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Projected iterative algorithms for complex symmetric systems arising in magnetized multicomponent transport

Vincent Giovangigli [a,*], Benjamin Graille [b]

[a] CMAP, CNRS, Ecole Polytechnique, 91128 Palaiseau, Cedex, France
[b] Laboratoire de Mathématiques d'Orsay, Université Paris sud, 91405 Orsay, France

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ABSTRACT

We investigate iterative algorithms for solving complex symmetric constrained singular systems arising in magnetized multicomponent transport. The matrices of the corresponding linear systems are symmetric with a positive semi-definite real part and an imaginary part with a compatible nullspace. We discuss well posedness, the symmetry of generalized inverses and Cholesky methods. We investigate projected stationary iterative methods as well as projected orthogonal residuals algorithms generalizing previous results on real systems. As an application, we consider the linear systems arising from the kinetic theory of gases and providing transport coefficients of partially ionized gas mixtures subjected to a magnetic field.

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1. Introduction

1.1. Transport linear systems

In nonionized gas mixtures, the evaluation of transport coefficients—such as the diffusion matrix or the thermal conductivity—requires solving real linear systems [10,7]. Similarly, in partially ionized gas mixtures subjected to strong magnetic fields, the evaluation of non-isotropic transport coefficients requires solving complex linear systems [10,16,17]. The linear systems associated with transport coef-

* Corresponding author. Tel.: +33 1 69 33 45 99; fax: +33 1 69 33 46 46.
E-mail address: vincent.giovangigli@polytechnique.edu (V. Giovangigli).

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ficients parallel to the magnetic field are real and similar to that of nonionized mixtures whereas the linear systems associated with transport coefficients perpendicular and transverse to the magnetic field are complex and are investigated in this paper. These linear systems arise—in a kinetic theory framework—from variational procedures used to solve approximately linearized Boltzmann integral equations [10,6,15].

The complex linear systems associated with partially ionized gas mixtures are constrained singular systems that can be written

$$\begin{cases} \mathscr{G}a = b, \\ a \in \mathscr{C}, \end{cases} \tag{1.1}$$

where $\mathscr{G} \in \mathbb{C}^{n,n}, \mathscr{C}$ is a linear subspace of $\mathbb{C}^n$, and $a, b \in \mathbb{C}^n$ are vectors. The matrix $\mathscr{G}$ and the constrained space $\mathscr{C}$ have a special structure derived from the kinetic theory of magnetized multicomponent transport [16,17]. The matrix $\mathscr{G}$ is in the form $\mathscr{G} = G + \mathrm{i}G'$ where $G \in \mathbb{R}^{n,n}$ is a symmetric positive semi-definite matrix, $G' \in \mathbb{R}^{n,n}$ a symmetric matrix with a 'compatible' nullspace, that is, such that $G'N(G) = 0$. The constrained subspace $\mathscr{C}$ is the complexification $\mathscr{C} = \mathcal{C} + \mathrm{i}\mathcal{C}$ of a real linear subspace $\mathcal{C} \subset \mathbb{R}^n$ complementary to $N(G)$. In some applications, there are n complex transport coefficients associated with the system (1.1) which are given by the components of a and in some others there is a single complex transport coefficient usually given by a scalar product $\mu = \langle a, b' \rangle$ where $b' \in \mathbb{C}^n$ is a vector. The constraint $a \in \mathscr{C}$ is generally a constraint on the transport coefficients which is important from a physical point of view and is typically associated with a conservation property.

In this paper, we generalize the mathematical tools introduced in [6,7] in the special situation $G' = 0$. We first relate the solution of (1.1) to generalized inverses naturally associated with the problem and investigate their symmetry. We also investigate regular reformulations of (1.1) involving symmetric matrices with a positive definite real part which can be inverted by using a complex Cholesky method. We then study the convergence of projected stationary iterative methods for solving the constrained singular system (1.1). We establish in particular that the convergence rate is never worse in the case $G' \neq 0$ upon properly choosing the splitting matrix.

Various generalized conjugated gradient techniques have been introduced in order to solve invertible complex symmetric linear systems [9,11,12]. In this paper, we investigate projected orthogonal residuals methods for solving the constrained singular system (1.1) and establish their convergence. Orthogonal residuals methods seem natural in this framework since they make use of the positivity properties of the real symmetric part G and they exactly correspond to previously introduced algorithms when $G' = 0$ [7]. Orthogonal residuals methods have a better convergence behavior than stationary methods and should generally be preferred. However they do not yield a linear dependency between the iterates and the right-hand side and this linear dependency may be important in some applications.

In order to illustrate the projected iterative algorithms we present an application to the species diffusion matrices perpendicular and transverse to the magnetic field in partially ionized magnetized mixtures.

After some mathematical preliminaries in Section 1, we investigate in Section 2 the properties of generalized inverses as well as regular reformulations and Cholesky type decompositions. In Section 3, we study the convergence of projected stationary iterative algorithms. In Section 4 we discuss projected orthogonal residuals algorithms. Finally, in Section 5, we present an application to multicomponent transport.

1.2. Notation and preliminaries

Let $\mathbb{K}$ be a field designating either $\mathbb{R}$ or $\mathbb{C}$, we denote by $\mathbb{K}^n$ the corresponding n-dimensional vector space, and by $\mathbb{K}^{n,n}$ the set of $n \times n$ matrices where $n \in \mathbb{N}, n \geqslant 1$. For a vector $z \in \mathbb{K}^n$, we denote by $z = (z_1, \dots, z_n)$ its components and by $\mathbb{K}z$ the subspace span(z) of $\mathbb{K}^n$. For $x, y \in \mathbb{C}^n$, $\langle x, y \rangle$ denotes the scalar product $\langle x, y \rangle = \sum_{1 \leqslant k \leqslant n} x_k \bar{y}_k$ and $\|x\| = \langle x, x \rangle^{1/2}$ the Hermitian norm of x. Therefore, if $x, y \in \mathbb{R}^n$, $\langle x, y \rangle$ also denotes the scalar product $\langle x, y \rangle = \sum_{1 \leqslant k \leqslant n} x_k y_k$ and $\|x\| = \langle x, x \rangle^{1/2}$ the Euclidean norm of x. For a subspace $\mathscr{S}$ of $\mathbb{R}^n$, we denote by $\mathscr{S}^\perp$ its orthogonal complement and for a nonzero vector $a \in \mathbb{R}^n$ we denote by $a^\perp$ the orthogonal complement of $\mathbb{R}a$. For $x, y \in \mathbb{C}^n$, (x, y) denotes the bilinear form $(x, y) = \sum_{1 \leqslant k \leqslant n} x_k y_k$, so that $\langle x, y\rangle = (x, \bar{y})$.

We use classical notation concerning complexifications and $z \in \mathbb{C}^n$ may be written $z = x + \mathrm{i}y$ where $x, y \in \mathbb{R}^n$. A subspace $\mathscr{F} \subset \mathbb{C}^n$ is the complexification of a subspace of $\mathbb{R}^n$ if and only if $\mathscr{F} = \overline{\mathscr{F}}$ in which case $\mathscr{F}$ is the complexification of $\mathscr{H} = \mathscr{F} \cap \mathbb{R}^n$ so that $\mathscr{F} = \mathscr{H} + \mathrm{i}\mathscr{H}$ and $\dim_{\mathbb{C}}(\mathscr{F}) = \dim_{\mathbb{R}}(\mathscr{H})$. If $\mathscr{S}_1$ and $\mathscr{S}_2$ are two complementary subspaces $\mathscr{S}_1 \oplus \mathscr{S}_2 = \mathbb{R}^n$, the corresponding complexifications are easily shown to satisfy $(\mathscr{S}_1 + \mathrm{i}\mathscr{S}_1) \oplus (\mathscr{S}_2 + \mathrm{i}\mathscr{S}_2) = \mathbb{C}^n$ as well as $(\mathscr{S}_1^\perp + \mathrm{i}\mathscr{S}_1^\perp) \oplus (\mathscr{S}_2^\perp + \mathrm{i}\mathscr{S}_2^\perp) = \mathbb{C}^n$. If $\mathscr{H}$ is a real vector space and $\mathscr{F} = \mathscr{H} + \mathrm{i}\mathscr{H}$ its complexification, $\mathscr{H}^\perp + \mathrm{i}\mathscr{H}^\perp$ is the orthogonal complement of $\mathscr{F}$ with respect to either the scalar product $\langle\,,\,\rangle$ or the bilinear form $(\,,\,)$.

For $A \in \mathbb{K}^{n,n}$, we write $A = (a_{kl})_{1 \leqslant k,l \leqslant n}$ the coefficients of the matrix A and A^t the transpose of A. The nullspace and the range of A are denoted by $N(A)$ and $R(A)$, respectively, and the rank of A is denoted by $\mathrm{rank}(A)$. For $x, y \in \mathbb{K}^n$, $x \otimes y \in \mathbb{K}^{n,n}$ denotes the tensor product matrix $x \otimes y = (x_k y_l)_{1 \leqslant k,l \leqslant n}$. The identity matrix is denoted by I and $\mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ is the diagonal matrix with diagonal elements $\lambda_1, \ldots, \lambda_n$. If $\mathscr{S}_1$ and $\mathscr{S}_2$ are two complementary subspaces of $\mathbb{K}^n$, i.e., $\mathscr{S}_1 \oplus \mathscr{S}_2 = \mathbb{R}^n$, we denote by $P_{\mathscr{S}_1,\mathscr{S}_2}$ the oblique projector matrix onto the subspace $\mathscr{S}_1$ along the subspace $\mathscr{S}_2$. For a matrix $A \in \mathbb{K}^{n,n}$, we denote by $\|A\|$ its Frobenius norm $\|A\| = \left(\sum_{1 \leqslant k,l \leqslant n} |a_{kl}|^2\right)^{1/2}$. If $A \in \mathbb{K}^{n,n}$ is such that $N(A) \oplus R(A) = \mathbb{K}^n$ we denote by $A^\sharp$ its group inverse [1,4]. The following proposition characterizes generalized inverses with prescribed range and nullspace and its proof is identical in the real or complex cases [1,4,15].

Proposition 1.1. *Let $\mathscr{G} \in \mathbb{C}^{n,n}$ be a matrix and let $\mathscr{C}$ and $\mathscr{S}$ be two subspaces of $\mathbb{C}^n$ such that $N(\mathscr{G}) \oplus \mathscr{C} = \mathbb{C}^n$ and $R(\mathscr{G}) \oplus \mathscr{S} = \mathbb{C}^n$. Then there exists a unique matrix $\mathscr{Z}$ such that $\mathscr{G}\mathscr{Z}\mathscr{G} = \mathscr{G}$, $\mathscr{Z}\mathscr{G}\mathscr{Z} = \mathscr{Z}$, $N(\mathscr{Z}) = \mathscr{S}$, and $R(\mathscr{Z}) = \mathscr{C}$. The matrix $\mathscr{Z}$ is called the generalized inverse of $\mathscr{G}$ with prescribed range $\mathscr{C}$ and nullspace $\mathscr{S}$ and is also such that $\mathscr{G}\mathscr{Z} = P_{R(\mathscr{G}),\mathscr{S}}$ and $\mathscr{Z}\mathscr{G} = P_{\mathscr{C},N(\mathscr{G})}$.*

For a matrix $\mathscr{T} \in \mathbb{C}^{n,n}$, $\sigma(\mathscr{T})$ and $\rho(\mathscr{T})$ denote, respectively, the spectrum and the spectral radius of $\mathscr{T}$, and we also define $\gamma(\mathscr{T}) = \max\{|\lambda|;\, \lambda \in \sigma(\mathscr{T}), \lambda \neq 1\}$. A matrix $\mathscr{T}$ is said to be convergent when $\lim_{i\to\infty} \mathscr{T}^i$ exists—not necessarily being zero [22]—and we have the following characterization [26,22].

Proposition 1.2. *A matrix $\mathscr{T} \in \mathbb{C}^{n,n}$ is convergent if and only if either $\rho(\mathscr{T}) < 1$ or $\rho(\mathscr{T}) = 1, 1 \in \sigma(\mathscr{T})$, $\gamma(\mathscr{T}) < 1$, and $(I - \mathscr{T})^\sharp$ exists, i.e., $\mathscr{T}$ has only elementary divisors corresponding to the eigenvalue 1.*

Next, for a matrix $\mathscr{G} \in \mathbb{C}^{n,n}$, the decomposition

$$\mathscr{G} = \mathscr{M} - \mathscr{W} \tag{1.2}$$

is a splitting if the matrix $\mathscr{M}$ is invertible. In order to solve the linear system $\mathscr{G}a = b$, where $b \in \mathbb{C}^n$, the splitting (1.2) induces the iterative scheme

$$z_{i+1} = \mathscr{T} z_i + \mathscr{M}^{-1} b, \quad i \geqslant 0, \tag{1.3}$$

where $\mathscr{T} = \mathscr{M}^{-1}\mathscr{W}$. Assuming that $b \in R(\mathscr{G})$, we have $\mathscr{M}^{-1}b \in R(I - \mathscr{T})$, and the behavior of the sequence of iterates (1.3) is given in the next lemma which can be found in [21,4] (some misprints in the matrix E are corrected in recent versions of Bermann and Plemmons [4]).

Lemma 1.3. *Let $\mathscr{T} \in \mathbb{C}^{n,n}$ and let $c \in \mathbb{C}^n$ such that $c \in R(I - \mathscr{T})$. Then the iterative scheme $z_{i+1} = \mathscr{T} z_i + c$, $i \geqslant 0$, converges for any $z_0 \in \mathbb{C}^n$ if and only if $\mathscr{T}$ is convergent. In this situation, the limit $\lim_{i\to\infty} z_i = z_\infty$ is given by $z_\infty = (I - \mathscr{T})^\sharp c + E z_0$ where $E = I - (I - \mathscr{T})(I - \mathscr{T})^\sharp$.*

2. Constrained singular systems

In this section we investigate well posedness of constrained singular systems, complex symmetric generalized inverses, regular symmetric reformulations of (1.1) and complex Cholesky methods.

2.1. Well posedness

Proposition 2.1. *Let $\mathscr{G} \in \mathbb{C}^{n,n}$ be a matrix and $\mathscr{C}$ be a subspace of $\mathbb{C}^n$. The constrained linear system (1.1) is well posed, i.e., admits a unique solution a for any $b \in R(\mathscr{G})$, if and only if*

$$N(\mathscr{G}) \oplus \mathscr{C} = \mathbb{C}^n. \tag{2.1}$$

In this situation, for any subspace $\mathscr{S}$ such that $R(\mathscr{G}) \oplus \mathscr{S} = \mathbb{C}^n$, the solution a can be written $a = \mathscr{Z}b$, where $\mathscr{Z}$ is the generalized inverse of $\mathscr{G}$ with prescribed range $\mathscr{C}$ and nullspace $\mathscr{S}$.

Proof. Assume first that the system (1.1) is well posed and let $x \in \mathbb{C}^n$. Then there exists a unique solution $y \in \mathscr{C}$ to the system $\mathscr{G}y = \mathscr{G}x$, and hence $x - y \in N(\mathscr{G})$ so that $N(\mathscr{G}) + \mathscr{C} = \mathbb{C}^n$. Furthermore, for any $z \in N(\mathscr{G}) \cap \mathscr{C}$, z satisfies $\mathscr{G}z = 0$ and $z \in \mathscr{C}$, so that we must have $N(\mathscr{G}) \cap \mathscr{C} = \{0\}$ by uniqueness. Conversely, if $N(\mathscr{G}) \oplus \mathscr{C} = \mathbb{C}^n$ and $b \in R(\mathscr{G})$, there exists $x \in \mathbb{C}^n$ such that $\mathscr{G}x = b$, and we may write $x = y + z$ where $y \in N(\mathscr{G})$ and $z \in \mathscr{C}$. Therefore, we have $\mathscr{G}z = b$ and $z \in \mathscr{C}$ so that (1.1) has at least one solution which is also unique since the difference between any two solutions is in $N(\mathscr{G}) \cap \mathscr{C} = \{0\}$. Let now $\mathscr{S}$ be a subspace such that $R(\mathscr{G}) \oplus \mathscr{S} = \mathbb{C}^n$. The generalized inverse $\mathscr{Z}$ then exists by Proposition 1.1 since $N(\mathscr{G}) \oplus \mathscr{C} = \mathbb{C}^n$ and $R(\mathscr{G}) \oplus \mathscr{S} = \mathbb{C}^n$. Moreover, the vector $\mathscr{Z}b$ satisfies $\mathscr{G}\mathscr{Z}b = P_{R(\mathscr{G}),\mathscr{S}}b = b$ since $b \in R(\mathscr{G})$, and we also have $\mathscr{Z}b \in \mathscr{C}$ since $R(\mathscr{Z}) = \mathscr{C}$, so that $a = \mathscr{Z}b$. $\square$

We also investigate in this section the range and nullspace of the complex matrices $\mathscr{G} = G + \mathrm{i}G'$ associated with the linear systems (1.1).

Lemma 2.2. *Let $\mathscr{G} = G + \mathrm{i}G'$ where G, G' are real symmetric matrices, G is positive semi-definite and $G'N(G) = 0$. Then we have $N(\mathscr{G}) = N(G) + \mathrm{i}N(G)$ and $R(\mathscr{G}) = N(G)^{\perp} + \mathrm{i}N(G)^{\perp}$. Moreover, for any subspace $\mathcal{C} \subset \mathbb{R}^n$ complementary to $N(G)$, we have $G' = (P_{\mathcal{C},N(G)})^t G' P_{\mathcal{C},N(G)}$, and denoting $\mathscr{C} = \mathcal{C} + \mathrm{i}\mathcal{C}$ the complexification of $\mathcal{C}$, we have $N(\mathscr{G}) \oplus \mathscr{C} = \mathbb{C}^n$ and $P_{\mathcal{C},N(G)} = P_{\mathscr{C},N(\mathscr{G})}$.*

Proof. For any $z = x + \mathrm{i}y$ where $x, y \in \mathbb{R}^n$, a direct calculation yields

$$\langle (G + \mathrm{i}G')z, z\rangle = \langle Gx, x\rangle + \langle Gy, y\rangle + \mathrm{i}(\langle G'x, x\rangle + \langle G'y, y\rangle),$$

since G and G' are symmetric. Assuming $(G + \mathrm{i}G')z = 0$ thus yields that $x, y \in N(G)$ since G is positive semi-definite and conversely, it is obvious that $N(G) + \mathrm{i}N(G) \subset N(G + \mathrm{i}G')$ since $G'N(G) = 0$. Since $N(G) \subset N(G')$, we also deduce by transposing that $N(G')^{\perp} \subset N(G)^{\perp}$ so that $R(G') \subset R(G)$ since G and G' are symmetric. As a consequence $R(G + \mathrm{i}G') \subset R(G) + \mathrm{i}R(G)$ and thus $R(G + \mathrm{i}G') = R(G) + \mathrm{i}R(G)$ since both subpaces of $\mathbb{C}^n$ are of dimension $n - \dim(N(G)) = n - \dim(N(\mathscr{G}))$. If $\mathcal{C}$ is complementary to $N(G)$, we can decompose any $x \in \mathbb{R}^n$ into $x = P_{\mathcal{C},N(G)}x + (I - P_{\mathcal{C},N(G)})x$ where $P_{\mathcal{C},N(G)}x \in \mathcal{C}$ and $(I - P_{\mathcal{C},N(G)})x \in N(G)$, and this implies that $G'x = G'P_{\mathcal{C},N(G)}x$ so that $G' = G'P_{\mathcal{C},N(G)}$. Upon transposing this relation we also obtain $G' = (P_{\mathcal{C},N(G)})^t G'$. Finally it is straightforward to establish that $N(\mathscr{G}) \oplus \mathcal{C} = \mathbb{C}^n$ and that $P_{\mathcal{C},N(G)} = P_{\mathscr{C},N(\mathscr{G})}$ upon decomposing vectors of $\mathbb{C}^n$ into their real and imaginary parts. $\square$

2.2. Symmetric generalized inverses

By using the symmetry of the matrix $\mathscr{G} = G + \mathrm{i}G'$ it is possible to select a symmetric generalized inverse of $\mathscr{G}$ with prescribed range $\mathscr{C} = \mathcal{C} + \mathrm{i}\mathcal{C}$.

Proposition 2.3. *Let $\mathscr{G} = G + \mathrm{i}G'$ where G, G' are real symmetric matrices, G is positive semi-definite and $G'N(G) = 0$. Let $\mathscr{C} = \mathcal{C} + \mathrm{i}\mathcal{C}$ where $\mathcal{C} \subset \mathbb{R}^n$ is a subspace complementary to $N(G)$. Let $\mathscr{Z}$ be the generalized* *inverse of $\mathscr{G}$ with prescribed nullspace $N(\mathscr{Z}) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ and range $R(\mathscr{Z}) = \mathcal{C} + \mathrm{i}\mathcal{C}$. Then the matrix $\mathscr{Z}$ is symmetric and is the unique symmetric generalized inverse of $\mathscr{G}$ with range $\mathscr{C}$, that is, the unique symmetric matrix $\mathscr{L}$ such that $\mathscr{L}\mathscr{G}\mathscr{L} = \mathscr{L}, \mathscr{G}\mathscr{L}\mathscr{G} = \mathscr{G}$ and $R(\mathscr{L}) = \mathscr{C}$. Upon decomposing $\mathscr{Z} = Z + \mathrm{i}Z'$, where $Z, Z' \in \mathbb{R}^{n,n}$, Z and Z' are symmetric matrices, Z is positive semidefinite, $Z'N(Z) = 0$ and $N(Z) = \mathcal{C}^\perp$. Furthermore, denoting by $u_1, \ldots, u_p$ a real basis of $N(G)$, where $p = \dim(N(G)) \geqslant 1$, there exist real vectors $v_1, \ldots, v_p$ spanning $\mathcal{C}^\perp$ such that $\langle v_i, u_j\rangle = \delta_{ij}, 1 \leqslant i, j \leqslant p$. Then for any positive numbers $\alpha_i, \beta_i, 1 \leqslant i \leqslant p$, such that $\alpha_i\beta_i = 1, 1 \leqslant i \leqslant p$, we have*

$$\mathscr{Z} = \left(\mathscr{G} + \sum_{1\leqslant i\leqslant p} \alpha_i v_i \otimes v_i\right)^{-1} - \sum_{1\leqslant i\leqslant p} \beta_i u_i \otimes u_i \tag{2.2}$$

and the real part $G + \sum_{1\leqslant i\leqslant p} \alpha_i v_i \otimes v_i$ of the matrix $\mathscr{G} + \sum_{1\leqslant i\leqslant p} \alpha_i v_i \otimes v_i$ is symmetric positive definite. Therefore, for $b \in R(\mathscr{G})$, the solution a of (1.1) obtained from Proposition 2.1 also satisfies the regular system

$$\left(\mathscr{G} + \sum_{1\leqslant i\leqslant p} \alpha_i v_i \otimes v_i\right) a = b \tag{2.3}$$

and we also have

$$P_{\mathcal{C},N(G)} = P_{\mathscr{C},N(\mathscr{G})} = I - \sum_{1\leqslant i\leqslant p} u_i \otimes v_i. \tag{2.4}$$

Proof. From $N(G) \oplus \mathcal{C} = \mathbb{R}^n$ we obtain that $N(G)^\perp \oplus \mathcal{C}^\perp = \mathbb{R}^n$ so that $R(G) \oplus \mathcal{C}^\perp = \mathbb{R}^n$ since G is symmetric. These relations implies that $N(\mathscr{G}) \oplus (\mathcal{C} + \mathrm{i}\mathcal{C}) = \mathbb{C}^n$ and $R(\mathscr{G}) \oplus (\mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp) = \mathbb{C}^n$ in such a way that the generalized inverse of $\mathscr{G}$ with prescribed range $\mathscr{C} = \mathcal{C} + \mathrm{i}\mathcal{C}$ and prescribed nullspace $\mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ is well defined. Furthermore, from $\mathscr{G}\mathscr{Z}\mathscr{G} = \mathscr{G}, \mathscr{Z}\mathscr{G}\mathscr{Z} = \mathscr{Z}, N(\mathscr{Z}) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp, R(\mathscr{Z}) = \mathcal{C} + \mathrm{i}\mathcal{C}$, and $\mathscr{G}^t = \mathscr{G}$, we first deduce that $\mathscr{G}\mathscr{Z}^t\mathscr{G} = \mathscr{G}, \mathscr{Z}^t\mathscr{G}\mathscr{Z}^t = \mathscr{Z}^t$, and we also have $N(\mathscr{Z}^t) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$, and $R(\mathscr{Z}^t) = \mathcal{C} + \mathrm{i}\mathcal{C}$. More specifically, let $z = x + \mathrm{i}y, x, y \in \mathbb{R}^n$ and assume that $\mathscr{Z}^t z = 0$. For any $c \in \mathcal{C}$ there exists $z' \in \mathbb{C}^n$ with $Zz' = c$ and $(z, c) = (z, \mathscr{Z}z') = (\mathscr{Z}^t z, z') = 0$ so that $(z, c) = \langle z, c\rangle = \langle x, c\rangle + \mathrm{i}\langle y, c\rangle = 0$. This yields $x, y \in \mathcal{C}^\perp, z \in \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ and $N(\mathscr{Z}^t) \subset \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ so that $N(\mathscr{Z}^t) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ since both subspaces of $\mathbb{C}^n$ are of dimension p over $\mathbb{C}$. Similarly, assume that $z = \mathscr{Z}^t z', z' \in \mathbb{C}^n$, and $z = x + \mathrm{i}y, x, y \in \mathbb{R}^n$. Then for any $d \in \mathcal{C}^\perp$ we have $(z, d) = (\mathscr{Z}^t z', d) = (z', \mathscr{Z}d) = 0$ since $N(\mathscr{Z}) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ and $\mathscr{Z}d = 0$. Thus $(z, d) = \langle z, d\rangle = \langle x, d\rangle + \mathrm{i}\langle y, d\rangle = 0$, so that $x, y \in \mathcal{C}, R(\mathscr{Z}^t) \subset \mathcal{C} + \mathrm{i}\mathcal{C}$ and finally $R(\mathscr{Z}^t) = \mathcal{C} + \mathrm{i}\mathcal{C}$. Since $R(\mathscr{Z}^t) = R(\mathscr{Z}), N(\mathscr{Z}^t) = N(\mathscr{Z}), \mathscr{G}\mathscr{Z}^t\mathscr{G} = \mathscr{G}$, and $\mathscr{Z}^t\mathscr{G}\mathscr{Z}^t = \mathscr{Z}^t$, we deduce from the uniqueness of the generalized inverse with prescribed range and nullspace that $\mathscr{Z} = \mathscr{Z}^t$ so that $\mathscr{Z}$ is symmetric. Any symmetric matrix $\mathscr{L}$ such that $\mathscr{L}\mathscr{G}\mathscr{L} = \mathscr{L}, \mathscr{G}\mathscr{L}\mathscr{G} = \mathscr{G}$ and $R(\mathscr{L}) = \mathcal{C}$ also satisfies $N(\mathscr{L}) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ by symmetry. Indeed, if $\mathscr{L}z = 0$ then for any $z' \in \mathbb{C}^n, (\mathscr{L}z, z') = 0 = (z, \mathscr{L}z')$. If $c \in \mathcal{C}$, there exists $z' \in \mathbb{C}^n$ such that $c = \mathscr{Z}z'$ and if $z = x + \mathrm{i}y, x, y \in \mathbb{R}^n, (z, c) = \langle z, c\rangle = \langle x, c\rangle + \mathrm{i}\langle y, c\rangle = 0$ for any $c \in \mathcal{C}$ and $x, y \in \mathcal{C}^\perp, N(\mathscr{L}) \subset \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ and $N(\mathscr{L}) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ so that $\mathscr{L}$ coincides with $\mathscr{Z}$.

Writing $\mathscr{Z} = Z + \mathrm{i}Z'$, where $Z, Z' \in \mathbb{R}^{n,n}$, we have already established that Z and Z' are symmetric. From the relation $(Z + \mathrm{i}Z')(G + \mathrm{i}G') = P$ where $P = P_{\mathcal{C},N(G)}$, we obtain that $ZG - Z'G' = P$ and $ZG' + Z'G = 0$. This implies that $Z = PZ = ZGZ - Z'G'Z = ZGZ + Z'GZ'$ so that $\langle Zx, x\rangle = \langle GZx, Zx\rangle + \langle GZ'x, Z'x\rangle$ and Z is positive semidefinite. Moreover, $Zx = 0$ implies that $Z'x \in N(G)$ and since $R(\mathscr{Z}) = \mathcal{C} + \mathrm{i}\mathcal{C}, Z'x \in \mathcal{C}$, so that $Z'x = 0$, and $Z'N(Z) = 0$. From Lemma 2.2 we deduce that $N(\mathscr{Z}) = N(Z) + \mathrm{i}N(Z)$ and since $N(\mathscr{Z}) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ we obtain $N(Z) = \mathcal{C}^\perp$. The vectors $v_i, 1 \leqslant i \leqslant p$, with $p = \dim(N(G))$ are then easily obtained by selecting for v_i a nonzero element in the one-dimensional subspace $\mathrm{span}(u_1, \ldots, u_{i-1}, u_{i+1}, \ldots, u_p)^\perp \cap \mathcal{C}^\perp$ and by normalizing it. It is then easily shown that $P_{R(\mathscr{Z}),N(\mathscr{G})} = I - \sum_{1\leqslant i\leqslant p} u_i \otimes v_i$ and $P_{R(\mathscr{G}),N(\mathscr{Z})} = I - \sum_{1\leqslant i\leqslant p} v_i \otimes u_i$, which yields (2.4) and implies that $\mathscr{G}\mathscr{Z} = I - \sum_{1\leqslant i\leqslant p} v_i \otimes u_i$ and the formula (2.2) directly follows. Eq. (2.3) is then a direct consequence of (2.2) since $b \in R(\mathscr{G}) = N(G)^\perp + \mathrm{i}N(G)^\perp$. $\square$

2.3. Cholesky method

Since the transport linear systems (1.1) can be rewritten into the nonsingular form (2.3) involving an invertible matrix $\mathscr{G} + \sum_{1\leqslant i\leqslant p} \alpha_i v_i \otimes v_i$ with a positive definite real part $G + \sum_{1\leqslant i\leqslant p} \alpha_i v_i \otimes v_i$ we investigate direct methods in this section. We first restate a classical result about Cholesky decomposition of complex symmetric matrices and next investigate the situation of matrices associated with the linear systems (1.1). Cholesky decomposition may also be used for large full systems arising from discretized integral equations [3].

Theorem 2.4. *Let $\mathscr{A}$ be a complex symmetric matrix such that all principal minors $\delta_i, 1 \leqslant i \leqslant n$, are nonzero. There exists an upper triangular matrix U with diagonal coefficient unity such that*

$$\mathscr{A} = U^t \mathscr{D} U, \tag{2.5}$$

where $\mathscr{D}$ is the diagonal matrix $\mathscr{D} = \mathrm{diag}(\delta_1, \delta_2/\delta_1, \ldots, \delta_n/\delta_{n-1})$.

Proof. Omitted. □

We now apply the preceding proposition to the symmetric complex regular form (2.3) of the transport linear system (1.1).

Proposition 2.5. *Keeping the assumptions of Proposition 2.3, the matrix $\mathscr{G} + \sum_{1 \leqslant i \leqslant p} \alpha_i v_i \otimes v_i$ can be decomposed in the form $U^t \mathscr{D} U$ where U is an upper triangular matrix with diagonal coefficients unity and $\mathscr{D}$ is a diagonal matrix whose diagonal coefficients have a positive real part.*

Proof. Denoting $\mathscr{A} = \mathscr{G} + \sum_{1 \leqslant i \leqslant p} \alpha_i v_i \otimes v_i$, $\mathscr{A} = (a_{ij})_{1 \leqslant i,j \leqslant n}$, and $\mathscr{A}^{[k]} = (a_{ij})_{1 \leqslant i,j \leqslant k}$, we have to check that the submatrix $\mathscr{A}^{[k]}$ is invertible. Assume that $\mathscr{A}^{[k]} z^{[k]} = 0$ where $z^{[k]} \in \mathbb{C}^k$ and define $z \in \mathbb{C}^n$ by $z_i = z_i^{[k]}$ if $1 \leqslant i \leqslant k$ and $z_i = 0$ otherwise. Then $\langle \mathscr{A} z, z \rangle = 0$ and from symmetry $\langle \mathscr{A} z, z \rangle = \langle A z, z \rangle + \mathrm{i} \langle G' z, z \rangle$ where $A = G + \sum_{1 \leqslant i \leqslant p} \alpha_i v_i \otimes v_i$ is positive definite. Upon decomposing $z = x + \mathrm{i} y, x, y \in \mathbb{R}^n$, we also have $\langle A z, z \rangle = \langle A x, x \rangle + \langle A y, y \rangle$ in such a way that $z = 0$, $\mathscr{A}^{[k]}$ is invertible and $\delta_k = \det(\mathscr{A}^{[k]}) \neq 0$.

The matrix U in Theorem 2.4 is constructed as the components in the canonical basis $e_1, \ldots, e_n$ of a family of vectors $f_1, \ldots, f_n$ orthogonal with respect to the bilinear form φ associated with $\mathscr{A}$, i.e., $\varphi(x, y) = (\mathscr{A} x, y) = \langle \mathscr{A} x, \bar{y} \rangle, x, y \in \mathbb{C}^n$. This family is constructed from $f_1 = e_1$ and $f_k = e_k + \sum_{1 \leqslant i \leqslant k-1} \alpha_{ik} e_i / \delta_{k-1}$ where α_{ik} is the cofactor of a_{ik} in $\mathscr{A}^{[k]}$. This family is such that $\varphi(f_k, e_i) = 0$ whenever $1 \leqslant i \leqslant k-1$, $\varphi(f_1, f_1) = \delta_1 = \mathscr{D}_{11}$, and $\varphi(f_k, e_k) = \delta_k / \delta_{k-1} = \mathscr{D}_{kk}$.

However, we can also write that $\varphi(f_k, f_k) = \varphi(f_k, e_k) = \varphi(f_k, \bar{f}_k)$ since the conjugate vector $\bar{f}_k$ is given by $\bar{f}_1 = f_1$ for $k = 1$ and $\bar{f}_k = e_k + \sum_{1 \leqslant i \leqslant k-1} \bar{\alpha}_{ik} e_i / \bar{\delta}_{k-1}$ otherwise, and thus $\mathscr{D}_{kk} = (\mathscr{A} f_k, \bar{f}_k) = \langle \mathscr{A} f_k, f_k \rangle = \langle A f_k, f_k \rangle + \mathrm{i} \langle G' f_k, f_k \rangle$ where A is positive definite. □

3. Stationary iterative algorithms

3.1. Convergence of projected iterative algorithms

We are now interested in solving the constrained singular system (1.1) by stationary iterative techniques. These techniques provide iterates which depend linearly on the right-hand side b, and this property may be important for some applications.

For a given splitting $\mathscr{G} = \mathscr{M} - \mathscr{W}$ and for $b \in R(\mathscr{G})$, assuming that the iteration matrix $\mathscr{T} = \mathscr{M}^{-1} \mathscr{W}$ is convergent, the iterates (1.3) will converge for any z_0. When the matrix $\mathscr{G}$ is singular, we have $\rho(\mathscr{T}) = 1$ since $\mathscr{T} z = z$ for $z \in N(\mathscr{G})$, and neither the iterates $\{z_i; i \geqslant 0\}$ nor the limit z_∞ are guaranteed to be in the constrained space $\mathscr{C}$. In order to overcome these difficulties, we will used a projected iterative scheme [14,7]

$$z'_{i+1} = \mathscr{P} \mathscr{T} z'_i + \mathscr{P} \mathscr{M}^{-1} b, \quad i \geqslant 0, \tag{3.1}$$

where $\mathscr{P} = P_{\mathscr{C}, N(\mathscr{G})}$ is the projector matrix onto the subspace $\mathscr{C}$ along $N(\mathscr{G})$. All the corresponding iterates $\{z'_i; i \geqslant 0\}$ then satisfy the constraint $z'_i \in \mathscr{C}$. Moreover, in order to obtain an iterative scheme with convergence properties valid for any matrix G' we will include the full imaginary part $\mathrm{i}G'$ of $\mathscr{G}$ in the splitting matrix $\mathscr{M}$. We will thus use splitting matrices in the form

$$\mathscr{M} = M + \mathrm{i}G', \tag{3.2}$$

where $G = M - W$ is a splitting of the symmetric positive semi-definite matrix G, so that $\mathscr{W} = \mathscr{M} - \mathscr{G} = W = M - G$ is a real matrix. In addition, $\mathscr{C}$ and $N(\mathscr{G})$ are in the form $\mathscr{C} = \mathcal{C} + \mathrm{i}\mathcal{C}$ and $N(\mathscr{G}) = N(G) + \mathrm{i}N(G)$ so that $\mathscr{P} = P_{\mathcal{C},N(\mathscr{G})} = P_{\mathcal{C},N(G)} = P$.

The spectral radius of the iteration matrix $\mathscr{P}\mathscr{T}$ associated with (3.1) can be estimated by using the following result of Neumann and Plemmons [22].

Theorem 3.1. *Let $\mathscr{T}$ be a matrix such that $(I - \mathscr{T})^\sharp$ exists, i.e., such that $R(I - \mathscr{T}) \cap N(I - \mathscr{T}) = \{0\}$. Let $\mathscr{C}$ be a subspace complementary to $N(I - \mathscr{T})$, i.e., such that $N(I - \mathscr{T}) \oplus \mathscr{C} = \mathbb{C}^n$, and let also $\mathscr{P}$ be the oblique projector matrix onto the subspace $\mathscr{C}$ along $N(I - \mathscr{T})$. Then we have*

$$\rho(\mathscr{P}\mathscr{T}) = \gamma(\mathscr{T}). \tag{3.3}$$

This result (3.3) has also been strengthened and the spectra of $\mathscr{T}$ and $\mathscr{P}\mathscr{T}$ are essentially the same [7]. Although the proof in [7] is given in a real framework it directly extends to the complex case *mutatis mutandis*.

Theorem 3.2. *Keep the assumptions of Theorem 3.1. Then,*

$$\sigma(\mathscr{P}\mathscr{T}) = \begin{cases} (\sigma(\mathscr{T})\backslash\{1\}) \cup \{0\}, & \text{if } N(I - \mathscr{T}) \neq \{0\}, \\ \sigma(\mathscr{T}), & \text{if } N(I - \mathscr{T}) = \{0\}. \end{cases}$$

Furthermore, the matrices $\mathscr{T}$ and $\mathscr{P}$ satisfy the relation $\mathscr{P}\mathscr{T} = \mathscr{P}\mathscr{T}\mathscr{P}$.

We now investigate the convergence and properties of the projected iterative algorithms (3.1) when applied to the complex symmetric constrained singular systems (1.1). Note that Keller's theorem [20] cannot be applied directly as in the real case [7] since $\mathscr{G}$ is not Hermitian when G' is nonzero.

Theorem 3.3. *Let $\mathscr{G} = G + \mathrm{i}G'$ where G, G' are real symmetric matrices, G is positive semi-definite and $G'N(G) = 0$. Let $\mathcal{C} \subset \mathbb{R}^n$ be a subspace complementary to $N(G)$ and let $\mathcal{C}$ be the complexification of $\mathcal{C}$. Consider a splitting $G = M - W$, assume that M is symmetric and that $M + W$ is positive definite, so that M is also symmetric positive definite. Define $\mathscr{M} = M + \mathrm{i}G', \mathscr{G} = \mathscr{M} - \mathscr{W}$, so that $\mathscr{W} = W$, and $\mathscr{T} = \mathscr{M}^{-1}\mathscr{W}, T = M^{-1}W$. Let $\mathscr{P} = P$ be the oblique projector matrix onto the subspace $\mathcal{C}$ along $N(G)$. Let also $b \in R(\mathscr{G}), z_0 \in \mathbb{C}^n, z'_0 = \mathscr{P}z_0$, and consider for $i \geqslant 0$ the iterates $z_{i+1} = \mathscr{T}z_i + M^{-1}b$ as in (1.3) and $z'_{i+1} = \mathscr{P}\mathscr{T}z'_i + \mathscr{P}M^{-1}b$ as in (3.1). Then $z'_i = \mathscr{P}z_i$ for all $i \geqslant 0$, the matrices $\mathscr{T}, \mathscr{P}\mathscr{T}, T$, and PT are convergent, $\rho(T) = \rho(\mathscr{T}) = 1$ when $\dim(N(G)) \geqslant 1, \rho(\mathscr{P}\mathscr{T}) = \gamma(\mathscr{T}) < 1, \rho(PT) = \gamma(T) < 1$, and*

$$\gamma(\mathscr{T}) \leqslant \gamma(T), \tag{3.4}$$

so that the convergence rate is never worse in the case $G' \neq 0$, and we have the following limits:

$$\lim_{i\to\infty} z'_i = \mathscr{P}(\lim_{i\to\infty} z_i) = a, \tag{3.5}$$

where a is the unique solution of (1.1). Moreover, for all $i \geqslant 1$, each partial sum

$$\mathscr{Z}_i = \sum_{0\leqslant j\leqslant i-1} (\mathscr{P}\mathscr{T})^j \mathscr{P}\mathscr{M}^{-1}\mathscr{P}^t \tag{3.6}$$

is symmetric and $\lim_{i\to\infty} \mathscr{Z}_i = \mathscr{Z}$ where

$$\mathscr{Z} = \sum_{0\leqslant j<\infty} (\mathscr{P}\mathscr{T})^j \mathscr{P}\mathscr{M}^{-1}\mathscr{P}^t \tag{3.7}$$

is the symmetric generalized inverse of $\mathscr{G}$ with prescribed nullspace $N(\mathscr{Z}) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ and range $R(\mathscr{Z}) = \mathscr{C} = \mathcal{C} + \mathrm{i}\mathcal{C}$.

In the proof of Theorem 3.3 we will use the following lemma whose proof is postponed.

Lemma 3.4. *Keeping the assumptions of Theorem 3.3, we have*

$$\gamma(T)=\sup\left\{\frac{|\langle Wx,x\rangle|}{\langle Mx,x\rangle};\quad x\in\mathbb{R}^n, x\neq 0, \forall u\in N(G), \langle Mx,u\rangle=0\right\}. \tag{3.8}$$

Proof. By applying Keller's theorem [20,7] to the splitting $G=M-W$ it is readily seen that the matrix T is convergent so that from Theorems 3.1 and 3.2 we deduce that $\gamma(T)=\rho(PT)<1, PT$ is convergent, and $\rho(T)=1$ when $\dim(N(G))\geqslant 1$.

With respect to $\mathscr{T}$, we first note that $1\in\sigma(\mathscr{T})$ when $\dim(N(G))\geqslant 1$ since then $\mathscr{G}$ is singular, $N(\mathscr{G})=N(G)+\mathrm{i}N(G)$, and $\mathscr{T}z=z$ for any $z\in N(\mathscr{G})$. Let now $\lambda\in\sigma(\mathscr{T}), \lambda\neq 1$, so that there exists $z\neq 0$ with $\mathscr{T}z=\lambda z$ and $z\notin N(\mathscr{G})$. Upon writing $z=x+\mathrm{i}y, x,y\in\mathbb{R}^n$, we have $\langle Gz,z\rangle=\langle Gx,x\rangle+\langle Gy,y\rangle$ and $\langle Gz,z\rangle=0$ implies $x,y\in N(G)$ and $z\in N(\mathscr{G})$. Since $z\notin N(\mathscr{G})$ we have $\langle Gz,z\rangle>0$ so that $\langle Wz,z\rangle<\langle Mz,z\rangle$ with $\langle Wz,z\rangle=\langle Wx,x\rangle+\langle Wy,y\rangle$ and $\langle Mz,z\rangle=\langle Mx,x\rangle+\langle My,y\rangle$. Similarly, we know that $M+W$ is symmetric positive definite so that $-\langle Mz,z\rangle<\langle Wz,z\rangle$ and finally $|\langle Wz,z\rangle|<\langle Mz,z\rangle$. On the other hand, since $\mathscr{T}z=\lambda z$, upon multiplying by $\mathscr{M}$ this identity we obtain that $Wz=\lambda\mathscr{M}z=\lambda(M+\mathrm{i}G')z$. Taking the scalar product with z we obtain $\lambda=\langle Wz,z\rangle/(\langle Mz,z\rangle+\mathrm{i}\langle G'z,z\rangle)$ so that

$$|\lambda|\leqslant\frac{|\langle Wz,z\rangle|}{\langle Mz,z\rangle}<1 \tag{3.9}$$

thanks to $\langle Mz,z\rangle\leqslant|\langle Mz,z\rangle+\mathrm{i}\langle G'z,z\rangle|$ and we have established that $\gamma(\mathscr{T})<1$.

In order to establish that $(I-\mathscr{T})^\sharp$ exists, we assume on the contrary that $N(I-\mathscr{T})\cap R(I-\mathscr{T})\neq 0$. In this situation, there exists $z,z'\in\mathbb{C}^n, z\neq 0, z'\neq 0$, such that $\mathscr{T}(z')=z+z'$ and $\mathscr{T}(z)=z$. This yields $Wz'=(M+\mathrm{i}G')(z'+z)$ and $Wz=(M+\mathrm{i}G')z$. Since $\mathscr{T}(z)=z$ we have $z\in N(G)+\mathrm{i}N(G)$ so that $G'z=0, Wz=Mz$, and

$$\langle Wz',z\rangle=\langle(M+\mathrm{i}G')(z'+z),z\rangle=\langle M(z'+z),z\rangle, \tag{3.10}$$

since $\langle G'(z'+z),z\rangle=\langle G'z',z\rangle=\langle z',G'z\rangle=0$ thanks to $G'z=0$. Therefore (3.10) implies that $\langle Mz',z\rangle+\langle Mz,z\rangle=\langle z',Wz\rangle=\langle z',Mz\rangle=\langle Mz',z\rangle$ and $\langle Mz,z\rangle=0$ and $z=0$ contradicting $z\neq 0$, and $\mathscr{T}$ is convergent.

In order to compare the values of $\gamma(T)$ and $\gamma(\mathscr{T})$ we now make use of Lemma 3.4. If $z\in\mathbb{C}^n, z\neq 0$ is such that $\mathscr{T}z=\lambda z$ with $\lambda\neq 1$, and if $u\in\mathbb{R}^n$ is such that $u\in N(G)$ we have $Wz=\lambda(M+\mathrm{i}G')z$ and $Wu=Mu$. Therefore, $\langle Wz,u\rangle=\lambda\langle(M+\mathrm{i}G')z,u\rangle=\lambda\langle Mz,u\rangle$ since $G'u=0$. Since W is symmetric we also have $\langle Wz,u\rangle=\langle z,Wu\rangle=\langle z,Mu\rangle=\langle Mz,u\rangle$ and we have thus shown that $\lambda\langle Mz,u\rangle=\langle Mz,u\rangle$. Since $\lambda\neq 1$ we conclude that $\langle Mz,u\rangle=0$ and thus, upon decomposing $z=x+\mathrm{i}y, x,y\in\mathbb{R}^n$, we deduce that $\langle Mx,u\rangle+\mathrm{i}\langle My,u\rangle=0$ so that finally $\langle Mx,u\rangle=\langle My,u\rangle=0$ for any $u\in N(G)$. We can now write from (3.9)

$$|\lambda|\leqslant\frac{|\langle Wz,z\rangle|}{\langle Mz,z\rangle}=\frac{|\langle Wx,x\rangle+\langle Wy,y\rangle|}{\langle Mx,x\rangle+\langle My,y\rangle},$$

but since $\langle Mx,u\rangle=\langle My,u\rangle=0$ for any $u\in N(G)$ we have $|\langle Wx,x\rangle|\leqslant\gamma(T)\langle Mx,x\rangle$ and $|\langle Wy,y\rangle|\leqslant\gamma(T)\langle My,y\rangle$ so that finally $|\lambda|\leqslant\gamma(T)$ and this yields $\gamma(\mathscr{T})\leqslant\gamma(T)$.

Since the matrices $\mathscr{T}$ and $\mathscr{P}\mathscr{T}$ are convergent, we know that both sequences $\{z_i;\, i\geqslant 0\}$ and $\{z_i';\, i\geqslant 0\}$ are convergent. Denoting by z_∞ and z_∞' the corresponding limits, we deduce from the relation $z_{i+1}=\mathscr{T}z_i+M^{-1}b$ that $z_\infty=\mathscr{T}z_\infty+\mathscr{M}^{-1}b$. This shows that $\mathscr{G}z_\infty=b$ and since $\mathscr{P}\mathscr{T}=\mathscr{P}\mathscr{T}\mathscr{P}$ it is easily established by induction that $z_i'=\mathscr{P}z_i$, for any $i\geqslant 0$. Therefore, $\mathscr{P}z_\infty=z_\infty'$ and since $\mathscr{G}\mathscr{P}=\mathscr{G}$ we obtain that $\mathscr{G}z_\infty'=\mathscr{G}z_\infty=b$. Finally, since $z_\infty'=\mathscr{P}z_\infty'$ we have $z_\infty'\in\mathscr{C}$ and z_∞' is the unique solution of the constrained singular system (1.1).

Assume now that $z_0=0$ so that $z_0'=0$ and then $z_i'=\mathscr{Z}_i b$ for any $i\geqslant 1$. We indeed have $z_1'=\mathscr{P}\mathscr{M}^{-1}b=\mathscr{Z}_1 b$, and assuming by induction that $z_i'=\mathscr{Z}_i b$ we obtain that

$$z_{i+1}'=\mathscr{P}\mathscr{T}z_i'+\mathscr{P}\mathscr{M}^{-1}b=(\mathscr{P}\mathscr{T}\mathscr{Z}_i+\mathscr{P}\mathscr{M}^{-1}\mathscr{P}^t)b=\mathscr{Z}_{i+1}b,$$

since $\mathscr{Z}_{i+1}=\mathscr{P}\mathscr{T}\mathscr{Z}_i+\mathscr{P}\mathscr{M}^{-1}\mathscr{P}^t$. Passing to the limit $i\to\infty$ and thanks to Proposition 2.1 we obtain for any $b\in R(\mathscr{G})$ that $\mathscr{Z}b=\sum_{i\geqslant 0}(\mathscr{P}\mathscr{T})^i\mathscr{P}\mathscr{M}^{-1}\mathscr{P}^t b$ so that $\mathscr{Z}$ and $\sum_{i\geqslant 0}(\mathscr{P}\mathscr{T})^i\mathscr{P}\mathscr{M}^{-1}\mathscr{P}^t$ coincide over $R(\mathscr{G})$ and $\mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ and therefore over $\mathbb{C}^n$. Finally, in order to establish that $\mathscr{Z}_i$ is symmetric, it is sufficient to establish that each term $(\mathscr{P}\mathscr{T})^j\mathscr{P}\mathscr{M}^{-1}\mathscr{P}^t$ in the series (3.6) is symmetric. However, from the relation $\mathscr{P}\mathscr{T} = \mathscr{P}\mathscr{T}\mathscr{P}$ we obtain $(\mathscr{P}\mathscr{T})^j\mathscr{P}\mathscr{M}^{-1}\mathscr{P}^t = \mathscr{P}\mathscr{T}^j\mathscr{M}^{-1}\mathscr{P}^t$ which is symmetric since $\mathscr{T} = \mathscr{M}^{-1}\mathscr{W}$ and $\mathscr{M}$ and $\mathscr{W}$ are symmetric. $\square$

Remark 3.5. The projector matrix $\mathscr{P} = P$ is needed for the convergence of the series (3.7). Indeed, the partial sums $\mathscr{Z}_i$ in (3.6) can be rewritten in the form $\mathscr{Z}_i = \mathscr{P}\left(\sum_{0\leqslant j\leqslant i-1}\mathscr{T}^j\mathscr{M}^{-1}\right)\mathscr{P}^t$ but the series $\sum_{0\leqslant j\leqslant i-1}\mathscr{T}^j\mathscr{M}^{-1}$ has no limit since $\sum_{0\leqslant j\leqslant i-1}\mathscr{T}^j\mathscr{M}^{-1}(\mathscr{M}u) = iu$ for $u \in N(\mathscr{G})$.

Remark 3.6. Upon writing $\mathscr{Z}_i = Z_i + \mathrm{i}Z_i'$, where $Z_i, Z_i' \in \mathbb{R}^{n,n}$, we have established that Z_i and Z_i' are symmetric and it should be true that Z_i is positive semi-definite, $Z_i'N(Z_i) = 0$, and $N(Z_i) = \mathcal{C}^\perp$. This can indeed be established for the first iterates $\mathscr{Z}_1 = \mathscr{P}\mathscr{M}^{-1}\mathscr{P}^t$ and $\mathscr{Z}_2 = \mathscr{P}\mathscr{M}^{-1}(\mathscr{M}+\mathscr{W})\mathscr{M}^{-1}\mathscr{P}^t$. More specifically, we first note that if $\mathscr{M}^{-1} = A + \mathrm{i}A', A, A' \in \mathbb{R}^{n,n}$, then we have $AM - A'G' = I$ and $AG' + A'M = 0$ so that $AMA + A'MA' = A$ and A is positive definite since $A = (M + G'M^{-1}G')^{-1}$. We then obtain after some algebra that $Z_1 = PAP^t$ and $Z_2 = P(A + AWA - A'WA')P^t$ so that $Z_2 = P(A(M+W)A + A'(M-W)A')P^t$ and Z_1 and Z_2 are positive semi-definite with nullspace $\mathcal{C}^\perp$. Since by construction $Z_1'\mathcal{C}^\perp = 0$ and $Z_2'\mathcal{C}^\perp = 0$ we get that $Z_1'N(Z_1) = 0$ and $Z_2'N(Z_2) = 0$. On the other hand, the next iterates $Z_i, i \geqslant 3$, are intricated expressions involving A, A', and W.

Remark 3.7. Iterative methods applied to the regular formulation (2.3) usually converge more slowly than those applied to the singular formulation (1.1) [6]. Moreover, the corresponding iterates do not generally satisfy the constraint at each step.

Proof of Lemma 3.4. Denote by $\langle\!\langle\, , \rangle\!\rangle$ the scalar product $\langle\!\langle x, y\rangle\!\rangle = \langle Mx, y\rangle, x, y \in \mathbb{R}^n$. With respect to this scalar product, the matrix $T = M^{-1}W$ is then symmetric since

$$\langle\!\langle Tx, y\rangle\!\rangle = \langle MTx, y\rangle = \langle Wx, y\rangle = \langle x, Wy\rangle = \langle M^{-1}Mx, Wy\rangle = \langle Mx, Ty\rangle = \langle\!\langle x, Ty\rangle\!\rangle.$$

As a direct application of spectral properties of symmetric matrices, we know that T has a complete set of real eigenvectors orthogonal with respect to $\langle\!\langle\, , \rangle\!\rangle$. In addition, the eigenspace associated with the eigenvalue 1 is the eigenspace $N(I - T) = N(G)$, so that

$$\gamma(T) = \sup\left\{\frac{|\langle\!\langle Tx, x\rangle\!\rangle|}{\langle\!\langle x, x\rangle\!\rangle} \quad x \in \mathbb{R}^n, x \neq 0, \forall u \in N(G), \langle Mx, u\rangle = 0\right\}$$

and (3.8) directly follows since $\langle\!\langle Tx, x\rangle\!\rangle = \langle Wx, x\rangle$ and $\langle\!\langle x, x\rangle\!\rangle = \langle Mx, x\rangle$. $\square$

3.2. Calculation of an inverse

The projected iterative algorithm (3.1) defined in Section 3.1 can readily be applied to solve the linear systems (1.1) provided that the inverse of the splitting matrix $\mathscr{M} = M + \mathrm{i}G'$ can easily be evaluated. In practical applications, even though the matrix G' may not be sparse, it generally has the special structure [16,17]

$$G' = P^tM'P, \tag{3.11}$$

where M' is diagonal and $P = P_{\mathcal{C},N(G)}$. We will thus assume that the matrix $M + \mathrm{i}M'$ is easily invertible and investigate the inverse of $\mathscr{M} = M + \mathrm{i}G'$ in terms of the inverse of $M + \mathrm{i}M'$.

We first consider—for the sake of simplicity—the special situation where the nullspaces of G and $\mathscr{G}$ are of dimension 1. In the following proposition, we evaluate the inverse of $M + \mathrm{i}G'$ when M is symmetric positive definite, $N(G) = \mathbb{R}\mathrm{u}, \mathcal{C} = \mathrm{y}^\perp$ in $\mathbb{R}^n$, $\langle \mathrm{y}, \mathrm{u}\rangle = 1$, so that $N(\mathscr{G}) = \mathbb{C}\mathrm{u}$ $\mathscr{C} = \mathrm{y}^\perp + \mathrm{i}\mathrm{y}^\perp$ in $\mathbb{C}^n$ and the well posedness property $N(G) \oplus \mathcal{C} = \mathbb{R}^n$ holds.

Proposition 3.8. *Assume that M is symmetric positive definite and that $G' \in \mathbb{R}^{n,n}$ is in the form*

$$G' = (I - \mathsf{y} \otimes \mathsf{u})M'(I - \mathsf{u} \otimes \mathsf{y}),$$

where $\mathsf{y}, \mathsf{u} \in \mathbb{R}^n$, $\langle \mathsf{y}, \mathsf{u}\rangle = 1$, *and* $M' \in \mathbb{R}^{n,n}$ *is a symmetric matrix. The matrices* $M + \mathrm{i}M'$ *and* $M + \mathrm{i}G'$ *are invertible,* $\langle (M + \mathrm{i}M')^{-1}\mathsf{y}, \mathsf{y}\rangle \neq 0$, *and we define the matrix E by*

$$E = (M + \mathrm{i}M')^{-1} - \frac{(M + \mathrm{i}M')^{-1}\mathsf{y} \otimes (M + \mathrm{i}M')^{-1}\mathsf{y}}{\langle (M + \mathrm{i}M')^{-1}\mathsf{y}, \mathsf{y}\rangle}. \tag{3.12}$$

Then $\langle (M - MEM)\mathsf{u}, \mathsf{u}\rangle \neq 0$ *and the inverse of* $M + \mathrm{i}G'$ *is given by*

$$(M + \mathrm{i}G')^{-1} = E + \frac{(I - EM)\mathsf{u} \otimes (I - EM)\mathsf{u}}{\langle (M - MEM)\mathsf{u}, \mathsf{u}\rangle}. \tag{3.13}$$

Proof. We introduce for convenience the compact notation $P = I - \mathsf{u} \otimes \mathsf{y}$ and $Q = I - \mathsf{y} \otimes \mathsf{u}$ in such a way that $G' = QM'P$. It is first easily checked that $M + \mathrm{i}M'$ and $M + \mathrm{i}G'$ are invertible since M is symmetric positive definite and M' and G' are symmetric. Moreover, defining $z = (M + \mathrm{i}M')^{-1}\mathsf{y}$ we have $\langle (M + \mathrm{i}M')^{-1}\mathsf{y}, \mathsf{y}\rangle = \langle z, (M + \mathrm{i}M')z\rangle = \langle (M - \mathrm{i}M')z, z\rangle$, and upon decomposing $z = x + \mathrm{i}y$, the real part of $\langle (M - \mathrm{i}M')z, z\rangle$ is $\langle Mz, z\rangle = \langle Mx, x\rangle + \langle My, y\rangle$ which is nonzero since z is nonzero and M is positive definite and this shows that $\langle (M + \mathrm{i}M')^{-1}\mathsf{y}, \mathsf{y}\rangle \neq 0$.

The matrix E is thus well defined and denoting $F = Q(M + \mathrm{i}M')P = QMP + \mathrm{i}G'$, E is the generalized inverse of F with nullspace $\mathbb{C}\mathsf{y}$ and range $\mathsf{y}^\perp + \mathrm{i}\mathsf{y}^\perp$, since it is easily checked that $EF = I - \mathsf{u} \otimes \mathsf{y}$ and $FE = I - \mathsf{y} \otimes \mathsf{u}$.

We introduce $\mathsf{u}' = (M + \mathrm{i}G')(\mathsf{u} - EM\mathsf{u})$ and u' is nonzero since $M + \mathrm{i}G'$ is invertible and $\mathsf{u} - EM\mathsf{u}$ is nonzero because $R(E) = \mathsf{y}^\perp + \mathrm{i}\mathsf{y}^\perp$ and $\mathsf{u} \notin \mathsf{y}^\perp$. We now establish that $\mathsf{u}' = \langle (M - MEM)\mathsf{u}, \mathsf{u}\rangle\mathsf{y}$. Indeed, we first have $\mathsf{u}' = M\mathsf{u} - MEM\mathsf{u} - \mathrm{i}QM'EM\mathsf{u}$ since $P\mathsf{u} = 0$ and $PE = E$ thanks to $E = E^t$ and $E\mathsf{y} = 0$. This yields $\mathsf{u}' = M\mathsf{u} - Q(M + \mathrm{i}M')EM\mathsf{u} - (I - Q)MEM\mathsf{u}$, and thus

$$\mathsf{u}' = M\mathsf{u} - Q\left(I - \frac{\mathsf{y} \otimes (M + \mathrm{i}M')^{-1}\mathsf{y}}{\langle (M + \mathrm{i}M')^{-1}\mathsf{y}, \mathsf{y}\rangle}\right)M\mathsf{u} - (I - Q)MEM\mathsf{u}.$$

Since $Q\mathsf{y} = 0$ we get $\mathsf{u}' = M\mathsf{u} - QM\mathsf{u} - (I - Q)MEM\mathsf{u} = (I - Q)(M\mathsf{u} - MEM\mathsf{u})$, and thus $\mathsf{u}' = \mathsf{y} \otimes \mathsf{u}(M\mathsf{u} - MEM\mathsf{u}) = \langle (M - MEM)\mathsf{u}, \mathsf{u}\rangle\mathsf{y}$ and this shows that $\langle (M - MEM)\mathsf{u}, \mathsf{u}\rangle \neq 0$ since u' is nonzero.

We now decompose $M + \mathrm{i}G' = M + \mathrm{i}QM'P = M - QMP + Q(M + \mathrm{i}M')P$ and evaluate the product of $M + \mathrm{i}G'$ by the right-hand side of (3.13) by forming

$$\left(E + \frac{(I - EM)\mathsf{u} \otimes (I - EM)\mathsf{u}}{\langle (M - MEM)\mathsf{u}, \mathsf{u}\rangle}\right)(M - QMP + Q(M + \mathrm{i}M')P). \tag{3.14}$$

The first contribution simplifies into $E(M - QMP) = E(M - MP) = EM(I - P) = EM\mathsf{u} \otimes \mathsf{y}$ since $EQ = E$ thanks to $Q = I - \mathsf{y} \otimes \mathsf{u}$ and $E\mathsf{y} = 0$. Moreover

$$EQ(M + \mathrm{i}M')P = E(M + \mathrm{i}M')P = \left(I - \frac{(M + \mathrm{i}M')^{-1}\mathsf{y} \otimes \mathsf{y}}{\langle (M + \mathrm{i}M')^{-1}\mathsf{y}, \mathsf{y}\rangle}\right)P = P,$$

since $a \otimes \mathsf{y}P = a \otimes (P^t\mathsf{y}) = a \otimes (Q\mathsf{y}) = 0$, and the whole contribution $E(M + \mathrm{i}G')$ finally sum up to $EM\mathsf{u} \otimes \mathsf{y} + I - \mathsf{u} \otimes \mathsf{y} = I - (\mathsf{u} - EM\mathsf{u}) \otimes \mathsf{y}$. We now form the product

$$(I - EM)\mathsf{u} \otimes (I - EM)\mathsf{u}(M + \mathrm{i}G') = (I - EM)\mathsf{u} \otimes ((M + \mathrm{i}G')(I - EM)\mathsf{u}),$$

and $\mathsf{u}' = (M + \mathrm{i}G')(\mathsf{u} - EM\mathsf{u}) = \langle (M - MEM)\mathsf{u}, \mathsf{u}\rangle\mathsf{y}$ so that gathering all terms of the product (3.14) we obtain $I - (\mathsf{u} - EM\mathsf{u}) \otimes \mathsf{y} + (\mathsf{u} - EM\mathsf{u}) \otimes \mathsf{y} = I$ and the proof is complete. □

We now consider the general situation where $N(G)$ and $\mathcal{C}^\perp$ are of dimension $p \geqslant 1$ and are spanned by basis vectors as in Proposition 2.3.

Proposition 3.9. *Assume that M is symmetric positive definite and that $G' \in \mathbb{R}^{n,n}$ is in the form*

$$G' = \left(I - \sum_{1 \leqslant i \leqslant p} v_i \otimes u_i\right) M' \left(I - \sum_{1 \leqslant i \leqslant p} u_i \otimes v_i\right), \tag{3.15}$$

where $p \geqslant 1, u_1, \ldots, u_p$ are real independent vectors, $v_1, \ldots, v_p$ are real independent vectors, $\langle v_i, u_j \rangle = \delta_{ij}, 1 \leqslant i,j \leqslant p$, and $M' \in \mathbb{R}^{n,n}$ is a symmetric matrix. The matrices $M + \mathrm{i}M'$ and $M + \mathrm{i}G'$ are invertible, and the matrix $(\langle (M + \mathrm{i}M')^{-1} v_i, v_j \rangle)_{1 \leqslant i,j \leqslant p}$ is invertible. Upon denoting by $(\gamma_{ij})_{1 \leqslant i,j \leqslant p}$ its inverse, we define the matrix E by

$$E = (M + \mathrm{i}M')^{-1} - \sum_{1 \leqslant i,j \leqslant p} \gamma_{ij} (M + \mathrm{i}M')^{-1} v_i \otimes (M + \mathrm{i}M')^{-1} v_j. \tag{3.16}$$

Then the matrix $(\langle (M - MEM)u_i, u_j \rangle)_{1 \leqslant i,j \leqslant p}$ is invertible, and denoting by $(\mu_{ij})_{1 \leqslant i,j \leqslant p}$ its inverse, the inverse of $M + \mathrm{i}G'$ is given by

$$(M + \mathrm{i}G')^{-1} = E + \sum_{1 \leqslant i,j \leqslant p} \mu_{ij} (I - EM)u_i \otimes (I - EM)u_j. \tag{3.17}$$

Proof. We only give a sketch of the proof and denote for convenience $P = I - \sum_{1 \leqslant i \leqslant p} u_i \otimes v_i$ and $Q = I - \sum_{1 \leqslant i \leqslant p} v_i \otimes u_i$ so that $G' = QM'P$. It is easily checked that $M + \mathrm{i}M'$ and $M + \mathrm{i}G'$ are invertible. The matrix $(\langle (M + \mathrm{i}M')^{-1} v_i, v_j \rangle)_{1 \leqslant i,j \leqslant p}$ is also invertible since upon defining $w_i = (M + \mathrm{i}M')^{-1} v_i, 1 \leqslant i \leqslant p$, we have $\langle (M + \mathrm{i}M')^{-1} v_i, v_j \rangle = \langle (M - \mathrm{i}M') w_i, w_j \rangle$ and the proof is similar to that of Corollary 2.5 since the real part of the symmetric matrix $M - \mathrm{i}M'$ is positive definite.

The matrix E is shown to be the generalized inverse of $Q(M + \mathrm{i}M')P = QMP + \mathrm{i}G'$ with range $\mathcal{C} + \mathrm{i}\mathcal{C}$ and nullspace $\mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ upon simply calculating that $Q(M + \mathrm{i}M')PE = Q$. In order to establish that the matrix $(\langle (M - MEM)u_i, u_j \rangle)_{1 \leqslant i,j \leqslant p}$ is invertible, one first note that

$$(M + \mathrm{i}QM'P)(u_i - EMu_i) = \sum_{1 \leqslant j \leqslant p} \langle (M - MEM)u_i, u_j \rangle v_j, \quad 1 \leqslant i \leqslant p. \tag{3.18}$$

The vectors $u_i - EMu_i, 1 \leqslant i \leqslant p$, are linearly independant since if there exists a linear relation $\sum_{1 \leqslant i \leqslant p} \theta_i (u_i - EMu_i) = 0$, we obtain upon taking the scalar product with v_j that $\theta_j = 0$ since $\langle u_i, v_j \rangle = \delta_{ij}, R(E) \subset \mathcal{C} + \mathrm{i}\mathcal{C}$, and $v_j, 1 \leqslant j \leqslant p$, form a basis of $\mathcal{C}^\perp$. As a consequence, the vectors $(M + \mathrm{i}QM'P)(u_i - EMu_i), 1 \leqslant i \leqslant p$, are independent, and from the relations (3.18) we deduce that $(\langle (M - MEM)u_i, u_j \rangle)_{1 \leqslant i,j \leqslant p}$ is invertible. Finally, a direct calculation shows that the right-hand side of (3.17) is the inverse of $M + \mathrm{i}QM'P$. $\square$

Remark 3.10. Assume that the splitting matrix M is diagonal and that G' is in the form (3.15) where the matrix M' is diagonal. Then each iteration of the scheme (1.3) costs $n^2 + O(n)$ (complex) flops thanks to the expression of (3.17) of $(M + \mathrm{i}QM'P)^{-1}$. The main costs are associated with the n^2 operations required by the multiplication of W by a complex vector. Similarly, each iteration of (3.1) requires approximately the same costs thanks to the decomposition $P_{\mathcal{C},N(G)} = I - \sum_{1 \leqslant i \leqslant p} u_i \otimes v_i$ obtained in Proposition 2.3.

4. Orthogonal residuals algorithms

Conjugate gradients-type methods—used in combination with preconditioning—are among the most effective iterative procedures for solving Hermitian systems [19,25,18]. Projected conjugate gradients methods have been introduced in particular to solve real symmetric constrained singular semi-definite systems [6,7]. For general linear systems, however, one cannot obtain short recurrence algorithms which globally minimize some error norm over the corresponding Krylov subspaces unless the matrix has certain rather special spectral properties [8]. Examples of short recurrence algorithms are CGS or BiCGStab whereas GMRES [27] corresponds to a global error minimization over the Krylov subspaces.

Complex symmetric systems have received much less attention than real systems even though symmetric complex systems arise in electromagnetic applications [9,11,12,3]. Special systems with diagonal positive imaginary parts have been investigated by Freund [11] as well as the Lanczos recursion and related algorithms [12]. Complex symmetric systems can be solved either in their complex form, since it is convenient and benefits from interesting numerical properties [12], or in their real equivalent form upon relying on good preconditioners [2,5].

We investigate in this section projected orthogonal residuals methods for solving the complex symmetric constrained singular systems (1.1). Orthogonal residuals methods are a natural generalization of conjugate gradient algorithms associated with Arnoldi algorithm [27] as well as with orthogonal errors methods introduced by Faber and Manteuffel [9]. Orthogonal residuals methods seem natural for the constrained singular systems (1.1) since they make use of the positivity properties of the real symmetric part.

The projected orthogonal residuals method usually has a better convergence behavior than the projected stationary method introduced in the previous section and should generally be preferred. However, the corresponding iterates depend nonlinearly on the right-hand side b because of the quadratic nature of conjugate gradients-type algorithms, and this prevents its use in some special applications.

4.1. A projected orthogonal residuals algorithm

In this section we investigate a projected orthogonal residuals method for solving the constrained singular linear systems (1.1). These algorithms correspond to the particular choice $B = A$ in the paper of Faber and Manteuffel on orthogonal errors methods in such a way that the errors are computable [9]. We consider again a matrix in the form $\mathscr{G} = G + \mathrm{i}G'$ where G, G' are real symmetric matrices, G is positive semi-definite and $G'N(G) = 0$, a vector $b \in R(\mathscr{G})$, a subspace $\mathcal{C} \subset \mathbb{R}^n$ complementary to $N(G)$ and $\mathscr{C}$ the complexification of $\mathcal{C}$.

The orthogonal residuals algorithm can be described as follows [9]. Let $z_0 \in \mathbb{C}^n$ be an initial guess, $r_0 = b - \mathscr{G}z_0$, and set $p_0 = r_0$. If $\langle \mathscr{G}p_0, p_0\rangle = 0$ then $r_0 = 0$ and we stop at step 0, and if $\langle \mathscr{G}p_0, p_0\rangle \neq 0$ we set $\sigma_0 = \langle r_0, p_0\rangle / \langle \mathscr{G}p_0, p_0\rangle$, $\nu_{00} = \langle \mathscr{G}^2 p_0, p_0\rangle / \langle \mathscr{G}p_0, p_0\rangle$, and we define $p_1 = \mathscr{G}p_0 - \nu_{00}p_0$, $z_1 = z_0 + \sigma_0 p_0$, and $r_1 = r_0 - \sigma_0\mathscr{G}p_0$. Assume now by induction that for $k \geqslant 1$ we have defined $\{p_i\}_{0\leqslant i\leqslant k}, \{z_i\}_{0\leqslant i\leqslant k}, \{r_i\}_{0\leqslant i\leqslant k}$, with $\prod_{0\leqslant i\leqslant k-1}\langle \mathscr{G}p_i, p_i\rangle \neq 0, r_i = b - \mathscr{G}z_i, 0 \leqslant i \leqslant k$, and

$$\langle r_i, r_j\rangle = 0, \quad 0 \leqslant j < i \leqslant k, \tag{4.1}$$

$$\langle \mathscr{G}p_i, p_j\rangle = 0, \quad 0 \leqslant j < i \leqslant k, \tag{4.2}$$

$$\langle r_i, p_j\rangle = 0, \quad 0 \leqslant j < i \leqslant k, \tag{4.3}$$

$$\mathscr{K}_i = \operatorname{span}(p_0, \ldots, p_i) = \operatorname{span}(r_0, \ldots, r_i) = \operatorname{span}(r_0, \ldots, \mathscr{G}^i r_0), \quad 0 \leqslant i \leqslant k, \tag{4.4}$$

where $\dim(\mathscr{K}_i) = i + 1$ for $0 \leqslant i \leqslant k-1$. Then $\langle \mathscr{G}p_k, p_k\rangle = 0$ if and only if $r_k = 0$ and in this situation we stop at step k, whereas if $\langle \mathscr{G}p_k, p_k\rangle \neq 0$ we define the coefficients $\nu_{kj}, 0 \leqslant j \leqslant k$, by solving the linear system

$$\begin{pmatrix} \langle \mathscr{G}p_0, p_0\rangle & & & \\ \langle \mathscr{G}p_0, p_1\rangle & \langle \mathscr{G}p_1, p_1\rangle & & \\ \vdots & \vdots & \ddots & \\ \langle \mathscr{G}p_0, p_k\rangle & \langle \mathscr{G}p_1, p_k\rangle & \ldots & \langle \mathscr{G}p_k, p_k\rangle \end{pmatrix} \begin{pmatrix} \nu_{k0} \\ \nu_{k1} \\ \vdots \\ \nu_{kk} \end{pmatrix} = \begin{pmatrix} \langle \mathscr{G}^2 p_k, p_0\rangle \\ \langle \mathscr{G}^2 p_k, p_1\rangle \\ \vdots \\ \langle \mathscr{G}^2 p_k, p_k\rangle \end{pmatrix}, \tag{4.5}$$

we define $\sigma_k = \langle r_k, p_k\rangle / \langle \mathscr{G}p_k, p_k\rangle$ and we set

$$p_{k+1} = \mathscr{G}p_k - \sum_{0\leqslant j\leqslant k} \nu_{kj}p_j, \quad z_{k+1} = z_k + \sigma_k p_k, \quad r_{k+1} = r_k - \sigma_k\mathscr{G}p_k. \tag{4.6}$$

Theorem 4.1. *The orthogonal residuals algorithm is well defined and converges in at most* $\operatorname{rank}(\mathscr{G})$ *steps towards the unique solution* z *of* $\mathscr{G}z = b$ *and* $z \in R(\mathscr{G})$.

Since we are interested in the solution of $\mathscr{G}z = b$ which is in $\mathscr{C}$, we now consider a projected version of the orthogonal residuals algorithm, constructed by using projected directions at each step. More specifically, we set $z_0' = \mathscr{P}z_0, p_0' = \mathscr{P}p_0, r_0' = b - \mathscr{G}z_0'$, and if $\langle \mathscr{G}p_0', p_0'\rangle = 0$ we stop at step 0, whereas if $\langle \mathscr{G}p_0', p_0'\rangle \neq 0$ we define $\sigma_0' = \langle r_0', p_0'\rangle / \langle \mathscr{G}p_0', p_0'\rangle$, $\nu_{00}' = \langle \mathscr{G}^2 p_0', p_0'\rangle / \langle \mathscr{G}p_0', p_0'\rangle$, and $p_1' = \mathscr{P}\mathscr{G}p_0' - \nu_{00}'p_0'$,

$z_1' = z_0' + \sigma_0' p_0'$, and $r_1' = r_0' - \sigma_0' \mathscr{G} p_0'$. Assume now by induction that for $k \geqslant 1$ we have defined $\{p_i'\}_{0\leqslant i\leqslant k}$, $\{z_i'\}_{0\leqslant i\leqslant k}$, $\{r_i'\}_{0\leqslant i\leqslant k}$, with $\prod_{0\leqslant i\leqslant k-1} \langle \mathscr{G} p_i', p_i'\rangle \neq 0$ and $r_i' = b - \mathscr{G} z_i', 0 \leqslant i \leqslant k$. Then $\langle \mathscr{G} p_k', p_k'\rangle = 0$ if and only if $r_k' = 0$ and in this situation we stop at step k. On the other hand if $\langle \mathscr{G} p_k', p_k'\rangle \neq 0$ we introduce the solution $\nu_{k0}', \dots, \nu_{kk}'$ of the linear system similar to (4.5) but using the directions $\{p_i'\}_{0\leqslant i\leqslant k}$ instead of $\{p_i\}_{0\leqslant i\leqslant k}$ to form the system coefficients, we define as well $\sigma_k' = \langle r_k', p_k'\rangle / \langle \mathscr{G} p_k', p_k'\rangle$ and we set

$$p_{k+1}' = \mathscr{P}\mathscr{G} p_k' - \sum_{0\leqslant j\leqslant k} \nu_{kj}' p_j', \quad z_{k+1}' = z_k' + \sigma_k' p_k', \quad r_{k+1}' = r_k' - \sigma_k' \mathscr{G} p_k'. \tag{4.7}$$

Theorem 4.2. *The projected orthogonal residuals algorithm is well defined and converges in at most* rank($\mathscr{G}$) *steps towards the unique solution a of $\mathscr{G} a = b$ and $a \in \mathscr{C}$. Moreover, at each step k, we have $r_k' = r_k, z_k' = \mathscr{P} z_k, p_k' = \mathscr{P} p_k, \sigma_k' = \sigma_k$, and $\nu_{ki}' = \nu_{ki}$, for $0 \leqslant i \leqslant k$. Finally, we have at step k*

$$\mathscr{K}_i' = \mathrm{span}(p_0', \dots, p_i') = \mathscr{P}\mathscr{K}_i, \quad \mathscr{K}_i = \mathscr{H}\mathscr{K}_i', \quad 0 \leqslant i \leqslant k, \tag{4.8}$$

where $\mathscr{H} = I - \sum_{1\leqslant i,j\leqslant p} \gamma_{ij} u_i \otimes u_j$ and $(\gamma_{ij})_{1\leqslant i,j\leqslant p}$ is the inverse of the matrix $(\langle u_i, u_j\rangle)_{1\leqslant i,j\leqslant p}$.

Proof of Theorems 4.1 and 4.2. Upon decomposing $r_0 = p_0 = x + \mathrm{i}y, x, y \in \mathbb{R}^n$, the real part of $\langle \mathscr{G} p_0, p_0\rangle$ is given by $\langle Gx, x\rangle + \langle Gy, y\rangle$ and $\langle \mathscr{G} p_0, p_0\rangle = 0$ implies that $x, y \in N(G)$. However, $r_0 \in N(G)^\perp + \mathrm{i}N(G)^\perp$ so that $\langle \mathscr{G} p_0, p_0\rangle = 0$ finally implies $x, y \in N(G) \cap N(G)^\perp$ and $r_0 = 0$. Conversely, $r_0 = 0$ obviously implies that $\langle \mathscr{G} p_0, p_0\rangle = 0$. On the other hand, if $\langle \mathscr{G} p_0, p_0\rangle \neq 0$, we can form $p_1 = \mathscr{G} p_0 - \nu_{00} p_0$, $z_1 = z_0 + \sigma_0 p_0$, and $r_1 = r_0 - \sigma_0 \mathscr{G} p_0$, with $\nu_{00} = \langle \mathscr{G}^2 p_0, p_0\rangle / \langle \mathscr{G} p_0, p_0\rangle$ and $\sigma_0 = \langle r_0, p_0\rangle / \langle \mathscr{G} p_0, p_0\rangle$ and $r_1 = b - \mathscr{G}(z_0 + \sigma_0 p_0) = b - \mathscr{G} z_1$. From the definition of ν_{00} we have $\langle \mathscr{G} p_1, p_0\rangle = 0$ and from the definition of σ_0 we obtain $\langle r_1, p_0\rangle = \langle r_1, r_0\rangle = 0$, and $\mathscr{K}_0 = \mathrm{span}(p_0) = \mathrm{span}(r_0)$ with $\dim(\mathscr{K}_0) = 1$ since $r_0 \neq 0$. From $p_1 = \mathscr{G} p_0 - \mu_{00} p_0$ we also have $\mathscr{G} p_0 \in \mathrm{span}(p_0, p_1)$ and $p_1 \in \mathrm{span}(p_0, \mathscr{G} p_0)$. Similarly since $r_1 = r_0 - \sigma_0 \mathscr{G} p_0$ and $\sigma_0 \neq 0$ we have $r_1 \in \mathrm{span}(r_0, \mathscr{G} r_0)$ and $\mathscr{G} r_0 \in \mathrm{span}(r_0, r_1)$ and all induction properties at step 1 are established.

Assume now that k steps of the algorithm have been taken. Suppose first that $\langle \mathscr{G} p_k, p_k\rangle = 0$. Then it is easily obtained as in the case $k = 0$ that $p_k \in N(\mathscr{G}) = N(G) + \mathrm{i}N(G)$, but we also deduce from (4.4) that $p_k \in \mathrm{span}(r_0, \dots, r_k) \subset R(\mathscr{G}) = N(G)^\perp + \mathrm{i}N(G)^\perp$. This shows that $p_k = 0$ and $r_k \in \mathrm{span}(p_0, \dots, p_{k-1})$. However, since r_k is orthogonal to $\mathrm{span}(p_0, \dots, p_{k-1})$, we deduce that $\langle r_k, r_k\rangle = 0$ and the algorithm is already converged. Conversely, if $r_k = 0$, then $p_k \in \mathrm{span}(r_0, \dots, r_{k-1})$ so that $p_k \in \mathrm{span}(p_0, \dots, p_{k-1})$ from (4.4) and $\langle \mathscr{G} p_k, p_k\rangle = 0$.

Supose now that $\langle \mathscr{G} p_k, p_k\rangle \neq 0$, then the scalars $\nu_{k0}, \dots, \nu_{kk}$ and σ_k are well defined and we can form $p_{k+1}, x_{k+1}, r_{k+1}$. We note that $\sigma_k \neq 0$ since $\sigma_k = 0$ implies that p_k is orthogonal to r_k, and then from $p_k \in \mathrm{span}(r_0, \dots, r_k)$ we obtain $p_k \in \mathrm{span}(r_0, \dots, r_{k-1})$ and $p_k \in \mathrm{span}(p_0, \dots, p_{k-1})$ in such a way that $\langle \mathscr{G} p_k, p_k\rangle = 0$. We next have $\langle \mathscr{G} p_{k+1}, p_i\rangle = 0, 0 \leqslant i \leqslant k$, from the definition of the coefficients $\nu_{k0}, \dots, \nu_{kk}$, and $\langle r_{k+1}, p_i\rangle = 0$ by definition of the coefficient σ_k. The recurrence relations (4.2) and (4.3) are then obtained at step $k + 1$ and (4.1) at step $k + 1$ follows from (4.3) at step $k + 1$ and (4.4) at step k. In addition $r_{k+1} = b - \mathscr{G} z_k - \sigma_k \mathscr{G} p_k = b - \mathscr{G}(z_k + \sigma_k p_k) = b - \mathscr{G} z_{k+1}$.

From $r_{k+1} = r_k - \sigma \mathscr{G} p_k$ we first obtain $r_{k+1} \in \mathrm{span}(r_0, \dots, \mathscr{G}^{k+1} r_0)$ since $p_k \in \mathscr{K}_k$ so that $\mathrm{span}(r_0, \dots, r_{k+1}) \subset \mathrm{span}(r_0, \dots, \mathscr{G}^{k+1} r_0)$. Conversely, since $\sigma_k \neq 0$, we have $\mathscr{G} p_k \in \mathrm{span}(r_0, \dots, r_{k+1})$ and if $0 \leqslant i \leqslant k - 1, \mathscr{G} p_i \in \mathscr{G}\mathscr{K}_{k-1} \subset \mathscr{K}_k$. This shows $\mathscr{G}\mathscr{K}_k \subset \mathrm{span}(r_0, \dots, r_{k+1})$ so that $\mathrm{span}(r_0, \dots, \mathscr{G}^{k+1} r_0) \subset \mathrm{span}(r_0, \dots, r_{k+1})$. Similarly, from $p_{k+1} = \mathscr{G} p_k - \sum_{0\leqslant j\leqslant k} \nu_{kj} p_j$, we have $\mathscr{G} p_k \in \mathrm{span}(p_0, \dots, p_{k+1})$ and if $0 \leqslant i \leqslant k - 1, \mathscr{G} p_i \in \mathscr{G}\mathscr{K}_{k-1} \subset \mathscr{K}_k$, so that $\mathscr{G}\mathscr{K}_k \subset \mathrm{span}(p_0, \dots, p_{k+1})$ and $\mathrm{span}(r_0, \dots, \mathscr{G}^{k+1} r_0) \subset \mathrm{span}(p_0, \dots, p_{k+1})$. Conversely, since $p_i \in \mathscr{K}_k$ if $0 \leqslant i \leqslant k$, $\mathrm{span}(p_0, \dots, p_{k+1}) \subset \mathrm{span}(r_0, \dots, \mathscr{G}^{k+1} r_0)$ and we have established (4.4) for $k + 1$. Finally, we also have $\dim(\mathscr{K}_k) = k + 1$ since r_k is nonzero and all induction properties at step $k + 1$ are established.

We now investigate the projected algorithm and establish by induction that $p_k' = \mathscr{P} p_k$ $z_k' = \mathscr{P} z_k$ and $r_k' = r_k$ at each step. We first note the relations $\mathscr{G} = \mathscr{G}\mathscr{P} = \mathscr{P}^t \mathscr{G}$ which imply in particular that for any $x, y \in \mathbb{C}^n, x' = \mathscr{P} x, y' = \mathscr{P} x$, we have $\langle \mathscr{G} x, y\rangle = \langle \mathscr{G} x', y\rangle = \langle \mathscr{G} x, y'\rangle = \langle \mathscr{G} x', y'\rangle$, and similarly that $\langle \mathscr{G}^2 x, y\rangle = \langle \mathscr{G}^2 x', y'\rangle$. Now for $k = 0$ we know by assumption that $p_0' = \mathscr{P} p_0$ and $z_0' = \mathscr{P} z_0$ so that $r_0' = b - \mathscr{G} z_0' = b - \mathscr{G} z_0 = r_0$ and $\langle \mathscr{G} p_0, p_0\rangle = \langle \mathscr{G} p_0', p_0'\rangle$. Therefore $\langle \mathscr{G} p_0', p_0'\rangle = 0$ if and only if $r_0' = 0$ and then we stop at step 0. When $\langle \mathscr{G} p_0, p_0\rangle \neq 0$ then it is easily checked that $\nu'_{00} = \nu_{00}$ and $\sigma'_0 = \sigma_0$. Since $p'_1 = \mathscr{P}\mathscr{G}p'_0 - \nu'_{00}p'_0$, and $z'_1 = z'_0 + \sigma'_0 p'_0$, we obtain that $p'_1 = \mathscr{P}(\mathscr{G}p'_0 - \nu_{00}p_0) = \mathscr{P}p_1$ and $z'_1 = \mathscr{P}(z_0 + \sigma_0 p_0) = \mathscr{P}z_1$ and thus $r'_1 = b - \mathscr{G}\mathscr{P}z_1 = r_1$. Assume now by induction that for $k \geqslant 1$ we have defined $\{p'_i\}_{0\leqslant i\leqslant k}, \{z'_i\}_{0\leqslant i\leqslant k}, \{r'_i\}_{0\leqslant i\leqslant k}$, with $\prod_{0\leqslant i\leqslant k-1} \langle \mathscr{G}p'_i, p'_i\rangle \neq 0$, and that $p'_i = \mathscr{P}p_i$ $z'_i = \mathscr{P}z_i$ and $r'_i = r_i$ for $0 \leqslant i \leqslant k$. Since $\langle \mathscr{G}p_k, p_k\rangle = \langle \mathscr{G}p'_k, p'_k\rangle$ and $r'_k = r_k$, $\langle \mathscr{G}p'_k, p'_k\rangle = 0$ if and only if $r'_k = 0$. On the other hand, when $\langle \mathscr{G}p'_k, p'_k\rangle \neq 0$ we define the coefficients ν'_{kj}, $0 \leqslant j \leqslant k$, by solving the linear system

$$\begin{pmatrix} \langle \mathscr{G}p'_0, p'_0\rangle & & & \\ \langle \mathscr{G}p'_0, p'_1\rangle & \langle \mathscr{G}p'_1, p'_1\rangle & & \\ \vdots & \vdots & \ddots & \\ \langle \mathscr{G}p'_0, p'_k\rangle & \langle \mathscr{G}p'_1, p'_k\rangle & \dots & \langle \mathscr{G}p'_k, p'_k\rangle \end{pmatrix} \begin{pmatrix} \nu'_{k0} \\ \nu'_{k1} \\ \vdots \\ \nu'_{kk} \end{pmatrix} = \begin{pmatrix} \langle \mathscr{G}^2 p'_k, p'_0\rangle \\ \langle \mathscr{G}^2 p'_k, p'_1\rangle \\ \vdots \\ \langle \mathscr{G}^2 p'_k, p'_k\rangle \end{pmatrix} \tag{4.9}$$

and define $\sigma'_k = \langle r'_k, p'_k\rangle / \langle \mathscr{G}p'_k, p'_k\rangle$. However, from the relations $p'_i = \mathscr{P}p_i, 0 \leqslant i \leqslant k$, we obtain that $\langle \mathscr{G}p_i, p_j\rangle = \langle \mathscr{G}p'_i, p'_j\rangle$ and $\langle \mathscr{G}^2 p_i, p_j\rangle = \langle \mathscr{G}^2 p'_i, p'_j\rangle$ in such a way that $\nu'_{kj} = \nu_{kj}, 0 \leqslant j \leqslant k$, and $\sigma'_k = \sigma_k$. The relations $p'_{k+1} = \mathscr{P}\mathscr{G}p'_k - \sum_{0\leqslant j\leqslant k} \nu'_{kj}p'_j, z'_{k+1} = z'_k + \sigma'_k p'_k$, and $r'_{k+1} = r'_k - \sigma'_k \mathscr{G}p'_k$ then directly yield that $p'_{k+1} = \mathscr{P}p_{k+1}, z'_{k+1} = \mathscr{P}z_{k+1}$ and $r'_{k+1} = r_{k+1}$, and the relation $\mathscr{K}'_i = \mathscr{P}\mathscr{K}_i$ is then obvious. Conversely, if $p' = \mathscr{P}p$ and $p \in N(G)^\perp + \mathrm{i}N(G)^\perp$, it is easily obtained that $p' = \mathscr{H}p$ where $\mathscr{H} = I - \sum_{1\leqslant i,j\leqslant p} \gamma_{ij} u_i \otimes u_j$ and $(\gamma_{ij})_{1\leqslant i,j\leqslant p}$ is the inverse of the matrix $(\langle u_i, u_j\rangle)_{1\leqslant i,j\leqslant p}$, and $\dim(\mathscr{K}_i) = \dim(\mathscr{K}'_i) = i + 1$ for $0 \leqslant i \leqslant k - 1$. Note that the projected iterates also satisfy the properties $\langle r'_i, r'_j\rangle = 0, \langle \mathscr{G}p'_i, p'_j\rangle = 0$, and $\langle r'_i, p'_j\rangle = 0$, for $0 \leqslant j < i \leqslant k$, and the projected algorithm can entirely be formulated in terms of projected quantities. $\square$

4.2. The preconditioned algorithm

We investigate in this section a preconditioned version of the projected orthogonal residuals algorithm. In order to precondition this algorithm, we rewrite the system (1.1) in the form

$$\begin{cases} \mathscr{B}^{-1}\mathscr{G}\mathscr{B}^{-*}(\mathscr{B}^* a) = \mathscr{B}^{-1}b, \\ \mathscr{B}^* a \in \mathscr{B}^*\mathscr{C}, \end{cases} \tag{4.10}$$

where $\mathscr{B}$ is an invertible matrix, $\mathscr{B}^*$ its adjoint and $\mathscr{B}^{-*}$ the inverse of the adjoint. The preconditioned algorithm is simply obtained upon writing the natural unpreconditioned algorithm presented in Section 4.1 in terms of the new matrix $\mathscr{B}^{-1}\mathscr{G}\mathscr{B}^{-*}$, the new right-hand side $\mathscr{B}^{-1}b$, the new unknown $\mathscr{B}^* a$, with the directions $\mathscr{B}^* p_i$ and residuals $\mathscr{B}^{-1}r_i$, and finally by reformulating back the resulting algorithm in terms of the original system with the help of the Hermitian matrix $M = \mathscr{B}\mathscr{B}^*$. The form (4.10) seems natural since $\langle \mathscr{B}^{-1}\mathscr{G}\mathscr{B}^{-*}z, z\rangle = \langle \mathscr{G}\mathscr{B}^{-*}z, \mathscr{B}^{-*}z\rangle$ in such a way that the positivity properties of the matrix $\mathscr{G}$ associated with (1.1) are maintained with the matrix $\mathscr{B}^{-1}\mathscr{G}\mathscr{B}^{-*}$ associated with (4.10).

Keeping the assumptions of Section 4.1 and assuming that $M \in \mathbb{R}^{n,n}$ is Hermitian positive definite, the preconditioned orthogonal residuals algorithm can be described as follows. Let $z_0 \in \mathbb{C}^n$ be an initial guess, $r_0 = b - \mathscr{G}z_0$, and set $p_0 = M^{-1}r_0$. If $\langle \mathscr{G}p_0, p_0\rangle = 0$ then $r_0 = 0$ and we stop at step 0, and if $\langle \mathscr{G}p_0, p_0\rangle \neq 0$ we set $\sigma_0 = \langle r_0, p_0\rangle / \langle \mathscr{G}p_0, p_0\rangle, \nu_{00} = \langle \mathscr{G}M^{-1}\mathscr{G}p_0, p_0\rangle / \langle \mathscr{G}p_0, p_0\rangle$, and we define $p_1 = M^{-1}\mathscr{G}p_0 - \nu_{00}p_0, z_1 = z_0 + \sigma_0 p_0$, and $r_1 = r_0 - \sigma_0 \mathscr{G}p_0$. Assume now by induction that for $k \geqslant 1$ we have defined $\{p_i\}_{0\leqslant i\leqslant k}, \{z_i\}_{0\leqslant i\leqslant k}, \{r_i\}_{0\leqslant i\leqslant k}$, with $\prod_{0\leqslant i\leqslant k-1} \langle \mathscr{G}p_i, p_i\rangle \neq 0, r_i = b - \mathscr{G}z_i, 0 \leqslant i \leqslant k$, and

$$\langle M^{-1}r_i, r_j\rangle = 0, \quad 0 \leqslant j < i \leqslant k, \tag{4.11}$$

$$\langle \mathscr{G}p_i, p_j\rangle = 0, \quad 0 \leqslant j < i \leqslant k, \tag{4.12}$$

$$\langle r_i, p_j\rangle = 0, \quad 0 \leqslant j < i \leqslant k, \tag{4.13}$$

$$\mathscr{K}_i = M\mathrm{span}(p_0, \dots, p_i) = \mathrm{span}(r_0, \dots, r_i) = \mathrm{span}(r_0, \dots, (\mathscr{G}M^{-1})^i r_0), \quad 0 \leqslant i \leqslant k, \tag{4.14}$$

where $\dim(\mathscr{K}_i) = i+1$ for $0 \leqslant i \leqslant k-1$. Then $\langle \mathscr{G}p_k, p_k\rangle = 0$ if and only if $r_k = 0$ and in this situation we stop at step k, whereas if $\langle \mathscr{G}p_k, p_k\rangle \neq 0$ we define the coefficients ν_{kj}, $0 \leqslant j \leqslant k$, by solving the linear system

$$\begin{pmatrix} \langle \mathscr{G}p_0, p_0\rangle & & & \\ \langle \mathscr{G}p_0, p_1\rangle & \langle \mathscr{G}p_1, p_1\rangle & & \\ \vdots & \vdots & \ddots & \\ \langle \mathscr{G}p_0, p_k\rangle & \langle \mathscr{G}p_1, p_k\rangle & \dots & \langle \mathscr{G}p_k, p_k\rangle \end{pmatrix} \begin{pmatrix} \nu_{k0} \\ \nu_{k1} \\ \vdots \\ \nu_{kk} \end{pmatrix} = \begin{pmatrix} \langle \mathscr{G}M^{-1}\mathscr{G}p_k, p_0\rangle \\ \langle \mathscr{G}M^{-1}\mathscr{G}p_k, p_1\rangle \\ \vdots \\ \langle \mathscr{G}M^{-1}\mathscr{G}p_k, p_k\rangle \end{pmatrix}, \tag{4.15}$$

we define $\sigma_k = \langle r_k, p_k\rangle / \langle \mathscr{G}p_k, p_k\rangle$ and we set

$$p_{k+1} = M^{-1}\mathscr{G}p_k - \sum_{0\leqslant j\leqslant k} \nu_{kj}p_j, \quad z_{k+1} = z_k + \sigma_k p_k, \quad r_{k+1} = r_k - \sigma_k \mathscr{G}p_k. \tag{4.16}$$

Theorem 4.3. *The preconditioned orthogonal residuals algorithm is well defined and converges in at most* $\mathrm{rank}(\mathscr{G})$ *steps towards the unique solution z of $\mathscr{G}z = b$ and $z \in R(\mathscr{G})$.*

We now consider a projected version of the preconditioned orthogonal residuals algorithm. We set $z_0' = \mathscr{P}z_0$, $p_0' = \mathscr{P}M^{-1}p_0$, $r_0' = b - \mathscr{G}z_0'$, and if $\langle \mathscr{G}p_0', p_0'\rangle = 0$ we stop at step 0, whereas if $\langle \mathscr{G}p_0', p_0'\rangle \neq 0$ we define $\sigma_0' = \langle r_0', p_0'\rangle / \langle \mathscr{G}p_0', p_0'\rangle$, $\nu_{00}' = \langle \mathscr{G}M^{-1}\mathscr{G}p_0', p_0'\rangle / \langle \mathscr{G}p_0', p_0'\rangle$, and $p_1' = \mathscr{P}M^{-1}\mathscr{G}p_0' - \nu_{00}'p_0'$, $z_1' = z_0' + \sigma_0'p_0'$, and $r_1' = r_0' - \sigma_0'\mathscr{G}p_0'$. Assume now by induction that for $k \geqslant 1$ we have defined $\{p_i'\}_{0\leqslant i\leqslant k}$, $\{z_i'\}_{0\leqslant i\leqslant k}$, $\{r_i'\}_{0\leqslant i\leqslant k}$, with $\prod_{0\leqslant i\leqslant k-1} \langle \mathscr{G}p_i', p_i'\rangle \neq 0$ and $r_i' = b - \mathscr{G}z_i'$, $0 \leqslant i \leqslant k$. Then $\langle \mathscr{G}p_k', p_k'\rangle = 0$ if and only if $r_k' = 0$ and in this situation we stop at step k. On the other hand if $\langle \mathscr{G}p_k', p_k'\rangle \neq 0$ we introduce the solution $\nu_{k0}', \dots, \nu_{kk}'$ of the linear systems similar to (4.15) but using the directions $\{p_i'\}_{0\leqslant i\leqslant k}$ instead of $\{p_i\}_{0\leqslant i\leqslant k}$ to form the system coefficients, as well as $\sigma_k' = \langle r_k', p_k'\rangle / \langle \mathscr{G}p_k', p_k'\rangle$ and we set

$$p_{k+1}' = \mathscr{P}M^{-1}\mathscr{G}p_k' - \sum_{0\leqslant j\leqslant k} \nu_{kj}'p_j', \quad z_{k+1}' = z_k' + \sigma_k'p_k', \quad r_{k+1}' = r_k' - \sigma_k'\mathscr{G}p_k'. \tag{4.17}$$

Theorem 4.4. *The projected preconditioned orthogonal residuals algorithm is well defined and converges in at most* $\mathrm{rank}(\mathscr{G})$ *steps towards the unique solution a of $\mathscr{G}a = b$ and $a \in \mathscr{C}$. Moreover, at each step k, we have $r_k' = r_k$, $z_k' = \mathscr{P}z_k$, $p_k' = \mathscr{P}p_k$, $\sigma_k' = \sigma_k$, and $\nu_{ki}' = \nu_{ki}$, for $0 \leqslant i \leqslant k$. Finally, we have*

$$\mathscr{K}_i' = \mathrm{span}(p_0', \dots, p_i') = \mathscr{P}M^{-1}\mathscr{K}_i, \quad \mathscr{K}_i = \mathscr{H}\mathscr{K}_i', \quad 0 \leqslant i \leqslant k, \tag{4.18}$$

where $\mathscr{H} = I - \sum_{1\leqslant i,j\leqslant p} \gamma_{ij} u_i \otimes Mu_j$ and $(\gamma_{ij})_{1\leqslant i,j\leqslant p}$ is the inverse of the matrix $(\langle Mu_i, u_j\rangle)_{1\leqslant i,j\leqslant p}$ and $\dim(\mathscr{K}_i) = \dim(\mathscr{K}_i') = i+1$ *for* $0 \leqslant i \leqslant k-1$.

Proof of Theorems 4.3 and 4.4. The proof is similar to that of the unpreconditioned algorithm. □

Remark 4.5. In order to precondition the orthogonal residuals algorithm one may also consider the following reformulation of (1.1)

$$\begin{cases} \mathscr{B}^{-1}\mathscr{G}\mathscr{B}^{-1}(\mathscr{B}a) = \mathscr{B}^{-1}b, \\ \mathscr{B}a \in \mathscr{B}\mathscr{C}, \end{cases} \tag{4.19}$$

where $\mathscr{B}$ is an invertible matrix. The corresponding iterative scheme is more complex than the algorithm associated with (4.10) and can be written in terms of the matrices $M = \mathscr{B}\mathscr{B}^*$, $\widetilde{M} = \mathscr{B}\mathscr{B}$ and $\widetilde{O} = \mathscr{B}\mathscr{B}^{-*}$. The coefficient of the linear system are $\langle \widetilde{O}^{-1}\mathscr{G}p_k, p_j\rangle$ and the right-hand sides $\langle \widetilde{O}^{-1}\mathscr{G}\widetilde{M}^{-1}\mathscr{G}p_k, p_j\rangle$. At step k the orthogonal relations are $\langle M^{-1}r_i, r_j\rangle = 0$, $\langle \widetilde{O}^{-1}\mathscr{G}p_i, p_j\rangle = 0$, $\langle \widetilde{O}^{-1}r_i, p_j\rangle = 0$, for $0 \leqslant j < i \leqslant k$. The new directions are defined from the relations $p_{k+1} = \widetilde{M}^{-1}\mathscr{G}p_k - \sum_{0\leqslant j\leqslant k} \nu_{kj}p_j$. This algorithm is not guarantee to converge unless $\mathscr{B}$ is such that $\langle \widetilde{O}^{-1}\mathscr{G}z, z\rangle = 0$ implies that $z \in N(\mathscr{G})$ and $\langle \widetilde{M}^{-1}z, z\rangle = 0$ implies that $z = 0$. Last but not least, the corresponding iterates defined with the projected directions generally *do not correspond* to the projected iterates. When $\mathscr{B}$ is Hermitian, we have $\widetilde{O} = I$, $\widetilde{M} = M$ and we recover the simpler algorithm introduced in Theorem 4.3.

5. Application to magnetized multicomponent transport

5.1. Transport coefficients in partially ionized gas mixtures

The equations governing partially ionized gas mixtures in the presence of a strong magnetic field can be derived from the kinetic theory of dilute gases and express the conservation of mass, momentum, and energy [10,16,17]. These equations contain the terms for transport fluxes, that is, the viscous tensor, the species diffusion velocities, and the heat flux vector, which are non-isotropic under the influence of the magnetic field. In this paper, we discuss the species diffusion velocities V_i, $1 \leqslant i \leqslant n^s$, which are vectors of $\mathbb{R}^3$, where n^s is the number of species in the mixture. We denote by B the magnetic field, assumed to be nonzero, by $B = \|\mathrm{B}\|$ its norm and by $\mathscr{B}$ the corresponding unitary vector $\mathscr{B} = \mathrm{B}/B$.

Upon neglecting thermal diffusion—for the sake of simplicity—the species diffusion velocities can be written in the form

$$V_i = -\sum_{1\leqslant j\leqslant n^s} (D^{\parallel}_{ij} d^{\parallel}_j + D^{\perp}_{ij} d^{\perp}_j + D^{\odot}_{ij} d^{\odot}_j), \quad 1 \leqslant i \leqslant n^s, \tag{5.1}$$

where d_j is the diffusion driving force of the jth species $d_j = (\nabla p_j - \rho_j f_j)/\bar{p}$ and

$$d^{\parallel}_j = \langle d_j, \mathscr{B}\rangle \mathscr{B}, \quad d^{\perp}_j = d_j - d^{\parallel}_j, \quad d^{\odot}_j = \mathscr{B} \wedge d_j$$

denote the corresponding parallel, perpendicular and transverse vectors. In these expressions, $D^{\parallel} = (D^{\parallel}_{ij})_{1\leqslant i,j\leqslant n^s}, D^{\perp} = (D^{\perp}_{ij})_{1\leqslant i,j\leqslant n^s}$ and $D^{\odot} = (D^{\odot}_{ij})_{1\leqslant i,j\leqslant n^s}$ denote the diffusion matrices parallel, perpendicular and transverse to the magnetic field, ∇ the space derivative operator, p_j the partial pressure of the jth species, $\bar{p} = \sum_{1\leqslant j\leqslant n^s} p_j$ the total pressure, ρ_j the partial density of the jth species, f_j the force per unit mass acting on the jth species, and $\wedge$ the vector product. We also denote by y_j the mass fraction of the jth species $\mathrm{y}_j = \rho_j/(\sum_{1\leqslant l\leqslant n^s} \rho_l)$, by y the mass fractions vector $\mathrm{y} = (\mathrm{y}_1, \dots, \mathrm{y}^s_n)$, and by $\overline{T}$ the temperature.

The diffusion matrices $D^{\parallel}, D^{\perp}$, and $D^{\odot}$, are functions of the variables $(\overline{T}, \bar{p}, \mathrm{y}_1, \dots, \mathrm{y}^s_n, B)$. However, these coefficients are not explicitly given by the kinetic theory. Their evaluation requires solving linear systems derived from orthogonal polynomial expansions of the species perturbed distribution functions [10,16,17]. The size of these systems is typically $n \approx \mathrm{r}n^s$ where $\mathrm{r} \in \{1, 2, 3\}$ and the number of species in the mixture n^s is generally in the range $10 \leqslant n^s \leqslant 100$—although very large chemical mechanisms involving several of hundreds of reactive species $100 \leqslant n^s \leqslant 1000$ are sometimes encountered. The resulting size of the transport linear systems is thus between $10 \leqslant n \leqslant 300$ and solving these linear systems by direct methods may become computationally expensive keeping in mind that transport properties have to be evaluated at each computational cell in space and time. Iterative techniques therefore constitute an appealing alternative and the mathematical and numerical theory of iterative algorithms for solving the transport linear systems in nonionized mixtures [6,7,15] has been generalized to the situation of ionized mixtures in strong magnetic fields [16,17].

In the next section we discuss the first order diffusion matrices in a multicomponent gas mixture of n^s components. We assume in the following that $n^s \geqslant 3$ and that the variables $(\overline{T}, \bar{p}, \mathrm{y}_1, \dots, \mathrm{y}^s_n, B)$ are given positive quantities. We also assume that the mass fractions satisfy the natural normalization condition $\sum_{1\leqslant i\leqslant n^s} \mathrm{y}_i = 1$.

5.2. Application to diffusion matrices

The transport linear systems associated with the evaluation of the diffusion matrices $D^{\parallel}, D^{\perp}$, and $D^{\odot}$, are the following n^s systems of size $n = n^s$ indexed by l, $1 \leqslant l \leqslant n^s$,

$$\begin{cases} \varDelta a^{l,1} = b^l, \\ a^{l,1} \in \mathrm{y}^{\perp}, \end{cases} \quad \begin{cases} (\varDelta + \mathrm{i}\varDelta')a^{l,2} = b^l, \\ a^{l,2} \in \mathrm{y}^{\perp} + \mathrm{i}\mathrm{y}^{\perp}, \end{cases} \tag{5.2}$$

where $\varDelta, \varDelta' \in \mathbb{R}^{n^s,n^s}$ and $a^{l,1}, b^l, \mathrm{y} \in \mathbb{R}^{n^s}$ and $a^{l,2} \in \mathbb{C}^{n^s}$ [10,16,17]. The coefficients of the matrices $\varDelta$ and $\varDelta'/B$ are functions of the state variables $(\overline{T}, \bar{p}, \mathrm{y}_1, \dots, \mathrm{y}^s_n)$ which usually have complex expressions and are omitted. The real part $\varDelta$ is thus independent of B but the imaginary part $\varDelta'$ is proportional to the intensity of the magnetic field B. Once the solutions of the transport linear systems (5.2) are obtained, the diffusion coefficients are evaluated from

$$D^{\parallel}_{kl} = a^{l,1}_k, \quad D^{\perp}_{kl} + \mathrm{i}D^{\odot}_{kl} = a^{l,2}_k. \tag{5.3}$$

The vectors $a^{l,1}, 1 \leqslant l \leqslant n^s$, are therefore the column vectors of the diffusion matrix $D^{\parallel}$, and the vectors $a^{l,2}, 1 \leqslant l \leqslant n^s$, are the column vectors of the diffusion matrix $D^{\perp} + \mathrm{i}D^{\odot}$.

In the framework of the kinetic theory of gases, where the transport linear systems arise from variational procedures, the authors have established the following properties for the matrices $\varDelta, \varDelta'$, and the vectors y, u, and $b^l, 1 \leqslant l \leqslant n^s$, when $n^s \geqslant 3$ [6,17] :

- $(\varDelta 1)$ $\varDelta$ is symmetric positive semi-definite.
- $(\varDelta 2)$ $N(\varDelta) = \mathbb{R}\mathsf{u}$ where $\mathsf{u} = (1, \dots, 1)$.
- $(\varDelta 3)$ $\langle \mathsf{y}, \mathsf{u} \rangle = 1$.
- $(\varDelta 4)$ $b^l_k = \delta_{lk} - \mathsf{y}_k, \quad 1 \leqslant k, l \leqslant n^s$.
- $(\varDelta 5)$ $2\mathrm{diag}(\varDelta) - \varDelta$ is symmetric positive definite.
- $(\varDelta 6)$ $\varDelta' = (I - \mathsf{y} \otimes \mathsf{u})M'(I - \mathsf{u} \otimes \mathsf{y})$.
- $(\varDelta 7)$ M' is a diagonal matrix.

In the situation of first order diffusion matrices, the properties $(\varDelta 1)$–$(\varDelta 7)$ can directly be deduced from the special structure of $\varDelta, \varDelta'$, and of the vectors y, u, and $b^l, 1 \leqslant l \leqslant n^s$, and the matrix $\varDelta$ is a singular M-Matrix [6,7,23]. From the properties $(\varDelta 1)$–$(\varDelta 7)$ we can now establish that the transport linear systems are well posed as well as several properties of the diffusion matrices.

Proposition 5.1. *Assume that the matrices $\varDelta, \varDelta'$, and the vectors y, u, and $b^l, 1 \leqslant l \leqslant n^s$, satisfy the properties $(\varDelta 1)$–$(\varDelta 7)$. Then the n^s systems (5.2) are well posed, the matrix $D^{\parallel}$ is symmetric and is the generalized inverse of $\varDelta$ with prescribed range $\mathsf{y}^{\perp}$ and prescribed nullspace $\mathbb{R}\mathsf{y}$, whereas the matrix $D^{\perp} + \mathrm{i}D^{\odot}$ is symmetric and is the generalized inverse of $\varDelta + \mathrm{i}\varDelta'$ with prescribed range $\mathsf{y}^{\perp} + \mathrm{i}\mathsf{y}^{\perp}$ and nullspace $\mathbb{C}\mathsf{y}$. The matrices $D^{\parallel}$ and $D^{\perp}$ are symmetric positive semi-definite and $N(D^{\parallel}) = N(D^{\perp}) = \mathbb{R}\mathsf{y}$. In addition, the diffusion matrices can be evaluated from $D^{\parallel} = (\varDelta + \alpha\mathsf{y} \otimes \mathsf{y})^{-1} - (1/\alpha)\mathsf{u} \otimes \mathsf{u}$ and $D^{\perp} + \mathrm{i}D^{\odot} = (\varDelta + \mathrm{i}\varDelta' + \alpha\mathsf{y} \otimes \mathsf{y})^{-1} - (1/\alpha)\mathsf{u} \otimes \mathsf{u}$ where $\alpha > 0$ is arbitrary.*

Proof. The proof is similar to that of the unmagnetized case thanks to Propositions 2.3 and 2.1 and since $b^l \in R(\varDelta) = \mathsf{u}^{\perp}$ and we refer to Ern and Giovangigli [7] for more details. □

Projected stationary iterative techniques as well as projected orthogonal residuals methods can be used to solve the constrained singular systems associated with the species diffusion coefficients (5.2). Iterative techniques for the real transport linear systems associated with $D^{\parallel}$ are similar to that of nonionized mixtures and have been investigated comprehensively [14,6,7]. We thus only discuss in the following the evaluation by iterative techniques of the complex matrix $D^{\perp} + \mathrm{i}D^{\odot}$ by solving the corresponding constrained linear systems (5.2). As a direct application of Theorem 3.3 we obtain an asymptotic expansion for $D^{\perp} + \mathrm{i}D^{\odot}$.

Theorem 5.2. *Let $\varDelta, \varDelta' \in \mathbb{R}^{n^s,n^s}$ be matrices, and $\mathsf{y}, \mathsf{u} \in \mathbb{R}^{n^s}, b^l \in \mathbb{R}^{n^s}$, $1 \leqslant l \leqslant n^s$, be vectors satisfying the properties $(\varDelta 1)$–$(\varDelta 7)$ and let $M = \mathrm{diag}(M_1, \dots, M^s_n)$ be such that $M_k \geqslant \varDelta_{kk}, 1 \leqslant k \leqslant n^s$. Consider the splittings $\varDelta = M - W$ and $\varDelta + \mathrm{i}\varDelta' = \mathscr{M} - \mathscr{W}$, where $\mathscr{M} = M + \mathrm{i}\varDelta'$, the iteration matrices $T = M^{-1}W$, and $\mathscr{T} = \mathscr{M}^{-1}\mathscr{W}$, and let $\mathscr{P} = P = I - \mathsf{u} \otimes \mathsf{y}$ denote the oblique projector matrix onto $\mathsf{y}^{\perp}$ along $\mathbb{R}\mathsf{u}$. Let $z^l_0 \in \mathbb{R}^n, z'^l_0 = \mathscr{P}z^l_0$, and consider for $i \geqslant 0$ and $1 \leqslant l \leqslant n^s$ the iterates $z^l_{i+1} = \mathscr{T}z^l_i + M^{-1}b^l$ and $z'^l_{i+1} = \mathscr{P}\mathscr{T}z'^l_i + \mathscr{P}\mathscr{M}^{-1}b^l$. Then $z'^l_i = \mathscr{P}z^l_i$ for all $i \geqslant 0$, the matrices $T, \mathscr{T}, PT$ and $\mathscr{P}\mathscr{T}$ are convergent, $\rho(T) = \rho(\mathscr{T}) = 1, \gamma(T) = \rho(PT) < 1, \gamma(\mathscr{T}) = \rho(\mathscr{P}\mathscr{T}) < 1, \gamma(\mathscr{T}) \leqslant \gamma(T)$, and we have the following limits:*

$$\lim_{i\to\infty} z'^l_i = P\Big(\lim_{i\to\infty} z^l_i\Big) = a^{l,2}, \quad 1 \leqslant l \leqslant n^s, \tag{5.4}$$

where $a^{l,2}$ is the unique solution of the (right) linear system of (5.2). *Moreover, for $i \geqslant 1$, the matrix iterates*

$$(D^{\perp} + \mathrm{i}D^{\odot})^{[i]} = \sum_{0 \leqslant j \leqslant i-1} (\mathscr{P}\mathscr{T})^{\mathrm{j}} \mathscr{P} \mathscr{M}^{-1} \mathscr{P}^{t} \tag{5.5}$$

are symmetric, and converge as $i \to \infty$ towards $D^{\perp} + \mathrm{i}D^{\odot}$, and we have the convergent asymptotic expansion

$$D^{\perp} + \mathrm{i}D^{\odot} = \sum_{0 \leqslant j < \infty} (\mathscr{P}\mathscr{T})^{\mathrm{j}} \mathscr{P} \mathscr{M}^{-1} \mathscr{P}^{t}.$$

The interest of these algorithms is that they perform well whatever the intensity of the magnetic field B since the complete matrix $\mathrm{i}\Delta'$ has been taken into account in the splitting matrix $\mathscr{M} = M + \mathrm{i}\Delta'$. They do not perform well, however, independently of the ionization degree and convergence rates deteriorate as ionization levels increase as investigated by García Muñ in the unmagnetized case [13,17]. The first approximation $\left(D^{\perp} + \mathrm{i}D^{\odot}\right)^{[1]} = \mathscr{P}\mathscr{M}^{-1}\mathscr{P}^{t}$ generalizes the Hirschfelder-Curtiss approximation with a mass corrector [24,14,15] to the magnetized case. Upon using Proposition 3.8 and $\mathscr{P}\mathrm{u} = 0$ we obtain the explicit formula

$$(D^{\perp} + \mathrm{i}D^{\odot})^{[1]} = E + \frac{EM\mathrm{u} \otimes EM\mathrm{u}}{\langle (M - MEM)\mathrm{u}, \mathrm{u}\rangle}, \tag{5.6}$$

where $E = (M + \mathrm{i}M')^{-1} - (M + \mathrm{i}M')^{-1}\mathrm{y} \otimes (M + \mathrm{i}M')^{-1}\mathrm{y} / \left\langle (M + \mathrm{i}M')^{-1}\mathrm{y}, \mathrm{y}\right\rangle$. The second order approximation can further be written

$$(D^{\perp} + \mathrm{i}D^{\odot})^{[2]} = (D^{\perp} + \mathrm{i}D^{\odot})^{[1]} + \mathscr{P}\mathscr{T}(D^{\perp} + \mathrm{i}D^{\odot})^{[1]} \tag{5.7}$$

and yields a more accurate approximation. Since $\mathscr{M}^{-1}$ is a rank two perturbation of the diagonal matrix $(M + \mathrm{i}M')^{-1}$, both iterates $\left(D^{\perp} + \mathrm{i}D^{\odot}\right)^{[1]}$ and $\left(D^{\perp} + \mathrm{i}D^{\odot}\right)^{[2]}$ are evaluated within $O(n^{s2})$ operations. The corresponding real parts $D^{\perp[1]}$ and $D^{\perp[2]}$ are shown to be positive semi-definite with nullspace $\mathbb{R}\mathrm{y}$.

Remark 5.3. When only the diffusion velocities are required—and not the diffusion coefficient matrices—a complex form of the Stefan–Maxwell equations can be solved by using orthogonal residuals algorithms [17]. These equations are in the form

$$-(\Delta + \mathrm{i}\Delta')(V^{\perp} - \mathrm{i}V^{\odot}) = d^{\perp} - \mathrm{i}d^{\odot} - \mathrm{y} \sum_{1 \leqslant l \leqslant n^s} (d_l^{\perp} - \mathrm{i}d_l^{\odot}) \tag{5.8}$$

and must be solved with the constraint $V^{\perp} - \mathrm{i}V^{\odot} \in \mathrm{y}^{\perp} + \mathrm{i}\mathrm{y}^{\perp}$, where $V^{\diamond} = (V_1^{\diamond}, \ldots, V_{n^s}^{\diamond})$, $d^{\diamond} = (d_1^{\diamond}, \ldots, d_{n^s}^{\diamond})$, $\diamond \in \{\|, \perp, \odot\}$. Only the diffusion velocities are required when an explicit time marching technique is use to compute a multicomponent flow for instance.

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