Projected Schur complement method for solving non-symmetric

systems arising from a smooth fictitious domain approach

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SUMMARY

The paper deals with a fast method for solving large scale algebraic saddle-point systems arising from fictitious domain formulations of elliptic boundary value problems. A new variant of the fictitious domain approach is analyzed. Boundary conditions are enforced by control variables introduced on an auxiliary boundary located outside of the original domain. This approach has a significantly higher convergence rate, however the algebraic systems resulting from finite element discretizations are typically non-symmetric. The presented method is based on the Schur complement reduction. If the stiffness matrix is singular, the reduced system can be formulated again as another saddle-point problem. Its modification by orthogonal projectors leads to an equation that can be efficiently solved by a projected Krylov subspace method for non-symmetric operators. For this purpose, the projected variant of the BiCGSTAB algorithm is derived from the non-projected one. The behavior of the method is illustrated by examples, in which the BiCGSTAB iterations are accelerated by a multigrid strategy. Copyright © 2007 John Wiley & Sons, Ltd.

KEY WORDS: saddle-point system, fictitious domain method, Schur complement, orthogonal projectors, BiCGSTAB algorithm, multigrid

1. INTRODUCTION

In this paper, we propose a fast method for finding a pair $(u, \lambda) \in \mathbb{R}^n \times \mathbb{R}^m$ that solves a linear system of algebraic equations called the *(generalized) saddle-point system*:

$$\begin{pmatrix} A & B_1^{\top} \\ B_2 & 0 \end{pmatrix} \begin{pmatrix} u \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix},$$
(1.1)

where the $(n \times n)$ diagonal block A is possibly singular, the $(m \times n)$ off-diagonal blocks B_1 , B_2 have full row-ranks and the vectors f, g are of order n, m, respectively. Motivated by a class of saddle-point systems arising from fictitious domain formulations of elliptic boundary value problems, we will be interested especially in systems (1.1) with n large, m much smaller than n and with the defect l of A, l = n - rank A, much smaller than m.

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Any fictitious domain formulation extends the original problem defined in a domain ω to a new fictitious domain Ω with a simple geometry (e.g. a box) which contains $\overline{\omega}$. The main advantage consists in possibility to use a structured mesh in Ω leading to a structured stiffness matrix represented by A in (1.1). Therefore actions of a generalized inverse A^{\dagger} (or inverse A^{-1}) are "cheap" and, in addition, the null-spaces of A and A^{\top} can be easily identified [7].

A class of fictitious domain methods enforces boundary conditions by Lagrange multipliers defined on the boundary γ of the original domain ω [5]. Therefore the fictitious domain solution has a singularity on γ that can result in an intrinsic error of the computed solution. The basic idea of our modification consists in introducing a new control variable instead of a Lagrange multiplier defined on an auxiliary boundary Γ located outside of $\overline{\omega}$ to realize the boundary condition on γ . In this approach, the singularity is moved away from $\overline{\omega}$ so that the computed solution is smoother in ω . Thus one may expect that the discretization error will be significantly smaller in ω . As B_1 and B_2 in (1.1) are determined by the geometries of Γ and γ , respectively, they are highly sparse and $B_1 \neq B_2$. Moreover, these matrices are usually non-structured.

There are several basic approaches for solving the saddle-point systems (1.1); see e.g. [2]. Due to the structure of our matrices, we focus on the class of methods that are based on the Schur complement reduction. Their key idea consists in eliminating the first component u of the solution pair (u, λ) . This leads (in the case of non-singular A) to the reduced system for the second component λ ,

$$B_2 A^{-1} B_1^{\dagger} \lambda = B_2 A^{-1} f - g, \qquad (1.2)$$

where $B_2 A^{-1} B_1^{\top}$ is the (negative) Schur complement -S. After computing λ from (1.2), one obtains u from

$$Au = f - B_1^{+}\lambda.$$

If an iterative method is used to solve (1.2), we do not need to form S explicitly as only the matrix-vector products with S are needed. The action of -S on μ can be computed successively as indicated by parentheses on the right hand-side of

$$-S\mu = B_2(A^{-1}(B_1^{\top}\mu)).$$

In the case A being singular u can not be completely eliminated from (1.1). Then the Schur complement reduction leads to another saddle-point system in terms of λ and a new unknown α , which corresponds to the null-space of A. Since (1.1) is non-symmetric, the reduced system again has two different off-diagonal blocks, say G_1 and G_2 . Therefore two orthogonal projectors on the respective null-spaces of G_1 and G_2 can be introduced. The first projector splits the saddle-point structure of the reduced system, the second one decomposes the unknown λ into two components $\lambda_{\mathbb{R}}$ and $\lambda_{\mathbb{N}}$, belonging to the range-space and to the null-space of G_2 , respectively. Considering both splittings together, we arrive at a projected equation for the component $\lambda_{\mathbb{N}}$ which can be solved by a *projected* Krylov method for non-symmetric operators. For this purpose, we will derive the projected BiCGSTAB algorithm from the non-projected one [8, 9].

The proposed method generalizes ideas of FETI domain decomposition methods [4], in which A is symmetric positive semidefinite and $B_1 = B_2$.

It should be noted that it is not appropriate to regularize the diagonal block of (1.1) by the penalized method [2] for our class of problems. The reason is that the corresponding Schur complement $S_{\rho} := -B_2(A + \rho B_2^{\top} B_2)^{-1} B_1^{\top}$, $\rho > 0$, requires actions of the inverse to the penalized matrix with two different parts: structured and non-structured. This excludes to

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apply highly efficient multiplying procedure discussed in Section 6 that is based on matrices with the circulant structure. Thus the usage of the penalized method destroys totally the main asset of the fictitious domain formulation.

The paper is organized as follows. In Section 2, we introduce a new variant of the fictitious domain approach. Section 3 describes the Schur complement reduction for the system (1.1) resulting in the algorithm presented in Section 4. The projected BiCGSTAB algorithm is proposed in Section 5 together with a hierarchical multigrid scheme which accelerates the iterative process. Finally, Section 6 describes some implementation details and presents results of numerical experiments illustrating the efficiency of our approach. Main aspects are concluded in Section 7.

2. A NEW FICTITIOUS DOMAIN APPROACH

We shall consider a non-homogeneous Dirichlet boundary value problem on a bounded domain $\omega \subset R^2$ with Lipschitz continuous boundary γ

$$\begin{array}{ccc} -\Delta u = f & \text{in } & \omega, \\ u = g & \text{on } & \gamma, \end{array} \right\}$$
 $(\mathcal{P}(\omega))'$

where $f \in L^2_{loc}(\mathbb{R}^2)$ and $g \in H^{1/2}(\gamma)$ are given. The weak formulation of $(\mathcal{P}(\omega))'$ is given by

$$\begin{cases} Find \ u \in H^1(\omega) \ such \ that \ u = g \ on \ \gamma \ and \\ \int_{\omega} \nabla u \cdot \nabla v \ dx = \int_{\omega} fv \ dx \quad \forall v \in H^1_0(\omega). \end{cases}$$
 $(\mathcal{P}(\omega))$

Let $\Xi \supset \overline{\omega}$ be another Lipschitz domain with boundary Γ such that $\delta = \text{dist}(\Gamma, \gamma) > 0$. Finally, $\Omega \supset \overline{\Xi}$ denotes the fictitious domain (e.g. a box), see Fig. 2.1.



Figure 2.1. Geometry.

Instead of $(\mathcal{P}(\omega))$, we propose to solve the extended problem:

$$Find (\hat{u}, \lambda) \in H_0^1(\Omega) \times H^{-1/2}(\Gamma) \text{ such that} \int_{\Omega} \nabla \hat{u} \cdot \nabla v \, dx = \int_{\Omega} fv \, dx + \langle \lambda, v \rangle_{\Gamma} \quad \forall v \in H_0^1(\Omega), \langle \mu, \hat{u} \rangle_{\gamma} = \langle \mu, g \rangle_{\gamma} \quad \forall \mu \in H^{-1/2}(\gamma), \end{cases}$$

where $\langle , \rangle_{\Gamma}, \langle , \rangle_{\gamma}$ stand for the duality pairings between $H^{-1/2}(\Gamma)$ and $H^{1/2}(\Gamma), H^{-1/2}(\gamma)$ and $H^{1/2}(\gamma)$, respectively.

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Suppose that $(\hat{\mathcal{P}}(\Omega))$ has a solution (\hat{u}, λ) . Then it is easy to see that (\hat{u}, λ) satisfies the following equations and boundary conditions:

$$\begin{array}{rcl} -\Delta \hat{u} &=& f \quad \text{in } \Xi \cup (\Omega \setminus \overline{\Xi}), \\ \hat{u} &=& g \quad \text{on } \gamma, \\ \hat{u} &=& 0 \quad \text{on } \partial \Omega, \\ \left[\frac{\partial \hat{u}}{\partial \nu} \right]_{\Gamma} &=& \lambda \quad \text{on } \Gamma, \end{array} \right\}$$

$$(2.1)$$

where $[]_{\Gamma}$ denotes the jump of the normal derivative $\frac{\partial \hat{u}}{\partial \nu}$ across Γ . In particular, we find that $\hat{u}_{|_{\omega}}$ solves the original problem $(\mathcal{P}(\omega))$.

Let us compare $(\hat{\mathcal{P}}(\Omega))$ with the classical fictitious domain formulation with boundary Lagrange multipliers on γ :

$$Find (\hat{w}, \chi) \in H_0^1(\Omega) \times H^{-1/2}(\gamma) \text{ such that} \int_{\Omega} \nabla \hat{w} \cdot \nabla v \, dx = \int_{\Omega} f v \, dx + \langle \chi, v \rangle_{\gamma} \quad \forall v \in H_0^1(\Omega), \langle \mu, \hat{w} \rangle_{\gamma} = \langle \mu, g \rangle_{\gamma} \quad \forall \mu \in H^{-1/2}(\gamma).$$

$$(2.2)$$

The second component χ in (2.2) plays the role of a Lagrange multiplier releasing the constraint u = g on γ . On the other hand, λ in $(\hat{\mathcal{P}}(\Omega))$ can be viewed as a control variable on Γ forcing \hat{u} to match g on γ . Suppose that Γ and γ are smooth enough so that $\hat{u}_{|\Xi} \in H^2(\Xi)$, $\hat{u}_{|_{\Omega\setminus\overline{\Xi}}} \in H^2(\Omega\setminus\overline{\Xi})$ if \hat{u} solves $(\hat{\mathcal{P}}(\Omega))$ and, similarly, $\hat{w}_{|_{\omega}} \in H^2(\omega)$, $\hat{w}_{|_{\Omega\setminus\overline{\omega}}} \in H^2(\Omega\setminus\overline{\omega})$ for \hat{w} solving (2.2). In both cases however, $\hat{u}, \hat{w} \in H^{3/2-\epsilon}(\Omega)$ for any $\epsilon > 0$ due to a in general non-zero jump of $\frac{\partial \hat{u}}{\partial \nu}, \frac{\partial \hat{w}}{\partial \nu}$ across Γ , respectively γ . Since the singularity of \hat{u} solving $(\hat{\mathcal{P}}(\Omega))$ is located on Γ which has a positive distance from γ , one can expect that the new variant of the fictitious domain approach will increase the convergence rate of approximate solutions in ω .

It remains to show under which conditions $(\hat{\mathcal{P}}(\Omega))$ has a solution. As we shall see this question is closely related to a controllability type problem. Indeed, consider for each $\lambda \in H^{-1/2}(\Gamma)$ the following elliptic problem:

$$Find \ \hat{u} := \hat{u}(\lambda) \in H^1_0(\Omega) \text{ such that} \\ \int_{\Omega} \nabla \hat{u} \cdot \nabla v \, dx = \int_{\Omega} f v \, dx + \langle \lambda, v \rangle_{\Gamma}. \end{cases}$$
 $(\hat{\mathcal{P}}(\lambda))$

Since $(\hat{\mathcal{P}}(\lambda))$ has a unique solution for every $\lambda \in H^{-1/2}(\Gamma)$, one can define a linear mapping $\Phi: H^{-1/2}(\Gamma) \mapsto H^{1/2}(\gamma)$ by

$$\Phi(\lambda) = \hat{u}(\lambda)|_{\gamma} \quad \forall \lambda \in H^{-1/2}(\Gamma), \tag{2.3}$$

where $\hat{u}(\lambda)$ solves $(\hat{\mathcal{P}}(\lambda))$.

Lemma 2.1. The range $\Phi(H^{-1/2}(\Gamma))$ is dense in $H^{1/2}(\gamma)$.

Proof. Without loss of generality we may suppose that $f \equiv 0$ in Ω . Let $\overline{\mu} \in H^{-1/2}(\gamma)$ be such that

$$\langle \overline{\mu}, \hat{u}(\lambda) \rangle_{\gamma} = 0 \quad \forall \lambda \in H^{-1/2}(\Gamma).$$
 (2.4)

We want to show that $\overline{\mu} = 0$ on γ . Let $z \in H^1_0(\Omega)$ be a unique solution of

$$\int_{\Omega} \nabla z \cdot \nabla v \, dx = \langle \overline{\mu}, v \rangle_{\gamma} \quad \forall v \in H_0^1(\Omega),$$
(2.5)

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i.e.,

$$\begin{aligned} \Delta z &= 0 \quad \text{in } \omega \cup (\Omega \setminus \overline{\omega}), \\ z &= 0 \quad \text{on } \partial \Omega, \\ [\frac{\partial z}{\partial \nu}]_{\gamma} &= \overline{\mu} \quad \text{on } \gamma. \end{aligned}$$
 (2.6)

Inserting $v := \hat{u}(\lambda)$ into (2.5) and v = z in $(\hat{\mathcal{P}}(\lambda))$ we obtain (recall $f \equiv 0$)

$$\langle \lambda, z \rangle_{\Gamma} = \int_{\Omega} \nabla z \cdot \nabla \hat{u}(\lambda) \, dx = \langle \overline{\mu}, \hat{u}(\lambda) \rangle_{\gamma} \quad \forall \lambda \in H^{-1/2}(\Gamma).$$

Taking into account (2.4), we have

$$\langle \lambda, z \rangle_{\Gamma} = 0 \quad \forall \lambda \in H^{-1/2}(\Gamma)$$

so that z = 0 on Γ . Since z is harmonic in $\Omega \setminus \overline{\omega}$ and z = 0 on $\partial\Omega$ and $\Gamma \subset \Omega \setminus \overline{\omega}$, we infer $z \equiv 0$ in $\Omega \setminus \overline{\omega}$ and hence z = 0 on γ . Since z is also harmonic in ω , we finally obtain $z \equiv 0$ in Ω implying $\overline{\mu} = 0$ on γ .

Corollary. Problem $(\hat{\mathcal{P}}(\Omega))$ has a solution provided that $g \in \Phi(H^{-1/2}(\Gamma))$. In addition, $\hat{u}_{|_{\omega}}$ is uniquely defined and solves $(\mathcal{P}(\omega))$. If $g \notin \Phi(H^{-1/2}(\Gamma))$ then for every $\epsilon > 0$ one can find $\tilde{g} \in \Phi(H^{-1/2}(\Gamma))$ such that

$$\|g - \widetilde{g}\|_{1/2,\gamma} \le \epsilon.$$

Denote by \hat{w} a solution of $(\hat{\mathcal{P}}(\Omega))$ with $g := \tilde{g}$. Then there exists a constant c > 0 such that

$$\|\hat{u} - \hat{w}\|_{1,\omega} \le c \|g - \widetilde{g}\|_{1/2,\gamma} \le c\epsilon,$$

i.e., $\hat{w}_{|_{\omega}}$ is a good approximation of the original problem $(\mathcal{P}(\omega))'$, too.

Remark 2.1. In the computations which will be presented in Section 6, the space $H_0^1(\Omega)$ will be replaced by $H_{per}^1(\Omega)$, the space of periodic functions from $H^1(\Omega)$. Then the approximate controllability result of Lemma 2.1 remains true with the following modifications. Let

$$\Lambda_f(\Gamma) = \{\lambda \in H^{-1/2}(\Gamma) | \langle \lambda, 1 \rangle_{\Gamma} + \int_{\Omega} f \, dx = 0\}$$

and

$$H_0^{1/2}(\gamma) = \{ \varphi \in H^{1/2}(\gamma) | \int_{\gamma} \varphi \, ds = 0 \}.$$

If $\lambda \in \Lambda_f(\Gamma)$ then $(\hat{\mathcal{P}}(\lambda))$ has a solution $\hat{u}(\lambda)$ determined up to an arbitrary constant. To choose a unique solution we require that $\hat{u}(\lambda)|_{\gamma} \in H_0^{1/2}(\gamma)$. This makes it possible to consider the mapping Φ , defined by (2.3) as a mapping from $\Lambda_f(\Gamma)$ into $H_0^{1/2}(\gamma)$. Then using the same

approach as in Lemma 2.1 one can show that $\Phi(\Lambda_f(\Gamma))$ is dense in $H_0^{1/2}(\gamma)$.

Let $V_h \subset H_0^1(\Omega)$, $L_H^{\gamma} \subset H^{-1/2}(\gamma)$, $L_H^{\Gamma} \subset H^{-1/2}(\Gamma)$, h, H > 0 be finite dimensional subspaces of the indicated spaces. Let $\dim V_h = n$ and in addition,

$$\dim L_H^{\gamma} = \dim L_H^{\Gamma} = m.$$

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A discretization of $(\hat{\mathcal{P}}(\Omega))$ results in the following problem:

$$\begin{cases} Find \ (\hat{u}_h, \lambda_H) \in V_h \times L_H^{\Gamma} \ such \ that \\ \int_{\Omega} \nabla \hat{u}_h \cdot \nabla v_h \ dx = \int_{\Omega} f v_h \ dx + \langle \lambda_H, v_h \rangle_{\Gamma} \quad \forall v_h \in V_h, \\ \langle \mu_H, \hat{u}_h \rangle_{\gamma} = \langle \mu_H, g \rangle_{\gamma} \quad \forall \mu_H \in L_H^{\gamma}, \end{cases}$$

where

$$\langle \lambda_H, v_h \rangle_{\Gamma} := \int_{\Gamma} \lambda_H v_h \, ds$$

and similarly for $\langle , \rangle_{\gamma}$.

The algebraic form of $(\hat{\mathcal{P}}(\Omega))_h^H$ is given by

Find
$$(\vec{u}, \vec{\lambda}) \in \mathbb{R}^n \times \mathbb{R}^m$$
 such that
 $\begin{pmatrix} A & B_1^\top \\ B_2 & 0 \end{pmatrix} \begin{pmatrix} \vec{u} \\ \vec{\lambda} \end{pmatrix} = \begin{pmatrix} \vec{f} \\ \vec{g} \end{pmatrix},$
 $(\vec{\mathcal{P}})$

where A is the standard $(n \times n)$ stiffness matrix, B_1, B_2 are $(m \times n)$ matrices with elements

$$b_{1,ij} = \int_{\Gamma} \mu_i^{\Gamma} \varphi_j \, ds, \quad b_{2,ij} = \int_{\gamma} \mu_i^{\gamma} \varphi_j \, ds, \quad i = 1, \dots, m, \ j = 1, \dots, n,$$

respectively, and $\vec{f} \in \mathbb{R}^n$, $\vec{g} \in \mathbb{R}^m$ are vectors whose components are

$$f_j = \int_{\Omega} f\varphi_j \, dx, \ j = 1, \dots, n, \quad g_i = \int_{\gamma} g\mu_i^{\gamma} \, ds, \ i = 1, \dots, m,$$

respectively. Above $\{\varphi_j\}_{j=1}^n$, $\{\mu_i^{\Gamma}\}_{i=1}^m$, $\{\mu_i^{\gamma}\}_{i=1}^m$ are basis functions of V_h , L_H^{Γ} and L_h^{γ} , respectively.

Remark 2.2. Denote by \mathcal{A} the $(n+m) \times (n+m)$ matrix of the system $(\vec{\mathcal{P}})$. If $\Gamma = \gamma$ then $B_1 = B_2$ and we arrive at the standard symmetric saddle-point formulation. If the stability condition

$$\langle \mu_H, v_h \rangle_{\gamma} = 0 \quad \forall v_h \in V_h \Rightarrow \mu_H = 0 \text{ on } \gamma$$

is satisfied then \mathcal{A} is non-singular. As the distance δ between γ and Γ is assumed to be small, the matrix B_2 can be considered to be a small perturbation of B_1 . Therefore the resulting matrix \mathcal{A} is a non-symmetric perturbation of the matrix from the symmetric case so that its non-singularity can be maintained. This observation can be proven by properties of the discrete Green function in 1D, see [3]. The proof in 2D case is still ongoing research.

Remark 2.3. In order to simplify the notation, we will omit the arrow over vectors in the rest of the paper.

3. SOLVABILITY OF SADDLE-POINT SYSTEMS

This section deals with basic properties of the saddle-point system (1.1). It should be noted that papers which analyze a general non-symmetric case are quite rare and many questions remain still open; see [2] and references therein. For this reason, we discuss in details necessary and

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sufficient conditions for the invertibility of the matrix in (1.1) and, in addition, we introduce the concept of the Schur complement reduction for the singular diagonal block A. Let us point out that our analysis generalizes ideas originally used for symmetric saddle-point systems arising from FETI domain decomposition methods, in which A is positive semidefinite [4].

First of all we introduce some notation. The null-space and the range-space of an $(m \times n)$ matrix B on \mathbb{V} will be denoted by

$$\begin{split} \mathbb{N}(B|\mathbb{V}) &:= \{ v \in \mathbb{V} : Bv = 0 \}, \\ \mathbb{R}(B|\mathbb{V}) &:= \{ \mu \in R^m : \mu = Bv, v \in \mathbb{V} \}, \end{split}$$

respectively, where $\mathbb{V} \subset \mathbb{R}^n$ is a subspace. If $\mathbb{V} = \mathbb{R}^n$, we simply write $\mathbb{N}(B) := \mathbb{N}(B|\mathbb{R}^n)$ and $\mathbb{R}(B) := \mathbb{R}(B|\mathbb{R}^n)$. The following lemma is well-known.

Lemma 3.1. $\mathbb{N}(B^{\top})$ is the orthogonal complement of $\mathbb{R}(B)$ in \mathbb{R}^m . In particular, if $v \perp \mathbb{N}(B^{\top})$, there is $w \in \mathbb{R}^n$ so that v = Bw.

Recall that \mathcal{A} is the matrix of the saddle-point system (1.1):

$$\mathcal{A} := \left(\begin{array}{cc} A & B_1^\top \\ B_2 & 0 \end{array} \right).$$

Theorem 3.1. A is invertible iff B_1 has full row-rank and the following two conditions hold

$$\mathbb{N}(A) \cap \mathbb{N}(B_2) = \{0\}, \tag{3.1}$$

$$\mathbb{R}(A|\mathbb{N}(B_2)) \cap \mathbb{R}(B_1^{\top}) = \{0\}.$$

$$(3.2)$$

Proof. Let $x = (u^{\top}, \lambda^{\top})^{\top}$ be such that $\mathcal{A}x = 0$. Hence $Au + B_1^{\top}\lambda = 0$ and $B_2u = 0$. It follows that $B_1^{\top}\lambda \in \mathbb{R}(A|\mathbb{N}(B_2))$ and $B_1^{\top}\lambda \in \mathbb{R}(B_1^{\top})$ so that $B_1^{\top}\lambda = 0$ by (3.2). Since B_1^{\top} has full column-rank, we obtain $\lambda = 0$. Moreover, $Au = -B_1^{\top}\lambda = 0$ so that $u \in \mathbb{N}(A) \cap \mathbb{N}(B_2)$ and therefore u = 0 by (3.1). This proves that \mathcal{A} is non-singular and that the conditions (3.1), (3.2) together with the rank condition for B_1 are sufficient.

The rank condition for B_1 is clearly necessary for the invertibility of \mathcal{A} . Assume now that $v \in \mathbb{R}(A|\mathbb{N}(B_2)) \cap \mathbb{R}(B_1^{\top}), v \neq 0$, i.e. $v = Au = -B_1^{\top}\lambda$ for some $u \in \mathbb{N}(B_2), u \neq 0$ and $\lambda \in \mathbb{R}^m$, $\lambda \neq 0$. Set $x = (u^{\top}, -\lambda^{\top})^{\top}$ then x is a nontrivial solution of $\mathcal{A}x = 0$. Hence, the condition (3.2) is necessary.

Finally, assume that $u \in \mathbb{N}(A) \cap \mathbb{N}(B_2)$, $u \neq 0$. Then for $x = (u^{\top}, 0^{\top})^{\top}$ we obtain $\mathcal{A}x = 0$ which implies that also condition (3.1) is necessary. \Box

Remark 3.1. The necessary and sufficient conditions of Theorem 3.1 do not explicitly contain any rank condition on B_2 . However, it is a consequence. If (3.1) holds, then dim $\mathbb{R}(A|\mathbb{N}(B_2)) =$ dim $\mathbb{N}(B_2) \ge n - m$. Since B_1 has full-row rank dim $\mathbb{R}(B_1^{\top}) = m$ and therefore (3.2) implies dim $\mathbb{R}(A|\mathbb{N}(B_2)) \le n - m$. We arrive at dim $\mathbb{N}(B_2) = n - m$ that is satisfied iff B_2 has full-row rank.

Suppose that A is singular with $l = \dim \mathbb{N}(A)$, $1 \leq l \ll m$ and consider $(n \times l)$ matrices N and M the columns of which span the null-spaces $\mathbb{N}(A)$ and $\mathbb{N}(A^{\top})$, respectively. Let A^{\dagger} be a generalized inverse to A. Note that the matrices A^{\dagger} , N and M satisfy

$$A = AA^{\dagger}A, \quad AN = 0 \quad \text{and} \quad A^{\top}M = 0.$$

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Since they are not determined uniquely we will consider below a fixed but arbitrary choice. The generalized Schur complement of A in \mathcal{A} is defined by

$$\mathcal{S} := \left(\begin{array}{cc} -B_2 A^{\dagger} B_1^{\top} & B_2 N \\ M^{\top} B_1^{\top} & 0 \end{array} \right).$$

Theorem 3.2. Assume that B_1 has full row-rank and that (3.1) and (3.2) are satisfied. Then S is invertible.

Proof. Using (3.1), it is easy to show that $N^{\top}B_2^{\top}$ has full row-rank. Therefore Theorem 3.1 will guarantee that S is invertible provided that

$$\mathbb{N}(-B_2A^{\dagger}B_1^{\top}) \cap \mathbb{N}(M^{\top}B_1^{\top}) = \{0\}, \tag{3.3}$$

$$\mathbb{R}(-B_2 A^{\dagger} B_1^{\top} | \mathbb{N}(M^{\top} B_1^{\top})) \cap \mathbb{R}(B_2 N) = \{0\}.$$

$$(3.4)$$

(i) Let $\lambda \in \mathbb{N}(-B_2A^{\dagger}B_1^{\top}) \cap \mathbb{N}(M^{\top}B_1^{\top})$ and denote $v = -B_1^{\top}\lambda$. Since $M^{\top}v = 0$ we have $v \perp \mathbb{N}(A^{\top})$ so that v = Aw by Lemma 3.1. Furthermore

$$0 = -B_2 A^{\dagger} B_1^{\top} \lambda = B_2 A^{\dagger} v = B_2 A^{\dagger} A w = B_2 w$$

for $u = A^{\dagger}Aw$ and

$$Au = AA^{\dagger}Aw = Aw = -B_1^{\top}\lambda.$$

This shows that $x = (u^{\top}, \lambda^{\top})^{\top}$ solves $\mathcal{A}x = 0$. However, \mathcal{A} is non-singular which implies $\lambda = 0$ and (3.3) holds.

(ii) Let $\lambda \in \mathbb{R}(-B_2A^{\dagger}B_1^{\top}|\mathbb{N}(M^{\top}B_1^{\top})) \cap \mathbb{R}(B_2N)$. Then there exist $\mu \in \mathbb{N}(M^{\top}B_1^{\top})$ and $\alpha \in R^l$ such that

$$\lambda = -B_2 A^{\dagger} B_1^{\dagger} \mu \quad \text{and} \quad \lambda = B_2 N \alpha.$$

Subtracting these equations, we obtain

$$0 = B_2(-A^{\dagger}B_1^{\top}\mu - N\alpha) =: B_2 u, \qquad (3.5)$$

where $u = -A^{\dagger}B_1^{\top}\mu - N\alpha$. Since $M^{\top}B_1^{\top}\mu = 0$ we have $B_1^{\top}\mu \perp \mathbb{N}(A^{\top})$ so that $B_1^{\top}\mu = Aw$ for some $w \in \mathbb{R}^n$ by Lemma 3.1. Finally,

$$Au = A(-A^{\dagger}B_{1}^{\top}\mu - N\alpha) = -AA^{\dagger}B_{1}^{\top}\mu = -AA^{\dagger}Aw = -Aw = -B_{1}^{\top}\mu.$$
 (3.6)

The equations (3.6), (3.5) imply that $x = (u^{\top}, \mu^{\top})^{\top}$ solves $\mathcal{A}x = 0$. Because \mathcal{A} is non-singular we obtain $\mu = 0$ and consequently $\lambda = 0$ so that (3.4) holds.

Example 3.1. Let us consider the matrix

$$\mathcal{A} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 2 & 3 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} A & B_1^\top \\ B_2 & 0 \end{pmatrix}.$$

It is easy to verify that (3.1), (3.2) hold and

$$A^{\dagger} = A^{\top}, \quad N = \begin{pmatrix} 0\\1\\0 \end{pmatrix}, \quad M = \begin{pmatrix} 0\\0\\1 \end{pmatrix}.$$

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The generalized Schur complement reads as follows:

$$S = \begin{pmatrix} -3 & -3 & 2\\ -1 & -1 & 1\\ \hline 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} -B_2 A^{\dagger} B_1^{\top} & B_2 N\\ M^{\top} B_1^{\top} & 0 \end{pmatrix}.$$

The following theorem describes the Schur complement reduction in the system (1.1).

Theorem 3.3. Assume S is invertible. Then A is invertible and the second component λ of the solution to (1.1) is the first component of the solution to the linear system

$$\begin{pmatrix} B_2 A^{\dagger} B_1^{\top} & -B_2 N \\ -M^{\top} B_1^{\top} & 0 \end{pmatrix} \begin{pmatrix} \lambda \\ \alpha \end{pmatrix} = \begin{pmatrix} B_2 A^{\dagger} f - g \\ -M^{\top} f \end{pmatrix}.$$
(3.7)

The first component u of the solution to (1.1) is given by

$$u = A^{\dagger}(f - B_1^{\top}\lambda) + N\alpha.$$
(3.8)

Proof. In order to show that \mathcal{A} is invertible we prove that \mathcal{A} is surjective. Given $(f,g) \in \mathbb{R}^n \times \mathbb{R}^m$ the second equation in (3.7) implies $M^{\top}(f - B_1^{\top}\lambda) = 0$ so that $f - B_1^{\top}\lambda \perp \mathbb{N}(\mathbb{A}^{\top})$ and therefore $f - B_1^{\top}\lambda = Aw$ for some $w \in \mathbb{R}^n$ by Lemma 3.1. Using (3.8) we get

$$Au + B_1^{\top}\lambda = A(A^{\dagger}(f - B_1^{\top}\lambda) + N\alpha) + B_1^{\top}\lambda = AA^{\dagger}Aw + B_1^{\top}\lambda = Aw + B_1^{\top}\lambda = f,$$

i.e., the first equation in the saddle-point system (1.1) is satisfied. Using (3.8) and the first equation in (3.7), we obtain:

$$B_2 u = B_2 (A^{\dagger} (f - B_1^{\top} \lambda) + N\alpha) = B_2 A^{\dagger} f - B_2 A^{\dagger} B_1^{\top} \lambda + B_2 N\alpha = g$$

so that the second equation in the saddle-point system (1.1) is satisfied, as well.

Corollary 3.1. Theorems 3.1-3.3 imply that the following three statements are equivalent:

- (i) B_1 has full row-rank and (3.1), (3.2) hold;
- (ii) \mathcal{A} is invertible;
- (iii) S is invertible.

Remark 3.2. In contrast to the symmetric case, the invertibility of \mathcal{A} is not guaranteed for A non-singular and B_1 , B_2 having full row-ranks. For instance, the generalized Schur complement of

$$\mathcal{A} = \left(\begin{array}{cc} I & B_1^{\top} \\ B_2 & 0 \end{array}\right)$$

is $\mathcal{S} = -B_2 B_1^{\top}$ that vanishes for B_1 and B_2 biorthogonal.

4. PROJECTED SCHUR COMPLEMENT METHOD

We will propose a solution method based on Theorem 3.3. In order to simplify our presentation, we introduce

$$\begin{split} F &:= B_2 A^{\dagger} B_1^{\top}, \quad G_1 := -N^{\top} B_2^{\top}, \quad G_2 := -M^{\top} B_1^{\top}, \\ d &:= B_2 A^{\dagger} f - g, \quad e := -M^{\top} f \end{split}$$

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which renders (3.7) into

$$\begin{pmatrix} F & G_1^\top \\ G_2 & 0 \end{pmatrix} \begin{pmatrix} \lambda \\ \alpha \end{pmatrix} = \begin{pmatrix} d \\ e \end{pmatrix}.$$
 (4.1)

Let us point out that the system (4.1) has formally the same saddle-point structure as (1.1), however its size is considerably smaller. It can be efficiently solved using orthogonal projectors.

Definition 4.1. Let G be an $(l \times m)$ matrix with full row-rank. The linear operator

$$P: \mathbb{R}^m \mapsto \mathbb{N}(G)$$

is called the orthogonal projector onto $\mathbb{N}(G)$ iff

(i)
$$P\mu = \mu \quad \forall \mu \in \mathbb{N}(G),$$

(ii) $(\mu - P\mu)^{\top}\nu = 0 \quad \forall \mu \in R^m \; \forall \nu \in \mathbb{N}(G).$

The orthogonal projector P is determined uniquely and it can be identified with the matrix

$$P := I - G^{\top} (GG^{\top})^{-1} G.$$

It is easy to verify that

$$GP = 0, \quad PG^{\top} = 0 \quad \text{and} \quad \mathbb{N}(P) = \mathbb{R}(G^{\top}).$$

In what follows, we will denote by P_1 , P_2 the orthogonal projectors associated with the matrices G_1 , G_2 , respectively.

Lemma 4.1. Let S be invertible. Then the linear operator $P_1F : \mathbb{N}(G_2) \mapsto \mathbb{N}(G_1)$ is invertible.

Proof. As both null-spaces $\mathbb{N}(G_1)$ and $\mathbb{N}(G_2)$ have the same dimension, it is enough to prove that P_1F is injective, i.e., $\mathbb{N}(P_1F|\mathbb{N}(G_2)) = \{0\}$. Let $\mu \in \mathbb{N}(G_2)$ be such that $P_1F\mu = 0$. Then $F\mu \in \mathbb{N}(P_1) = \mathbb{R}(G_1^{\top})$ and there exists $\beta \in \mathbb{R}^l$ such that

$$F\mu = G_1^\top \beta$$
 and $G_2\mu = 0$.

Setting $y = (\mu^{\top}, -\beta^{\top})^{\top}$ we get $-\mathcal{S}y = 0$ which implies $\mu = 0$ using the invertibility of \mathcal{S} . \Box

The following theorem is fundamental for the proposed method.

Theorem 4.1. Assume that S is invertible and decompose $\lambda \in \mathbb{R}^m$ according to

$$\lambda := \lambda_{\mathbb{N}} + \lambda_{\mathbb{R}},\tag{4.2}$$

where $\lambda_{\mathbb{N}} \in \mathbb{N}(G_2)$ and $\lambda_{\mathbb{R}} \in \mathbb{R}(G_2^{\top})$. Then λ is the first component of the solution to (4.1) iff

$$\lambda_{\mathbb{R}} = G_2^{+} (G_2 G_2^{+})^{-1} e \tag{4.3}$$

and $\lambda_{\mathbb{N}}$ is unique solution of

$$P_1 F \lambda_{\mathbb{N}} = P_1 (d - F \lambda_{\mathbb{R}}). \tag{4.4}$$

The second component of the solution to (4.1) is given by

$$\alpha = (G_1 G_1^{\top})^{-1} G_1 (d - F\lambda).$$
(4.5)

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Proof. Let λ be the first component of the solution to (4.1) and decompose λ according to (4.2). This decomposition is unique by Lemma 3.1. The second equation in (4.1) gives $G_2\lambda = G_2\lambda_{\mathbb{R}} = e$ that is obviously satisfied by (4.3). Inserting (4.2) in the first equation of (4.1) we obtain

$$F\lambda_{\mathbb{N}} = d - F\lambda_{\mathbb{R}} - G_1^{\mathsf{T}}\alpha$$

and the statement (4.4) follows by applying P_1 to both sides.

Conversely, let $\lambda_{\mathbb{N}} \in \mathbb{N}(G_2)$ and $\lambda_{\mathbb{R}} \in \mathbb{R}(G_2^{\top})$ be given by (4.3), respectively (4.4). Since P_1F is invertible by Lemma 4.1, it follows that $\lambda_{\mathbb{N}}$ satisfying (4.4) is unique. Therefore λ defined by (4.2) is also unique. In view of $F\lambda_{\mathbb{N}} + F\lambda_{\mathbb{R}} - d = F\lambda - d \in \mathbb{N}(P_1) = \mathbb{R}(G_1^{\top})$ there exists $\alpha \in \mathbb{R}^l$ such that $F\lambda - d = -G_1^{\top}\alpha$, i.e.

$$F\lambda + G_1^\top \alpha = d.$$

As before one verifies $G_2\lambda = e$. This implies that λ is the first component of the solution to (4.1).

Finally, (4.5) follows multiplying the first equation in (4.1) by G_1 :

$$G_1F\lambda + G_1G_1^\top \alpha = G_1d,$$

and solving for α .

Example 4.1. Let us consider the saddle-point system

$$\mathcal{A}\left(\begin{array}{c} u\\ \lambda\end{array}\right) = \left(\begin{array}{c} f\\ g\end{array}\right),$$

where \mathcal{A} is as in Example 3.1, $f = (1,3,1)^{\top}$ and $g = (5,2)^{\top}$. The reduced system (4.1) is described by

$$\begin{pmatrix} F & G_1^{\top} \\ G_2 & 0 \end{pmatrix} = \begin{pmatrix} 3 & 3 & | & -2 \\ 1 & 1 & | & -1 \\ \hline 0 & -1 & | & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} d \\ e \end{pmatrix} = \begin{pmatrix} 4 \\ 1 \\ \hline -1 \end{pmatrix}.$$

The orthogonal projectors P_1 , P_2 on

$$\begin{split} \mathbb{N}(G_1) &= \{ (\lambda_1, \lambda_2)^\top \in R^2 : -2\lambda_1 - \lambda_2 = 0 \}, \\ \mathbb{N}(G_2) &= \{ (\lambda_1, \lambda_2)^\top \in R^2 : -\lambda_2 = 0 \} \end{split}$$

are given by

$$P_1 = \begin{pmatrix} 1/5 & -2/5 \\ -2/5 & 4/5 \end{pmatrix}, \quad P_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

respectively. Using (4.3), we obtain

$$\lambda_{\mathbb{R}} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} (1)^{-1} (-1) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

As

$$P_1F = \begin{pmatrix} 1/5 & 1/5 \\ -2/5 & -2/5 \end{pmatrix}$$
 and $P_1(d - F\lambda_{\mathbb{R}}) = \begin{pmatrix} 1/5 \\ -2/5 \end{pmatrix}$,

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we see that the equation (4.4) reads as

$$\frac{1/5\,\lambda_1 + 1/5\,\lambda_2}{-2/5\,\lambda_1 - 2/5\,\lambda_2} = \frac{1/5}{-2/5},$$
(4.6)

where $\lambda_{\mathbb{N}} = (\lambda_1, \lambda_2)^{\top}$. Since $\lambda_{\mathbb{N}} \in \mathbb{N}(G_2)$, we get $\lambda_2 = 0$ so that (4.6) implies $\lambda_1 = 1$ and

$$\lambda = \lambda_{\mathbb{N}} + \lambda_{\mathbb{R}} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Then (4.5) yields

$$\alpha = (5)^{-1}(-2, -1)\left(\left(\begin{array}{c}4\\1\end{array}\right) - \left(\begin{array}{c}6\\2\end{array}\right)\right) = 1$$

and, finally, the formulae (3.8) gives $u = (1, 1, 1)^{+}$.

Let us algorithmically summarize the previous results. Since our aim is to solve systems (\mathcal{P}) arising from fictitious domain approaches, it turns out to be reasonable to form and store the $(l \times m)$ matrices G_1, G_2 and the $(l \times l)$ matrices $H_1 := (G_1 G_1^\top)^{-1}, H_2 := (G_2 G_2^\top)^{-1}$ because l is small. On the other hand, the $(m \times m)$ matrices F, P_1 and P_2 are not assembled explicitly since only their matrix-vector products are needed. The actions on μ can be evaluated successively as indicated by parentheses on the right hand-sides of

$$F\mu := B_2(A^{\dagger}(B_1^{\top}\mu))$$
 and $P_k\mu := \mu - G_k(H_k(G_k^{\top}\mu)), \quad k = 1, 2.$

The actions of B_1 and B_2 are inexpensive compute since these matrices are highly sparse. Finally, let us point out that actions of A^{\dagger} , N and M can be easily performed bacause A is a stiffness matrix on a fictitious domain with a simple geometry. Efficient multiplication procedures will be discussed in Section 6.

Algorithm: Projected Schur Complement Method (PSCM)

 $\begin{array}{lll} \text{Step 1.a:} & \text{Assemble } G_1 := -N^\top B_2^\top, \ G_2 := -M^\top B_1^\top, \ d := B_2 A^\dagger f - g \ \text{and} \ e := -M^\top f.\\ \text{Step 1.b:} & \text{Assemble } H_1 := (G_1 G_1^\top)^{-1} \ \text{and} \ H_2 := (G_2 G_2^\top)^{-1}.\\ \text{Step 1.c:} & \text{Assemble } \lambda_{\mathbb{R}} := G_2^\top H_2 e.\\ \text{Step 1.d:} & \text{Assemble } \tilde{d} := P_1 (d - F \lambda_{\mathbb{R}}).\\ \text{Step 1.e:} & \text{Solve the equation } P_1 F \lambda_{\mathbb{N}} = \tilde{d} \ \text{on } \mathbb{N}(G_2).\\ \text{Step 1.f:} & \text{Assemble } \lambda := \lambda_{\mathbb{N}} + \lambda_{\mathbb{R}}.\\ \text{Step 2:} & \text{Assemble } \alpha := H_1 G_1 (d - F \lambda).\\ \text{Step 3:} & \text{Assemble } u := A^\dagger (f - B_1^\top \lambda) + N\alpha. \end{array}$

The heart of the algorithm consists in Step 1.e. Its solution can be computed by a *projected* Krylov subspace method for non-symmetric operators.

5. PROJECTED BICGSTAB AND MULTIGRID

In this section, we will show how to solve efficiently the equation

$$P_1 F \lambda_{\mathbb{N}} = d \quad \text{on} \quad \mathbb{N}(G_2). \tag{5.1}$$

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Although P_1F is an $(m \times m)$ matrix, we only need its restriction to the m - l dimensional subspace $\mathbb{N}(G_2)$. For this purpose, we will derive the projected variant of the BiCGSTAB algorithm from the non-projected one [9, 8].

As the solution of (5.1) belongs to $\mathbb{N}(G_2)$, all BiCGSTAB iterations $\lambda_{\mathbb{N}}^k$ must also belong to this subspace. This can be achieved by choosing the first iteration $\lambda_{\mathbb{N}}^0$ in $\mathbb{N}(G_2)$ and by projecting each BiCGSTAB directions p^k and s^k onto $\mathbb{N}(G_2)$. Therefore the step generating a new iteration takes the form

$$\lambda_{\mathbb{N}}^{k+1} = \lambda_{\mathbb{N}}^{k} + \alpha_k P_2 p^k + \omega_k P_2 s^k.$$
(5.2)

It follows from the construction of the BiCGSTAB algorithm that the projector P_2 can be shifted from (5.2) to applications of P_1F while the initial residual is projected onto $\mathbb{N}(G_2)$.

Algorithm: ProjBiCGSTAB[$\epsilon, \lambda_{\mathbb{N}}^0, F, P_1, P_2, \widetilde{d}$] $\rightarrow \lambda_{\mathbb{N}}$

Initialize: Let $\lambda_{\mathbb{N}}^0 \in \mathbb{N}(G_2)$ be given, $r^0 := P_2 F^{\top}(\widetilde{d} - P_1 F \lambda_{\mathbb{N}}^0), p^0 := r^0, \widetilde{r}^0$ arbitrary, k := 0. While $||r^k|| > \epsilon$

$$\begin{split} \widetilde{p}^k &:= P_2 F^\top P_1 F p^k, \, \alpha_k := (r^k)^\top \widetilde{r}^0 / (\widetilde{p}^k)^\top \widetilde{r}^0, \, s^k := r^k - \alpha_k \widetilde{p}^k, \\ \widetilde{s}^k &:= P_2 F^\top P_1 F s^k, \, \omega_k := (\widetilde{s}^k)^\top s^k / (\widetilde{s}^k)^\top \widetilde{s}^k, \, \lambda_{\mathbb{N}}^{k+1} := \lambda_{\mathbb{N}}^k + \alpha_k p^k + \omega_k s^k, \\ r^{k+1} &:= s^k - \omega_k \widetilde{s}^k, \, \beta_{k+1} := (\alpha_k / \omega_k) (r^{k+1})^\top \widetilde{r}^0 / (r^k)^\top \widetilde{r}^0, \, p^{k+1} := r^{k+1} + \beta_{k+1} (p^k - \omega_k \widetilde{p}^k), \\ k &:= k+1 \\ \text{end.} \\ \text{Potume } \lambda &:= \lambda^k \end{split}$$

Return: $\lambda_{\mathbb{N}} := \lambda_{\mathbb{N}}^k$.

It should be noted that the projected BiCGSTAB algorithm differs from the non-projected one only in the initialization step and in the occurrence of the operator $P_2F^{\top}P_1F$.

In the rest of this section, we will show how to accelerate BiCGSTAB iterations. As the fictitious domain Ω has a simple geometry, it is easy to define a multilevel family of nested partitions and corresponding spaces V_{h_j} with stepsizes h_j , $0 \le j \le J$, so that $h_{j+1} < h_j$ (e.g., $h_{j+1} = h_j/2$). In order to accelerate BiCGSTAB iterations on the finest *J*-th level, one can apply the hierarchical multigrid scheme, which is formulated below. Note that upper indices *j* refer to the *j*-th level.

The computation starts on the coarsest level, j = 0, with the first iterate $\lambda_{\mathbb{N}}^{0,(0)}$ arbitrarily chosen in $\mathbb{N}(G_2^{(0)})$ (e.g., $\lambda_{\mathbb{N}}^{0,(0)} = 0$). The first iterate on each subsequent level is determined as the prolongated and projected result from the nearest lower level. The terminating tolerance ϵ on the *j*-th level is set proportionally to an expected discretization error that is $\epsilon := Ch_j^p$, where *p* is an expected convergence rate (in the $L^2(\omega)$ -norm) and *C* is a control parameter. The result obtained with such ϵ can be viewed as an inexact solution of the discretized system $(\vec{\mathcal{P}})$ with the same convergence rate as the exact one [1].

Algorithm: Hierarchical Multigrid Scheme

Initialize: Let $\lambda_{\mathbb{N}}^{0,(0)} \in \mathbb{N}(G_2^{(0)})$ be given. PROJBiCGSTAB $[Ch_0^p, \lambda_{\mathbb{N}}^{0,(0)}, F^{(0)}, P_1^{(0)}, P_2^{(0)}, \tilde{d}^{(0)}] \rightarrow \lambda_{\mathbb{N}}^{(0)}$.

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For j = 1, ..., J,

$$\begin{split} & \text{prolongate } \lambda_{\mathbb{N}}^{(j-1)} \to \widetilde{\lambda}_{\mathbb{N}}^{0,(j)}, \\ & \text{project } \widetilde{\lambda}_{\mathbb{N}}^{0,(j)} \to \lambda_{\mathbb{N}}^{0,(j)} := P_2^{(j)} \widetilde{\lambda}_{\mathbb{N}}^{0,(j)}, \\ & \text{ProjBiCGSTAB}[Ch_j^p, \lambda_{\mathbb{N}}^{0,(j)}, F^{(j)}, P_1^{(j)}, P_2^{(j)}, \widetilde{d}^{(j)}] \to \lambda_{\mathbb{N}}^{(j)}, \\ & \text{end.} \end{split}$$

Return: $\lambda_{\mathbb{N}} := \lambda_{\mathbb{N}}^{(J)}$.

6. NUMERICAL EXAMPLES

We will assess experimentally two aspects analyzed in the paper. Firstly, we will illustrate the increased accuracy and improved convergence properties of the new variant of the fictitious domain approach compared to the standard one based on boundary Lagrange multipliers. Secondly, we will demonstrate the computational efficiency of the PSCM algorithm for solving non-symmetric saddle-point systems arising from finite element discretizations.

We will consider two model problems $(\mathcal{P}(\omega))'$ with different geometries of ω represented by the ellipse and by the (non-convex) Cassini oval both lying inside of the unit box $\Omega = (0,1) \times (0,1)$. The right hand-side f and g in $(\mathcal{P}(\omega))'$ are computed as $f = -\Delta \hat{u}$ in R^2 , $g = \hat{u}_{|_{\gamma}}$, where $\hat{u}(x,y) = 100 ((x-0.5)^3 - (y-0.5)^3) - x^2$, $(x,y) \in R^2$. In the examples below the exact solution u_{ex} is given by $\hat{u}_{|_{\gamma}}$.

In the fictitious domain formulation $(\hat{\mathcal{P}}(\Omega))$, we replace $H_0^1(\Omega)$ by

 $H^1_{per}(\Omega) := \{ v \in H^1(\Omega) | v \text{ is periodic on } \partial \Omega \}.$

It should be noted that the theoretical results of Section 2 remain valid also for this modification of the state space. The advantage of this choice consists in the fact that the resulting stiffness matrix A in $(\vec{\mathcal{P}})$ has a block circulant structure which allows to use the highly efficient Poisson solver [7] based on the discrete Fourier transform (DFT). For the convenience of the reader, we recall the main ideas.

We consider $(\hat{\mathcal{P}}(\Omega))_h^H$ with the following choice of subspaces: $V_h \subset H_{per}^1(\Omega)$ is formed by piecewise bilinear functions on a rectangulation of Ω with the stepsizes h_x , h_y ; L_H^{γ} and L_H^{Γ} are defined by piecewise constant functions on partitions of polygonal approximations of γ and Γ . The stepsizes H on γ and Γ respectively, are chosen to guarantee the requirement dim $L_H^{\gamma} = \dim L_H^{\Gamma}$. The stiffness matrix in $(\vec{\mathcal{P}})$ can be written as

$$A = A_x \otimes M_y + M_x \otimes A_y, \tag{6.1}$$

where

$$A_x = \frac{1}{h_x} \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & -1 \\ -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 \\ -1 & 0 & 0 & \dots & -1 & 2 \end{pmatrix}, \quad M_x = \frac{h_x}{6} \begin{pmatrix} 4 & 1 & 0 & \dots & 0 & 1 \\ 1 & 4 & 1 & \dots & 0 & 0 \\ 0 & 1 & 4 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 4 & 1 \\ 1 & 0 & 0 & \dots & 1 & 4 \end{pmatrix}$$

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are the circulants of the order $n_x \sim 1/h_x$ and A_y , M_y are the analogous circulants of the order $n_y \sim 1/h_y$; the symbol \otimes stands for the Kronecker tensor product. It is well-known that eigenvalues of any circulant can be obtained by the DFT of its first column while eigenvectors are columns of the inverse to the DFT matrix [6]. Introducing notation X_x and X_y for the DFT matrices of the order n_x and n_y , respectively, we can write

$$A_k = X_k^{-1} D_{A_k} X_k, \quad M_k = X_k^{-1} D_{M_k} X_k, \quad k = x, y,$$

where D_{A_k} , D_{M_k} are the respective diagonal matrices of eigenvalues. Substituting these expressions into (6.1) and using properties of the Kronecker tensor product, we obtain

$$A = X_x^{-1} D_{A_x} X_x \otimes X_y^{-1} D_{M_y} X_y + X_x^{-1} D_{M_x} X_x \otimes X_y^{-1} D_{A_y} X_y$$

= $(X_x \otimes X_y)^{-1} (D_{A_x} \otimes D_{M_y} + D_{M_x} \otimes D_{A_y}) (X_x \otimes X_y).$

Then the generalized inverse to A can be written as

$$A^{\dagger} := (X_x \otimes X_y)^{-1} (D_{A_x} \otimes D_{M_y} + D_{M_x} \otimes D_{A_y})^{\dagger} (X_x \otimes X_y), \tag{6.2}$$

where $(D_{A_x} \otimes D_{M_y} + D_{M_x} \otimes D_{A_y})^{\dagger}$ is defined just by inverting the non-zero diagonal entries in $D_{A_x} \otimes D_{M_y} + D_{M_x} \otimes D_{A_y}$. Let us point out that actions of A^{\dagger} based on (6.2) require to perform two DFT (in 2D) and one product by a diagonal matrix. Therefore the total complexity is $\mathcal{O}(2n \log_2 n + n)$ with $n = n_x n_y$ provided n_x and n_y are powers of two. Finally, let us point out that the null-spaces of A and A^{\top} are the same and their bases are given by

$$N = M = (1, 1, \dots, 1)^{\top} \in \mathbb{R}^{n \times 1}$$

This makes it possible to perform matrix-vector products by N with the complexity $\mathcal{O}(n)$.

In the tables below, we report the number of primal (n) and control (m) variables, the number of BiCGSTAB iterations, the computational time and the absolute errors of the approximate solution \hat{u}_h with respect to the exact one in the following norms:

$$\operatorname{Err}_{L_2(\omega)} = \|\hat{u}_h - u_{ex}\|_{L_2(\omega)}, \quad \operatorname{Err}_{H^1(\omega)} = \|\hat{u}_h - u_{ex}\|_{H^1(\omega)}, \quad \operatorname{Err}_{L_2(\gamma)} = \|\hat{u}_h - u_{ex}\|_{L_2(\gamma)}.$$

From the computed errors, we determine convergence rates of the fictitious domain solution in the $L_2(\omega)$, $H^1(\omega)$ and $L_2(\gamma)$ -norm, respectively. The parameters in the multigrid scheme are set to p = 2 and $C = \|\tilde{d}\|$. We consider partitions with the nonconstant ratio of stepsizes $H/h = |\log_2(h)|$ found experimentally with $h = \max(h_x, h_y)$ which leads to a smooth behavior of the approximations λ_H as $H \to 0 +$.

Example 6.1. (ellipse) Let ω be given by the interior of an ellipse

$$\omega = \{ (x, y) \in \mathbb{R}^2 | \frac{(x - 0.5)^2}{0.4^2} + \frac{(y - 0.5)^2}{0.2^2} < 1 \}.$$

The auxiliary boundary Γ is constructed by shifting γ eight h units in the direction of the outward normal vector ν ; see Figures 6.1-6.8 for h = 1/256. Table 6.1 summarizes results of the classical fictitious domain approach while the results of the new variant are presented in Tables 6.2, 6.3. The computed errors and the convergence rates confirm the predictions of Section 2. The number of BiCGSTAB iterations is small in comparison with the size of the problems and, in addition, it is considerably reduced by the multigrid scheme.

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Figure 6.9 illustrates a smoothing effect of δ . If the auxiliary boundary Γ is shifted far enough from the original γ the smoothness of the computed solution increases inside ω which in turn results in smaller discretization errors. On the other hand, Figure 6.10 shows that the condition number of P_1F (on $\mathbb{N}(G_2)$) increases exponentially with respect to δ . Finally, Figure 6.11 shows the deviation of P_1F from normality.



Figure 6.1. Geometry of ω .

Figure 6.2. Right hand side f.

Figure 6.3. Ex. solution u_{ex} .







Figure 6.4. Comp. sol. \hat{u}_h .

Figure 6.5. Comp. sol. \hat{u}_h in ω . Figure 6.6. Diffr. $\hat{u}_h - u_{ex}$ in ω .



Figure 6.7. Diffr. $\hat{u}_h - u_{ex}$ on γ .



Figure 6.8. Control variable λ_H on Γ .

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Step h	n/m	Iters.	S.time[s]	$\operatorname{Err}_{L^2(\omega)}$	$\operatorname{Err}_{H^1(\omega)}$	$\operatorname{Err}_{L^2(\gamma)}$
1/128	16641/35	8	0.14	2.0860e-2	1.9647e + 0	6.6516e-2
1/256	66049/62	9	0.56	1.1092e-2	1.2884e + 0	3.2175e-2
1/512	263169/110	12	5.19	5.3989e-3	8.6517e-1	1.5019e-2
1/1024	1050625/198	20	33.05	2.7453e-3	6.0511e-1	7.3265e-3
1/2048	4198401/360	26	167.00	1.3349e-3	4.4015e-1	3.6245e-3
Convergence rates:				0.995	0.541	1.053

Table 6.1. Ellipse, classical FD approach.

Table 6.2. Ellipse, new FD approach; ProjBiCGSTAB, $\epsilon = h^2 \| \widetilde{d} \|$.

Step h	n/m	Iters.	S.time[s]	$\operatorname{Err}_{L^2(\omega)}$	$\operatorname{Err}_{H^1(\omega)}$	$\operatorname{Err}_{L^2(\gamma)}$
1/128	16641/35	13	0.17	2.2550e-4	1.6884e-2	1.1689e-3
1/256	66049/62	25	1.33	5.4869e-5	7.7891e-3	2.9342e-4
1/512	263169/110	40	14.97	1.4177e-5	4.0160e-3	1.1504e-4
1/1024	1050625/198	55	83.56	3.4507e-6	1.9028e-3	2.4769e-5
1/2048	4198401/360	94	571.50	9.0638e-7	9.9895e-4	1.2495e-5
Convergence rates:				1.991	1.019	1.666

Table 6.3. Ellipse, new FD approach; Multigrid.

Step h	n/m	Iters.	S.time[s]	$\operatorname{Err}_{L^2(\omega)}$	$\operatorname{Err}_{H^1(\omega)}$	$\operatorname{Err}_{L^2(\gamma)}$
1/128	16641/34	11	0.22	2.4444e-4	1.8988e-2	1.4694e-3
1/256	66049/62	13	0.88	5.5030e-5	7.6303e-3	2.5171e-4
1/512	263169/110	19	8.41	1.3952e-5	3.8638e-3	8.3976e-5
1/1024	1050625/198	22	41.91	3.3209e-6	1.8681e-3	2.5253e-5
1/2048	4198401/360	31	243.50	8.5762e-7	9.6771e-4	1.1555e-5
Convergence rates:				2.036	1.062	1.730



Figure 6.9. $H_1(\omega)$ -error sensitivity with δ .

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Figure 6.10. $cond(P_1F|\mathbb{N}(G_2))$ sensitivity with δ .



Figure 6.11. Violation of normality as a function of δ , i.e. $||KK^{\top} - K^{\top}K||$, $K = P_1F$.

Example 6.2. (Cassini oval) Let ω be the interior of the Cassini oval

$$\gamma = \left\{ (x, y) = (r \cos \varphi, r \sin \varphi) \in \mathbb{R}^2, \ \varphi \in [0, 2\pi), \ r = a \sqrt{\cos(2\varphi) + \sqrt{(b/a)^4 - \sin^2(2\varphi)}} \right\},$$

where a = 0.25 and b = 0.255; see Figures 6.12-6.19 for h = 1/256. The auxiliary boundary Γ is constructed as in the previous example with $\delta = 6h$. The results in Tables 6.4-6.6 are similar to those computed in Example 6.1. The number of BiCGSTAB iterations is now greater. This may be due to the non-convexity of the domain ω .

Table 6.4. Cassini oval, classical FD approach.

Step h	n/m	Iters.	S.time[s]	$\operatorname{Err}_{L^2(\omega)}$	$\operatorname{Err}_{H^1(\omega)}$	$\operatorname{Err}_{L^2(\gamma)}$
1/128	16641/32	7	0.11	1.8469e-2	1.4316e+0	4.9200e-2
1/256	66049/57	9	0.56	8.5003e-3	9.9211e-1	2.5737e-2
1/512	263169/101	13	5.27	4.0795e-3	6.9436e-1	1.1640e-2
1/1024	1050625/182	17	27.77	1.9695e-3	4.9840e-1	5.9052e-3
1/2048	4198401/332	21	136.80	9.9397e-4	3.5127e-1	3.0024e-3
Convergence rates:				1.054	0.505	1.019

Table 6.5. Cassini oval, new FD approach; ProjBiCGSTAB, $\epsilon = h^2 \|\tilde{d}\|$.

Step h	n/m	Iters.	S.time[s]	$\operatorname{Err}_{L^2(\omega)}$	$\operatorname{Err}_{H^1(\omega)}$	$\operatorname{Err}_{L^2(\gamma)}$
1/128	16641/32	16	0.20	4.8818e-4	4.3430e-2	5.2433e-3
1/256	66049/57	30	1.59	5.8574e-5	1.0141e-2	7.0059e-4
1/512	263169/101	51	18.86	1.3846e-5	4.6618e-3	2.1672e-4
1/1024	1050625/182	100	149.70	2.7136e-6	1.8784e-3	4.6878e-5
1/2048	4198401/332	186	1135.00	7.5260e-7	1.0081e-3	1.9824e-5
Convergence rates:				2.311	1.329	2.000

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Step h	n/m	Iters.	S.time[s]	$\operatorname{Err}_{L^{2}(\omega)}$	$\operatorname{Err}_{H^{1}(\omega)}$	$\operatorname{Err}_{L^2(\gamma)}$
1/128	16641/32	15	0.2031	4.2930e-4	3.8333e-2	4.5419e-3
1/256	66049'/56	29	1.672	4.6345e-5	8.1012e-3	4.5772e-4
1/512	263169/100	30	12.33	1.0902e-5	3.7576e-3	1.3216e-4
1/1024	1050625/182	44	76	2.6887e-6	1.8829e-3	4.8691e-5
1/2048	4198401/332	63	439.3	7.3218e-7	9.8655e-4	1.8763e-5
Convergence rates:				2.250	1.267	1.907

Table 6.6. Cassini oval, new FD approach; Multigrid.





Figure 6.12. Geometry of $\omega.$

Figure 6.13. Right hand side f.

Figure 6.14. Ex. solution u_{ex} .



Figure 6.15. Comp. sol. \hat{u}_h .





Figure 6.16. Comp. sol. \hat{u}_h in ω . Figure 6.17. Diffr. $\hat{u}_h - u_{ex}$ in ω .



Figure 6.18. Diffr. $\hat{u}_h - u_{ex}$ on γ .

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Figure 6.19. Control variable λ_H on Γ .

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7. CONCLUSIONS AND COMMENTS

The objective of the paper was twofold: a) to introduce a new, more regular fictitious domain approach, in which the singularity of a solution is shifted away from the original domain, b) to present an efficient method for solving non-symmetric singular systems of saddle point type arising from a discretized fictitious domain approach. Numerical experiments illustrate the high efficiency of our approach. Unlike the standard fictitious domain method with the convergence rate of order 1/2, the present version has the same rate of convergence as a classical finite element method. It is worth noticing that the errors on the coarsest grid (16641 of primal variables) used in the new approach are smaller than the ones on the finest grid (4198401 primal variables) in the standard fictitious domain method.

The saddle-point system of algebraic equations arising from a finite element discretization is typically non-symmetric with a possibly singular diagonal block. Our solution method combines two basic algorithms: the Schur complement method and the null-space method [2]. The resulting equation is solved iteratively by the projected BiCGSTAB algorithm. This procedure is easy to implement and converges fast as demonstrated by numerical examples.

Finally, we used a hierarchical multigrid scheme. This preconditioning technique connects theoretical results on convergence rates of finite element discretizations with the terminating tolerance for the BiCGSTAB algorithm. The numerical experiments demonstrate considerable accelerations of the BiCGSTAB iterations.

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