

where

$$A = \begin{pmatrix} X & O \\ O & O \end{pmatrix}, B = \begin{pmatrix} O \\ Y \end{pmatrix}, x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \quad (26)$$

$X \in \mathbb{R}^{n_1 \times n_1}$, $C \in \mathbb{R}^{m \times m}$ are symmetric positive definite, $Y \in \mathbb{R}^{n_2 \times m}$ has full rank, $x_1, f_1 \in \mathbb{R}^{n_1}$, $x_2, f_2 \in \mathbb{R}^{n_2}$, $y, g \in \mathbb{R}^m$ and $n = n_1 + n_2$. In this example, we set $n_1 = 2n_2$.

The matrices X and C are generated using the function `sprandsym` of MATLAB as follows:

$$X = 10 \times \text{sprandsym}(n_1, 5/n_1, 10^{-2}, 1),$$

$$C = 0.1 \times \text{sprandsym}(m, 5/m, 10^{-4}, 1).$$

Here, the function `sprandsym(size, density, rc, kind)` returns a symmetric random, $size \times size$, sparse, positive definite matrix with a reciprocal condition number equal to rc and approximately $density \times size \times size$ nonzeros. The matrix Y is generated using the function `sprand` of MATLAB as follows:

$$Y = \text{sprand}(n_2, m, 5/n_2, 10^{-1}).$$

Here, the function `sprand(row, col, density, rc)` returns a random, $row \times col$, sparse matrix with a reciprocal condition number equal to rc and approximately $density \times row \times col$ nonzeros. The vectors f_1, f_2, g are defined as $\mathcal{H}u$ where u is all-ones vector.

An approximate solution of (25) is obtained using the function `mldivide` of MATLAB. In this example, since A is singular, we set $W = \frac{\alpha}{\|C\|_2}I$ where $\alpha = 0.5$.

In Figure 4.1, error bounds of each methods for example 1 and exact errors are shown. Since we know an exact solution u^* and have an approximation u , we calculate an upper bound of $\|u^* - u\|_2$ and show it as the exact error.

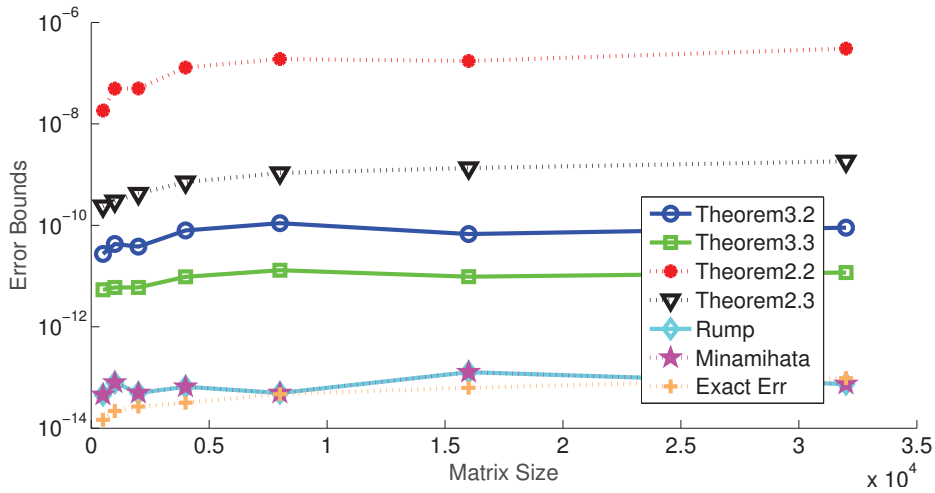


FIGURE 4.1. Error bounds for example 1.

In Figure 4.2, CPU time of each methods for example 1 are shown.

In Table 4.1, we show numerical results of error bounds and CPU time for example 1. In this table, quantities inside square brackets are CPU time (sec). Moreover, “Apptime” is CPU time (sec) of computing the approximation, and “Cond Num” is the condition number of the coefficient matrix. Residual $\|b - \mathcal{H}u\|_2$ are shown in 4th row.

Since we know the exact solution, we show the upper bounds of $\|u^* - u\|_2$ as the exact error in the 5th row. In the 6th to 8th rows of this table, we show the upper bounds of the norm of quantities needed in Theorem 3.2. Similarly, in the 13th to

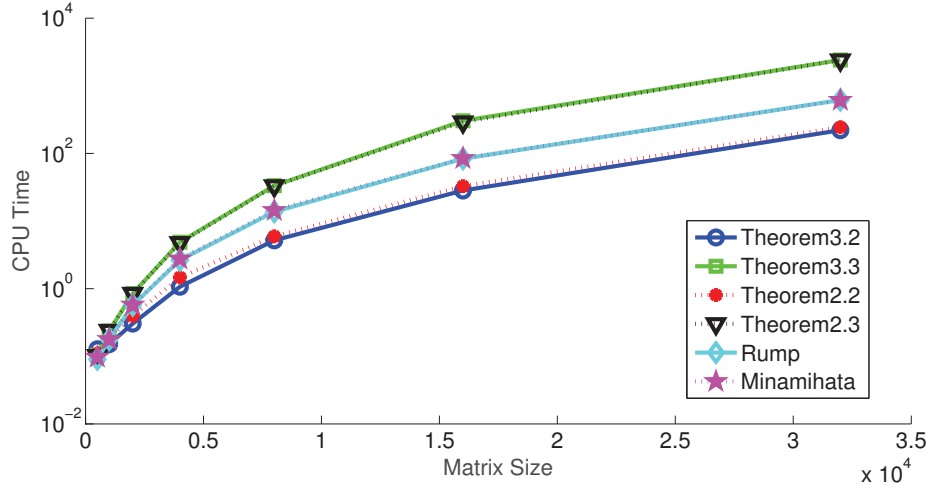


FIGURE 4.2. CPU time for example 1.

15th rows, we show the upper bounds of the norm of quantities needed in Theorem 3.3.

In this example, since we know the eigenvalues of X and C and the singular values of Y , we can calculate the 2-norm of the inverse of \tilde{A} . $\|\tilde{A}^{-1}\|_2 = \max(\|X^{-1}\|_2, 2\|C\|_2 \|(YY^T)^{-1}\|_2) \approx 2.000 * 10$. It is shown that the computed values of the norm are near the calculated ones. The error bounds are as in Table 4.1.

The new method and the new preconditioned method give error bounds sharper than those obtained by the methods based on Theorems 2.2 and 2.3. CPU time of the methods based on Theorem 3.2 and 2.2 are almost same. The method on Theorem 3.2 is faster than the verification methods for general linear systems. CPU time of the preconditioned methods based on Theorems 3.3 and 2.3 are almost same. However, only in this example, CPU time of the preconditioned methods are longer than the verification methods for general linear systems. Because L in this example is more dense than one in other examples. Therefore, the computing cost of $\|L^{-1}\|_2$ and $\|L^T(\tilde{B}^T\tilde{B})^{-1}L\|_2$ become high.

TABLE 4.1. Error bounds and CPU time for example 1.

(n, m)	(1500, 500)	(3000, 1000)	(6000, 2000)	(12000, 4000)	(24000, 8000)
Apptime	[5.128e-02s]	[2.852e-01s]	[1.676e+00s]	[1.195e+01s]	[1.094e+02s]
Cond Num	2.163e+02	2.773e+02	3.454e+02	4.321e+02	3.700e+02
$\ b - \mathcal{H}u\ _2$	1.421e-14	1.776e-14	2.309e-14	2.132e-14	2.309e-14
$\ u^* - u\ _2$	2.680e-14	3.176e-14	4.696e-14	6.255e-14	9.653e-14
$\ \tilde{A}^{-1}\ _2$	2.020e+01	2.020e+01	2.020e+01	2.020e+01	2.020e+01
$\ \tilde{S}^{-1}\ _2$	1.651e+03	2.748e+03	2.947e+03	1.948e+03	2.400e+03
$\ \tilde{b} - \tilde{\mathcal{H}}u\ _2$	1.423e-14	1.776e-14	2.309e-14	2.132e-14	2.309e-14
Theorem 3.2 (New)	3.800e-11 [3.037e-01s]	7.899e-11 [1.068e+00s]	1.101e-10 [5.177e+00s]	6.717e-11 [2.818e+01s]	8.966e-11 [2.204e+02s]
Theorem 2.2 (Previous)	4.971e-08 [3.948e-01s]	1.290e-07 [1.467e+00s]	1.895e-07 [5.936e+00s]	1.741e-07 [3.281e+01s]	3.049e-07 [2.441e+02s]
$\ S_l^{-1}\ _2$	1.010e+01	1.010e+01	1.010e+01	1.010e+01	1.010e+01
$\ L^{-1}\ _2$	1.283e+01	1.664e+01	1.725e+01	1.395e+01	1.552e+01
$\ \mathcal{P}_l(\tilde{b} - \tilde{\mathcal{H}}u)\ _2$	1.423e-14	1.776e-14	2.309e-14	2.132e-14	2.309e-14
Theorem 3.3 (New)	5.966e-12 [8.413e-01s]	9.664e-12 [4.848e+00s]	1.302e-11 [3.325e+01s]	9.723e-12 [3.028e+02s]	1.172e-11 [2.400e+03s]
Theorem 2.3 (Previous)	4.216e-10 [8.451e-01s]	7.118e-10 [4.770e+00s]	1.077e-09 [3.301e+01s]	1.349e-09 [2.896e+02s]	1.829e-09 [2.394e+03s]
Rump's method	4.949e-14 [5.677e-01s]	6.547e-14 [2.635e+00s]	4.942e-14 [1.369e+01s]	1.269e-13 [8.318e+01s]	7.438e-14 [6.155e+02s]
Minamihata's method	4.949e-14 [5.739e-01s]	6.547e-14 [2.741e+00s]	4.942e-14 [1.433e+01s]	1.269e-13 [8.443e+01s]	7.438e-14 [6.099e+02s]

Note: Quantities inside square brackets are CPU time (sec), ‘‘Apptime’’ is CPU time(sec) of computing the approximation, and ‘‘Cond Num’’ is the condition number of the coefficient matrix.

4.2. EXAMPLE 2

We consider linear systems as follows:

$$\mathcal{H}u = \left(\begin{array}{cc|cc} \alpha I & 0 & & 0 \\ 0 & 0 & & \beta I \\ \hline 0 & \beta I & 0 & 0 \\ 0 & & 0 & -\gamma I \end{array} \right) \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}, \quad (27)$$

where $\alpha = 2.0$, $\beta = 1.2$, $\gamma = 1.5$. The vectors f , g are defined as $\mathcal{H}u$ where u is all-ones vector.

An approximate solution of (27) is obtained using the function `mldivide` of MATLAB. In this example, since A is singular, we set $W = \frac{\alpha}{\|C\|_2} I$ where $\alpha = 0.5$.

In Figure 4.3, error bounds of each methods for example 2 are shown.

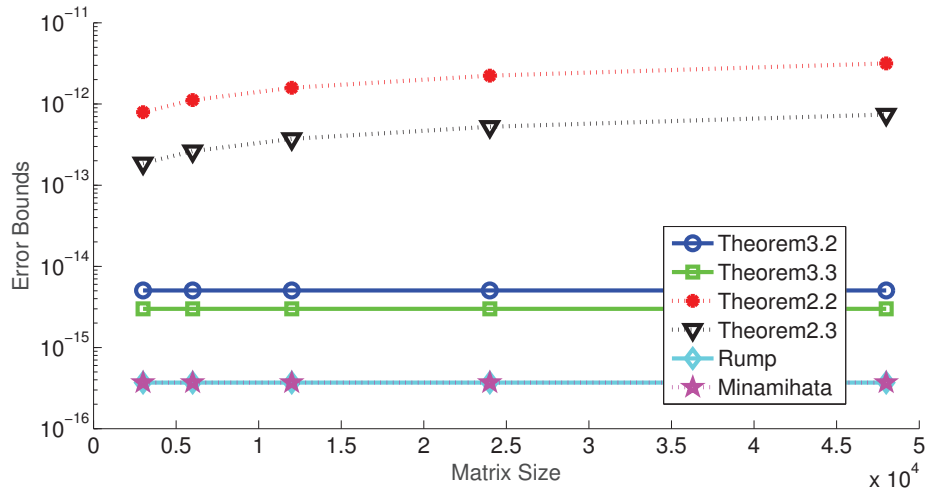


FIGURE 4.3. Error bounds for example 2.

In Figure 4.4, CPU time of each methods for example 2 are shown.

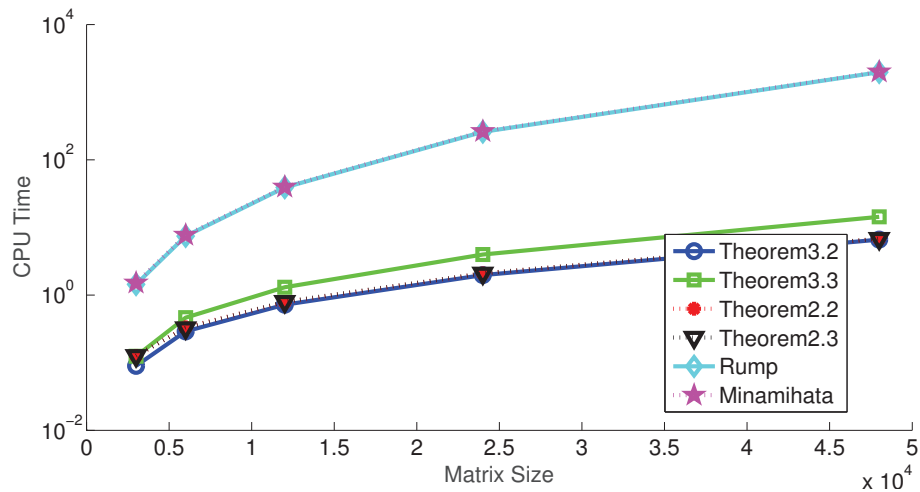


FIGURE 4.4. CPU time for example 2.

In Table 4.2, we show numerical results of error bounds and CPU time for example 2.

The new method and the new preconditioned method give error bounds sharper than those obtained by the methods based on Theorems 2.2 and 2.3. The new method

TABLE 4.2. Error bounds and CPU time for example 2.

(n, m)	(2001, 1001)	(4001, 2001)	(8001, 4001)	(16001, 8001)	(32001, 16001)
Apptime	1.777e-03	4.130e-03	7.690e-03	1.515e-02	3.271e-02
Cond Num	7.111e+00	7.111e+00	7.111e+00	7.111e+00	7.111e+00
$\ b - \mathcal{H}u\ _2$	4.441e-16	4.441e-16	4.441e-16	4.441e-16	4.441e-16
Theorem 3.2 (New)	5.050e-15 [8.969e-02s]	5.050e-15 [2.903e-01s]	5.050e-15 [7.210e-01s]	5.050e-15 [1.969e+00s]	5.050e-15 [6.597e+00s]
Theorem 2.2 (Previous)	7.933e-13 [1.257e-01s]	1.121e-12 [3.331e-01s]	1.584e-12 [7.824e-01s]	2.240e-12 [2.081e+00s]	3.167e-12 [6.774e+00s]
Theorem 3.3 (New)	3.000e-15 [1.245e-01s]	3.000e-15 [4.630e-01s]	3.000e-15 [1.303e+00s]	3.000e-15 [3.977e+00s]	3.000e-15 [1.431e+01s]
Theorem 2.3 (Previous)	1.863e-13 [1.262e-01s]	2.631e-13 [3.256e-01s]	3.716e-13 [7.971e-01s]	5.252e-13 [2.092e+00s]	7.423e-13 [6.804e+00s]
Rump's method	3.701e-16 [1.439e+00s]	3.701e-16 [7.429e+00s]	3.701e-16 [3.891e+01s]	3.701e-16 [2.591e+02s]	3.701e-16 [1.973e+03s]
Minamihata's method	3.701e-16 [1.511e+00s]	3.701e-16 [7.690e+00s]	3.701e-16 [3.962e+01s]	3.701e-16 [2.626e+02s]	3.701e-16 [1.995e+03s]

Note: Quantities inside square brackets are CPU time (sec), “Apptime” is CPU time(sec) of computing the approximation, and “Cond Num” is the condition number of the coefficient matrix.

is faster than other verification methods. The new preconditioned method is faster than the verification methods for general linear systems.

4.3. EXAMPLE 3 (STOKES EQUATION [4, §6])

We consider saddle point linear systems arising from the mixed finite element discretization of the stationary Stokes equation:

$$\left\{ \begin{array}{l} -\nu\Delta u + \nabla p = f \quad \text{in } \Omega, \\ -\operatorname{div} u = 0 \quad \text{in } \Omega, \\ u = 0 \quad \text{on } \partial\Omega, \\ \int_{\Omega} p \, dx = 0, \end{array} \right.$$

where $\Omega = (0, 1) \times (0, 1)$, $\partial\Omega$ is the boundary of Ω , ν is a positive parameter, f is a given force field, $u : \Omega \rightarrow \mathbb{R}^2$ is a velocity field, and $p : \Omega \rightarrow \mathbb{R}$ is a pressure field.

We reformulate the stationary Stokes equation into a weak formulation with a penalty term [4, §6] as follows:

$$\begin{cases} \nu(\nabla u, \nabla v) + (\nabla p, v) = (f, v) & , \quad \forall v \in H_0^1, \\ (\operatorname{div} u, q) - t^2(p, q) = 0 & , \quad \forall q \in L_0^2. \end{cases}$$

In this example, we set $\nu = 1$ and $t = 10^{-2}$.

We apply a mixed finite element approximation with uniform triangular meshes, where the velocity is approximated by the standard piecewise quadratic basis functions and the pressure is approximated by the standard piecewise linear basis functions. Then, we obtain a discretized equation (11). An approximate solution of (11) is obtained using the function `mldivide` of MATLAB. We set $\alpha = 0$ because A is symmetric positive definite.

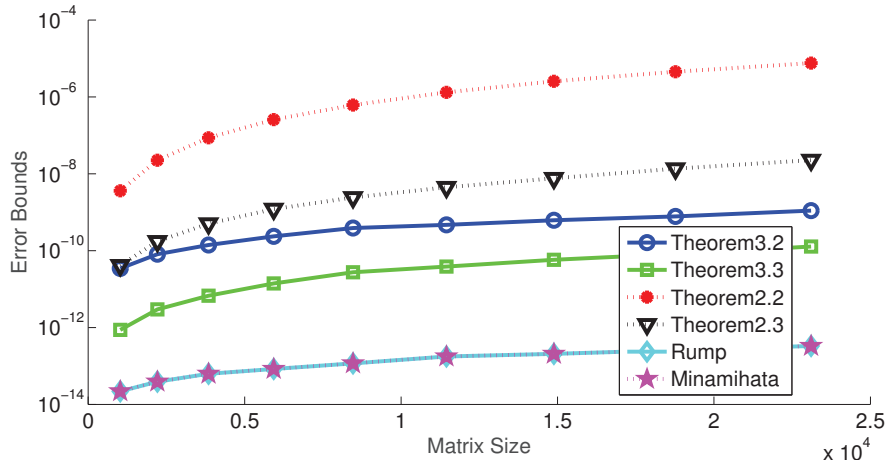


FIGURE 4.5. Error bounds for the Stokes equation.

In Figure 4.5, error bounds of each methods for the Stokes equation are shown.

In Figure 4.6, CPU time of each methods for the Stokes equation are shown.

In Table 4.3, we show numerical results of error bounds and CPU time for the Stokes equation. The new method gives error bounds sharper than those obtained by the method based on Theorem 2.2, although CPU time of two methods are almost same. Similarly, the new preconditioned method gives error bounds sharper than

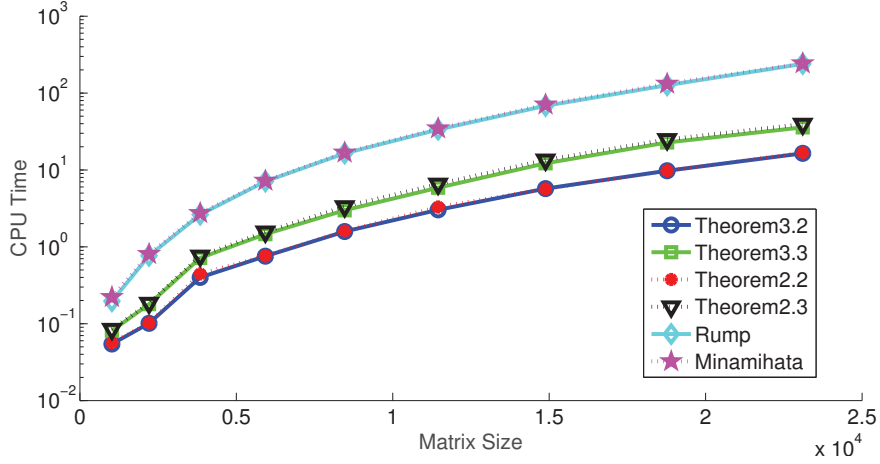


FIGURE 4.6. CPU time for the Stokes equation.

TABLE 4.3. Error bounds and CPU time for the Stokes equation.

(n,m)	(882,143)	(3362,483)	(7442,1023)	(13122,1763)	(20402,2703)
Apptime	7.038e-03	1.152e-01	8.546e-01	3.822e+00	1.247e+01
Cond Num	4.098e+05	1.477e+06	3.205e+06	5.595e+06	8.645e+06
$\ b - \mathcal{H}u\ _2$	5.708e-16	1.047e-15	1.590e-15	2.073e-15	2.594e-15
Theorem 3.2 (New)	3.435e-11 [5.441e-02s]	1.400e-10 [4.004e-01s]	3.870e-10 [1.580e+00s]	6.193e-10 [5.720e+00s]	1.098e-09 [1.645e+01s]
Theorem 2.2 (Previous)	8.697e-13 [8.094e-02s]	6.726e-12 [7.163e-01s]	2.741e-11 [2.985e+00s]	5.799e-11 [1.220e+01s]	1.279e-10 [3.571e+01s]
Theorem 3.3 (New)	3.609e-09 [5.652e-02s]	8.649e-08 [4.438e-01s]	6.152e-07 [1.603e+00s]	2.542e-06 [5.657e+00s]	7.545e-06 [1.675e+01s]
Theorem 2.3 (Previous)	4.137e-11 [8.482e-02s]	5.050e-10 [7.615e-01s]	2.419e-09 [3.339e+00s]	7.640e-09 [1.349e+01s]	2.265e-08 [3.947e+01s]
Rump's method	2.197e-14 [1.962e-01s]	6.250e-14 [2.626e+00s]	1.168e-13 [1.643e+01s]	2.060e-13 [6.831e+01s]	3.314e-13 [2.396e+02s]
Minamihata's method	2.197e-14 [2.214e-01s]	6.250e-14 [2.738e+00s]	1.168e-13 [1.676e+01s]	2.060e-13 [7.078e+01s]	3.314e-13 [2.430e+02s]

Note: Quantities inside square brackets are CPU time (sec), “Apptime” is CPU time(sec) of computing the approximation, and “Cond Num” is the condition number of the coefficient matrix.

those obtained by the method based on Theorem 2.3, although CPU time of two methods are almost same. Moreover, the new methods are faster than the verification methods for approximate solutions of general linear systems.

4.4. EXAMPLE 4 (THE BRINKMAN PROBLEM [12])

We consider saddle point linear systems arising from the finite element discretization of the Brinkman problem:

$$\begin{cases} -\nu\Delta\mathbf{u} + \mathbf{u} + \nabla p = \mathbf{f}(x) & \forall x \in \Omega, \\ \operatorname{div} \mathbf{u} = g(x) & \forall x \in \Omega, \end{cases} \quad (28)$$

where ν is the fluid viscosity and $\Omega = (0, 1) \times (0, 1) \times (0, 1)$, $\mathbf{f}(x)$ and $g(x)$ are given force fields, $\mathbf{u} : \Omega \rightarrow \mathbb{R}^3$ is a velocity field, and $p : \Omega \rightarrow \mathbb{R}$ is a pressure field.

By introducing the vorticity variable

$$\boldsymbol{\sigma} = \epsilon \operatorname{curl} \mathbf{u}, \quad \epsilon = \sqrt{\nu},$$

then we have the following weak formulation:

$$\begin{cases} (\boldsymbol{\sigma}, \boldsymbol{\tau}) & -\epsilon(\mathbf{u}, \operatorname{curl} \boldsymbol{\tau}) & = & 0, \\ & (\operatorname{div} \mathbf{u}, q) & = & (g, q), \\ -\epsilon(\operatorname{curl} \boldsymbol{\sigma}, \mathbf{v}) & + (p, \operatorname{div} \mathbf{v}) & - \epsilon^2(\operatorname{div} \mathbf{u}, \operatorname{div} \mathbf{v}) - (\mathbf{u}, \mathbf{v}) & = -(\mathbf{f}, \mathbf{v}), \end{cases}$$

where

$$\forall \boldsymbol{\tau} \in H_0^1(\operatorname{curl}; \Omega) := \{\boldsymbol{\tau} \in H_0^1 \mid \operatorname{curl} \boldsymbol{\tau} \in H_0^1, \boldsymbol{\tau} \times \mathbf{n} = \mathbf{0} \text{ on } \partial\Omega\},$$

$$\forall \mathbf{v} \in H_0^1(\operatorname{div}; \Omega) := \{\mathbf{v} \in H_0^1 \mid \operatorname{div} \mathbf{v} \in H_0^1, \mathbf{v} \cdot \mathbf{n} = \mathbf{0} \text{ on } \partial\Omega\},$$

$$\forall q \in L_0^2,$$

and $\mathbf{n} \in \mathbb{R}^3$ is the unit outward normal vector.

By applying the Q1 finite element method on a uniform cubic mesh to the above weak formulation, we obtain a discretized equation (1). An approximate solution of (1) is obtained using the function `mldivide` of MATLAB.

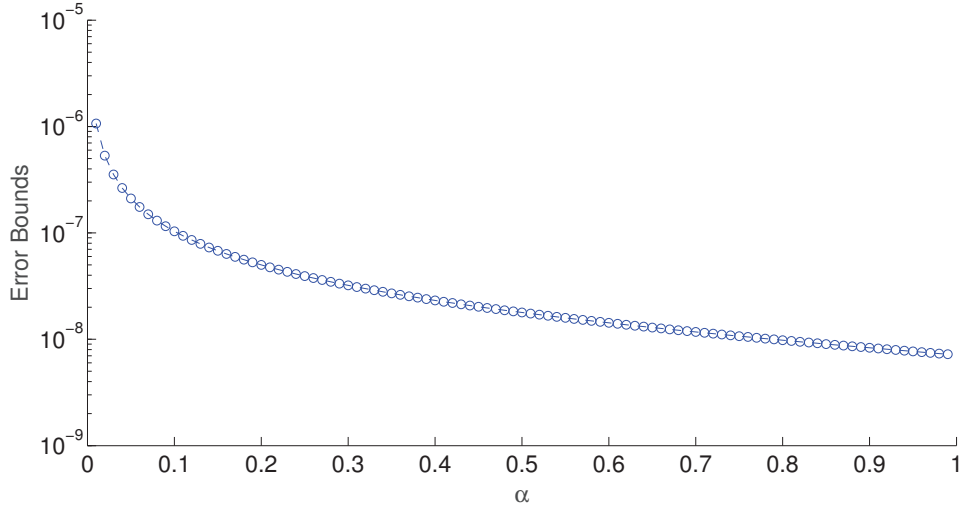


FIGURE 4.7. Error bounds of Theorem 3.2 for the Brinkman problem with different α . $(n, m) = (256, 192)$.

In this example, $\mathbf{f}(x)$, $g(x)$ and Dirichlet boundary conditions are chosen such that

$$\boldsymbol{\sigma}_{ex} = \epsilon\pi \begin{bmatrix} \sin(\pi x) \cos(\pi y) - \cos(\pi z) \sin(\pi x) \\ \sin(\pi y) \cos(\pi z) - \cos(\pi x) \sin(\pi y) \\ \sin(\pi z) \cos(\pi x) - \cos(\pi y) \sin(\pi z) \end{bmatrix},$$

$$\mathbf{u}_{ex} = \begin{bmatrix} \sin(\pi y) \sin(\pi z) \\ \sin(\pi z) \sin(\pi x) \\ \sin(\pi x) \sin(\pi y) \end{bmatrix},$$

and

$$p_{ex} = 8.0 \sin(\pi x) \sin(\pi y) \sin(\pi z),$$

are the exact solutions of (28). We set $\nu = 1$.

In this example, since A is singular, we set $W = \frac{\alpha}{\|C\|_2} I$ where $0 < \alpha < 1$. Figure 4.7 shows error bounds obtained by Theorem 3.2 for the Brinkman problem with $(n, m) = (256, 192)$ changing α from 0.01 to 0.99. Note that error bounds don't diverge when

$\alpha = 1$, because the error bound of $\|\tilde{A}^{-1}\|_2$ is larger than one of $\|\tilde{S}^{-1}\|_2$ regardless of the changing of α .

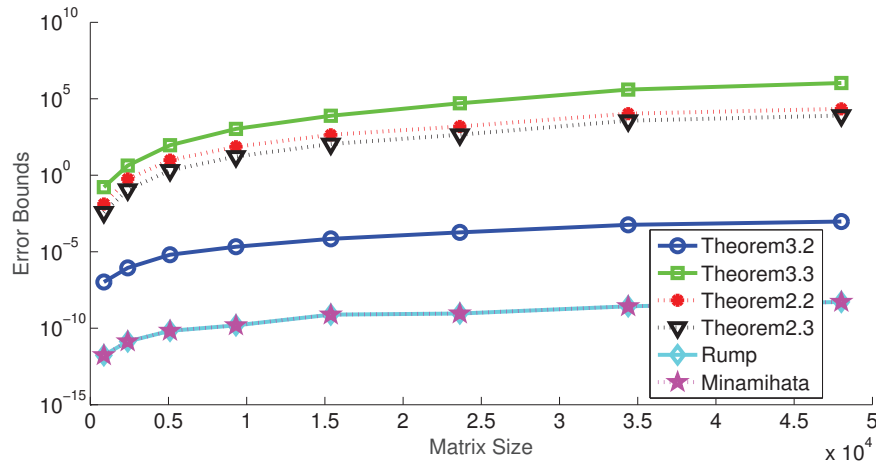


FIGURE 4.8. Error bounds for the Brinkman problem.

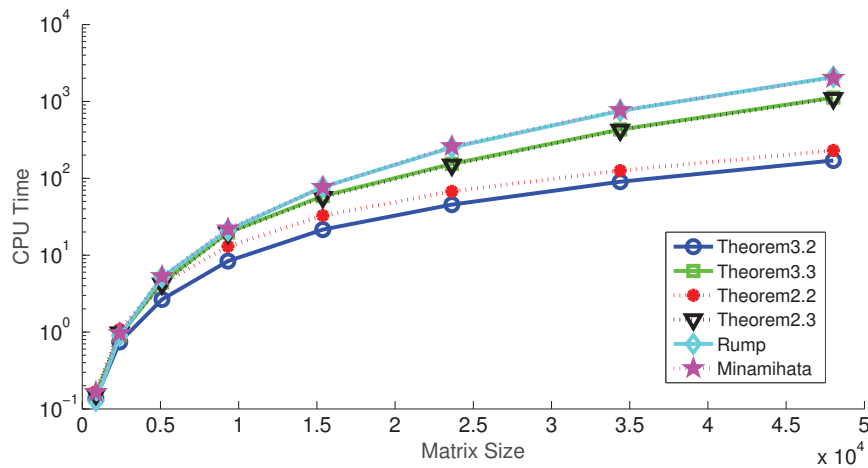


FIGURE 4.9. CPU time for the Brinkman problem.

In Figure 4.8, error bounds of each methods for the Brinkman problem are shown.

In Figure 4.9, CPU time of each methods for the Brinkman problem are shown.

In Table 4.4, we show numerical results of error bounds and CPU time for the Brinkman problem with $\alpha = 0.99$.

TABLE 4.4. Error bounds and CPU time for example 3. $\alpha = 0.99$.

(n,m)	(5324,3993)	(8788,6591)	(13500,10125)	(19652,14739)	(27436,20577)
Apptime	[2.610e-01s]	[8.142e-01s]	[2.398e+00s]	[6.339e+00s]	[1.553e+01s]
Cond Num	2.058e+08	5.054e+08	8.492e+08	2.890e+09	4.115e+09
Residual	5.854e-14	9.106e-14	1.353e-13	1.966e-13	2.496e-13
Theorem 3.2 (New)	2.139e-05 [8.354e+00s]	6.977e-05 [2.150e+01s]	1.842e-04 [4.549e+01s]	5.712e-04 [9.031e+01s]	9.487e-04 [1.705e+02s]
Theorem 2.2 (Previous)	1.068e+03 [1.967e+01s]	7.770e+03 [5.860e+01s]	5.048e+04 [1.540e+02s]	3.998e+05 [4.313e+02s]	1.066e+06 [1.119e+03s]
Theorem 3.3 (New)	7.265e+01 [1.301e+01s]	4.437e+02 [3.272e+01s]	1.531e+03 [6.762e+01s]	1.059e+04 [1.258e+02s]	2.201e+04 [2.307e+02s]
Theorem 2.3 (Previous)	1.676e+01 [1.942e+01s]	1.094e+02 [5.663e+01s]	4.462e+02 [1.490e+02s]	3.712e+03 [4.245e+02s]	8.051e+03 [1.095e+03s]
Rump's method	1.543e-10 [2.111e+01s]	7.788e-10 [7.711e+01s]	9.099e-10 [2.515e+02s]	2.710e-09 [7.536e+02s]	5.251e-09 [2.077e+03s]
Minamihata's method	1.543e-10 [2.215e+01s]	7.788e-10 [7.686e+01s]	9.099e-10 [2.613e+02s]	2.710e-09 [7.669e+02s]	5.251e-09 [2.014e+03s]

Note: Quantities inside square brackets are CPU time (sec), “Apptime” is CPU time(sec) of computing the approximation, and “Cond Num” is the condition number of the coefficient matrix.

In this example, the method based on Theorem 3.2 gives error bounds sharper than those obtained by the methods based on Theorems 2.2 and 2.3, although CPU time of Theorem 3.2 is less than those of Theorems 2.2 and 2.3.

REMARK 4.1. *In four examples, numerical results show that CPU time of the proposed method is less than those of other methods and error bounds of the proposed method is sharper than those based on Theorem 2.2.*

CHAPTER 5
CONCLUSION

For a symmetric saddle point linear systems with both diagonal block matrices A and C are symmetric positive semidefinite, we proposed fast verification methods based on Schur complement.

First, because Schur complement require the regularity of A in the coefficient matrix \mathcal{H} , we proposed a proposition and presented the method to regularize a matrix A . we defined the preconditioner with Schur complement and proposed the theorem of an inclusion of all eigenvalues of the preconditioned matrix. Using the absolute minimum eigenvalue obtained by the above theorem, we proposed the theorem of a new error bound for an approximation of the saddle point linear systems. In addition, we showed the theorem of another new error bound applying the technique studied in the previous works. We provided a verification method based on the above theorems.

We carried out four numerical experiments for illustrating the usefulness of proposed verification methods. These experiments include artificial ones and ones arising from actual problems. We compared proposed methods with the methods studied by Chen and Hashimoto and the methods using an approximate solution of the inverse of the coefficient matrix. The proposed method could be computed faster than other methods. And the error bound obtained by the proposed method is smaller than one by Chen and Hashimoto's methods.

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国際会議 講演	[2] <u>Ryo Kobayashi</u> , Kouta Sekine, Masahide Kashiwagi, Shin'ichi Oishi, "Verified numerical integration for function with power-type singularity using partial integration", INVA2017(The International Workshop on Numerical Verification and its Applications), HOTEL BREEZE BAY MARINA OKINAWA, Japan, (2017/3/18). [3] <u>Ryo Kobayashi</u> , Kouta Sekine, Masahide Kashiwagi, Shin'ichi Oishi, "Verified quadrature for integrand with power-type singularity using partial integral", ANZIAM2017, The Adelaide Hills Convention Centre, Australia, (2017/2/6). [4] <u>Ryo Kobayashi</u> , Takuma Kimura, Shin'ichi Oishi, "A method of verified computation for convex programming", SCAN2016(The 17th International Symposium on Scientific Computing, Computer Arithmetics and Verified Numerics.), UPPSALA UNIVERSITY, (2016/9/27) [5] <u>Ryo Kobayashi</u> , Takuma Kimura, Shin'ichi Oishi, "Validated Solutions for Symmetric Saddle Point Linear Systems", The 14th Asia Simulation Conference & The 33rd JSST Annual Conference, International Conference on Simulation Technology, Kitakyusyu, Japan, Oct.2014.
国内講演	[6] <u>小林 領</u> , 関根 晃太, 柏木 雅英, 大石 進一, "部分積分と Euler-Maclaurin の公式を用いたベキ型特異点を持つ関数の精度保証付き数値積分", 日本応用数理学会 2016 年度年会, 北九州国際会議場 (2016/9/14). [7] <u>Ryo Kobayashi</u> , Takuma Kimura, Shin'ichi Oishi, "A Numerical Verification Method for Solutions of Symmetric Saddle point Linear Systems", Joint Seminar on Numerical Analysis at Niigata University, Niigata, Japan, Sep.2015. [8] <u>小林 領</u> , 木村 拓馬, 大石 進一, "カントロビッチの定理を用いた凸二次計画問題の精度保証", 日本応用数理学会 2015 年度年会, 金沢大学 (2014/9/9). [9] 木村拓馬、 <u>小林 領</u> 、大石 進一, "SADDLE POINT MATRIX EQUATIONS の近似解に対する誤差評価について", 2014 年度応用数学合同研究集会、龍谷大学瀬田キャンパス (2014/12)

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