

ECOLE POLYTECHNIQUE

CENTRE DE MATHÉMATIQUES APPLIQUÉES

UMR CNRS 7641

91128 PALAISEAU CEDEX (FRANCE). Tél: 01 69 33 41 50. Fax: 01 69 33 30 11

<http://www.cmap.polytechnique.fr/>

**PROJECTED ITERATIVE ALGORITHMS
FOR COMPLEX SYMMETRIC SYSTEMS
ARISING IN MAGNETIZED
MULTICOMPONENT TRANSPORT**

Vincent Giovangigli and Benjamin Graille

R.I. 638

Juillet 2008

Projected Iterative Algorithms for Complex Symmetric Systems Arising in Magnetized Multicomponent Transport

Vincent Giovangigli* and Benjamin Graille†

*CMAP, CNRS, Ecole Polytechnique, 91128 Palaiseau, France

†Laboratoire de Mathématiques d’Orsay, Univ Paris-Sud, 91405 Orsay, France

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 standard iterative methods as well as projected orthogonal residuals algorithms generalizing previous results on real systems. As an application, we consider the complex linear systems arising from the kinetic theory of gases and providing transport coefficients of partially ionized gas mixtures subjected to a magnetic field. We obtain convergent iterative algorithms as well as low-cost accurate approximate expressions for transport coefficients that can be used in multicomponent flow models.

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 [5, 12, 6, 8]. Similarly, in partially ionized gas mixtures subjected to strong magnetic fields, the evaluation of non-isotropic transport coefficients requires solving complex linear systems [12, 18, 19]. The linear systems associated with transport coefficients 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 linear integral equations. These integral equations are obtained from the Enskog-Chapman expansion and involve a linearized Boltzmann integral collision operator [5, 12, 6, 17, 18, 19].

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

$$\begin{cases} \mathcal{G}\alpha = \beta, \\ \alpha \in \mathcal{C}, \end{cases} \quad (1.1)$$

where $\mathcal{G} \in \mathbb{C}^{\omega, \omega}$, \mathcal{C} is a linear subspace of \mathbb{C}^{ω} , and $\alpha, \beta \in \mathbb{C}^{\omega}$ are vectors. The matrix \mathcal{G} and the constrained space \mathcal{C} have a special structure derived from the kinetic theory of magnetized multicomponent transport [12, 18, 19]. The matrix \mathcal{G} is in the form $\mathcal{G} = G + iG^B$ where $G \in \mathbb{R}^{\omega, \omega}$ is a symmetric positive semi-definite matrix, $G^B \in \mathbb{R}^{\omega, \omega}$ a symmetric matrix with a ‘compatible’ nullspace, that is, such that $G^B N(G) = 0$, and G^B is proportional to the intensity of the magnetic field. The constrained subspace \mathcal{C} is the complexification $\mathcal{C} = \mathcal{C} + i\mathcal{C}$ of a real linear

subspace $\mathcal{C} \subset \mathbb{R}^\omega$ complementary to $N(G)$. In some applications, there are ω complex transport coefficients associated with the system (1.1) which are given by the components of α . This situation arises with the species diffusion coefficients for instance and will be referred to as “the vector case”. The constraint $\alpha \in \mathcal{C}$ is then a constraint on the transport coefficients which is important from a physical point of view and is typically associated with a conservation property. In other applications, there is a single complex transport coefficient associated with the system (1.1) which is usually given by a scalar product $\mu = \langle \alpha, \beta' \rangle$ where $\beta' \in \mathbb{C}^\omega$ is a vector. This situation occurs with the thermal conductivities coefficients for instance and will be referred to as “the scalar case”.

In this paper, we generalize the mathematical tools introduced in [6, 7, 8] in order to investigate the real constrained singular linear systems associated with nonmagnetized multicomponent transport. 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 standard iterative methods for solving the constrained singular system (1.1). We establish in particular that the convergence rate is always better in the presence of a magnetic field upon properly choosing the splitting matrix.

On the other hand, various generalized conjugated gradient techniques have been introduced in order to solve invertible complex symmetric linear systems [11, 13, 14]. In this paper, we investigate projected orthogonal residuals methods for solving the constrained singular system (1.1) and establish their convergence. Orthogonal residuals methods are generalized conjugate gradient methods which usually have a better convergence behavior than standard methods and should generally be preferred. However, as opposed to standard methods, they do not yield a linear dependency between the iterates and the second members as standard methods do, and this linear dependency turns out to be important in some applications as for instance with the species diffusion matrices. Thus, when this linear dependency is needed, only standard iterative methods should be used.

We then present typical applications associated with the species diffusion matrices and the thermal conductivities coefficients perpendicular and transverse to the magnetic field in partially ionized magnetized mixtures. We also present numerical results concerning these coefficients for a mixture associated with weakly ionized air at high temperature.

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 standard iterative algorithms. In Section 4 we discuss projected orthogonal residuals algorithms. Finally, in Section 5, we present the applications together with the numerical results.

1.2 Notation and preliminaries

Let \mathbb{K} be a field designating either \mathbb{R} or \mathbb{C} , we denote by \mathbb{K}^ω the corresponding ω -dimensional vector space, and by $\mathbb{K}^{\omega, \omega}$ the set of $\omega \times \omega$ matrices where $\omega \in \mathbb{N}, \omega \geq 1$. For a vector $z \in \mathbb{K}^\omega$, we denote by $z = (z_1, \dots, z_\omega)$ its components and by $\mathbb{K}z$ the subspace $\text{span}(z)$ of \mathbb{K}^ω .

For $a, b \in \mathbb{C}^\omega$, $\langle a, b \rangle$ denotes the scalar product $\langle a, b \rangle = \sum_{1 \leq k \leq \omega} a_k \bar{b}_k$ and $\|a\| = \langle a, a \rangle^{1/2}$ the Hermitian norm of a . Therefore, if $x, y \in \mathbb{R}^\omega$, $\langle x, y \rangle$ also denotes the scalar product $\langle x, y \rangle = \sum_{1 \leq k \leq \omega} x_k y_k$ and $\|x\| = \langle x, x \rangle^{1/2}$ the Euclidean norm of x . For a subspace S of \mathbb{R}^ω , we denote by S^\perp its orthogonal and for a nonzero vector $a \in \mathbb{R}^\omega$ we denote by a^\perp the orthogonal of $\mathbb{R}a$. For $x, y \in \mathbb{C}^\omega$, (x, y) denotes the bilinear form $(x, y) = \sum_{1 \leq k \leq \omega} x_k y_k$, so that $\langle x, y \rangle = (x, \bar{y})$.

We use classical notation concerning complexifications and $z \in \mathbb{C}^\omega$ may be written $z = x + iy$ where $x, y \in \mathbb{R}^\omega$. A subspace $F \subset \mathbb{C}^\omega$ is the complexification of a subspace of \mathbb{R}^ω if and only if $F = \bar{F}$ in which case F is the complexification of $H = F \cap \mathbb{R}^\omega$ so that $F = H + iH$

and $\dim_{\mathbb{C}}(F) = \dim_{\mathbb{R}}(H)$. If A and B are two complementary subspaces $A \oplus B = \mathbb{R}^\omega$, the corresponding complexifications are easily shown to satisfy $(A + iA) \oplus (B + iB) = \mathbb{C}^\omega$ as well as $(A^\perp + iA^\perp) \oplus (B^\perp + iB^\perp) = \mathbb{C}^\omega$. If H is a real vector space and $F = H + iH$ its complexification, $H^\perp + iH^\perp$ is the orthogonal of F with respect to either the scalar product $\langle \cdot, \cdot \rangle$ or the bilinear form (\cdot, \cdot) .

For $A \in \mathbb{K}^{\omega, \omega}$, we write $A = (A_{kl})_{1 \leq k, l \leq \omega}$ 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 $\text{rank}(A)$. For $x, y \in \mathbb{K}^\omega$, $x \otimes y \in \mathbb{K}^{\omega, \omega}$ denotes the tensor product matrix $x \otimes y = (x_k y_l)_{1 \leq k, l \leq \omega}$. The identity matrix is denoted by I and $\text{diag}(\lambda_1, \dots, \lambda_\omega)$ is the diagonal matrix with diagonal elements $\lambda_1, \dots, \lambda_\omega$. If S_1 and S_2 are two complementary subspaces of \mathbb{K}^ω , i.e., $S_1 \oplus S_2 = \mathbb{K}^\omega$, we denote by P_{S_1, S_2} the oblique projector matrix onto the subspace S_1 along the subspace S_2 . For a matrix $A \in \mathbb{K}^{\omega, \omega}$, we denote by $\|A\|$ its Frobenius norm $\|A\| = (\sum_{1 \leq k, l \leq \omega} |A_{kl}|^2)^{1/2}$. If $A \in \mathbb{K}^{\omega, \omega}$ is such that $N(A) \oplus R(A) = \mathbb{K}^\omega$ we denote by A^\sharp its group inverse [1, 3]. The following proposition characterizes generalized inverses with prescribed range and nullspace and its proof is identical in the real or complex cases [1, 3, 17].

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

For a matrix $\mathcal{T} \in \mathbb{C}^{\omega, \omega}$, $\sigma(\mathcal{T})$ and $\rho(\mathcal{T})$ denote respectively the spectrum and the spectral radius of \mathcal{T} , and we also define $\gamma(\mathcal{T}) = \max\{|\lambda|; \lambda \in \sigma(\mathcal{T}), \lambda \neq 1\}$. A matrix \mathcal{T} is said to be convergent when $\lim_{i \rightarrow \infty} \mathcal{T}^i$ exists—not necessarily being zero [25]—and we have the following characterization [29, 25].

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

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

$$\mathcal{G} = \mathcal{M} - \mathcal{W}, \tag{1.2}$$

is a splitting if the matrix \mathcal{M} is invertible. In order to solve the linear system

$$\mathcal{G}\alpha = \beta, \tag{1.3}$$

where $\beta \in \mathbb{C}^\omega$, the splitting (1.2) induces the iterative scheme

$$z_{i+1} = \mathcal{T}z_i + \mathcal{M}^{-1}\beta, \quad i \geq 0, \tag{1.4}$$

where $\mathcal{T} = \mathcal{M}^{-1}\mathcal{W}$. Assuming that $\beta \in R(\mathcal{G})$, we have $\mathcal{M}^{-1}\beta \in R(I - \mathcal{T})$, and the behavior of the sequence of iterates (1.4) is given in the next lemma which can be found in [24, 3] (some misprints in the matrix E are corrected in recent versions of [3]).

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

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

We investigate well posedness of the constrained singular system (1.1) and relate its solution to generalized inverses naturally associated with the problem.

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

$$N(\mathcal{G}) \oplus \mathcal{C} = \mathbb{C}^{\omega}. \quad (2.1)$$

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

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

We also investigate in this section the range and nullspace of the complex matrices $\mathcal{G} = G + iG^B$ arising from magnetized transport.

Lemma 2.2. *Let $\mathcal{G} = G + iG^B$ where G, G^B are real symmetric matrices, G is positive semi-definite and $G^B N(G) = 0$. Then we have $N(\mathcal{G}) = N(G) + iN(G)$ and $R(\mathcal{G}) = N(G)^{\perp} + iN(G)^{\perp}$. Moreover, for any subspace $\mathcal{C} \subset \mathbb{R}^{\omega}$ complementary to $N(G)$, we have $G^B = (P_{\mathcal{C}, N(G)})^t G^B P_{\mathcal{C}, N(G)}$, and denoting $\mathcal{C} = \mathcal{C} + i\mathcal{C}$ the complexification of \mathcal{C} , we have $N(\mathcal{G}) \oplus \mathcal{C} = \mathbb{C}^{\omega}$ and $P_{\mathcal{C}, N(\mathcal{G})} = P_{\mathcal{C}, N(G)}$.*

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

$$\langle (G + iG^B)z, z \rangle = \langle Gx, x \rangle + \langle Gy, y \rangle + i(\langle G^B x, x \rangle + \langle G^B y, y \rangle),$$

since G and G^B are symmetric. Assuming $(G + iG^B)z = 0$ thus yields that $x, y \in N(G)$ since G is positive semi-definite and conversely, it is obvious that $N(G) + iN(G) \subset N(G + iG^B)$ since $G^B N(G) = 0$. Since $N(G) \subset N(G^B)$, we also deduce by transposing that $N(G^B)^{\perp} \subset N(G)^{\perp}$ so that $R(G^B) \subset R(G)$ since G and G^B are symmetric. As a consequence $R(G + iG^B) \subset R(G) + iR(G)$ and thus $R(G + iG^B) = R(G) + iR(G)$ since both subspaces of \mathbb{C}^{ω} are of dimension $\omega - \dim(N(G)) = \omega - \dim(N(\mathcal{G}))$. If \mathcal{C} is complementary to $N(G)$, we can decompose any $x \in \mathbb{R}^{\omega}$ 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 $G^B x = G^B P_{\mathcal{C}, N(G)}x$ so that $G^B = G^B P_{\mathcal{C}, N(G)}$. Upon transposing this relation we also obtain $G^B = (P_{\mathcal{C}, N(G)})^t G^B$. Finally it is straightforward to establish that $N(\mathcal{G}) \oplus \mathcal{C} = \mathbb{C}^{\omega}$ and that $P_{\mathcal{C}, N(\mathcal{G})} = P_{\mathcal{C}, N(G)}$ upon decomposing vectors of \mathbb{C}^{ω} into their real and imaginary parts. \square

2.2 Symmetric generalized inverses

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

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

$$\mathcal{Z} = (\mathcal{G} + \sum_{1 \leq i \leq p} a_i v_i \otimes v_i)^{-1} - \sum_{1 \leq i \leq p} b_i u_i \otimes u_i, \quad (2.2)$$

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

$$(\mathcal{G} + \sum_{1 \leq i \leq p} a_i v_i \otimes v_i)\alpha = \beta, \quad (2.3)$$

and we also have

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

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

Writing $\mathcal{Z} = Z + iZ^B$, where $Z, Z^B \in \mathbb{R}^{\omega,\omega}$, we have already established that Z and Z^B are symmetric. From the relation $(Z + iZ^B)(G + iG^B) = P$ where $P = P_{\mathcal{C}, N(\mathcal{G})}$, we obtain that $ZG - Z^B G^B = P$ and $ZG^B + Z^B G = 0$. This implies that $Z = PZ = ZGZ - Z^B G^B Z = ZGZ + Z^B G Z^B$ so that $\langle Zx, x \rangle = \langle GZx, Zx \rangle + \langle GZ^B x, Z^B x \rangle$ and Z is positive semidefinite. Moreover, $Zx = 0$ implies that $Z^B x \in N(G)$ and since $R(\mathcal{Z}) = \mathcal{C} + i\mathcal{C}$, $Z^B x \in \mathcal{C}$, so that $Z^B x = 0$, and $Z^B N(Z) = 0$. From Lemma 2.2 we deduce that $N(\mathcal{Z}) = N(Z) + iN(Z)$ and since $N(\mathcal{Z}) = \mathcal{C}^\perp + i\mathcal{C}^\perp$ we obtain $N(Z) = \mathcal{C}^\perp$. The vectors v_i , $1 \leq i \leq p$, with $p = \dim(N(G))$ are then easily obtained by selecting for v_i a nonzero element in the one-dimensional subspace

$$\left(\text{span}(u_1, \dots, u_{i-1}, u_{i+1}, \dots, u_p) \right)^\perp \cap \mathcal{C}^\perp, \quad (2.5)$$

and by normalizing it. It is then easily shown that $P_{R(\mathcal{Z}), N(\mathcal{G})} = I - \sum_{1 \leq i \leq p} u_i \otimes v_i$ and $P_{R(\mathcal{G}), N(\mathcal{Z})} = I - \sum_{1 \leq i \leq p} v_i \otimes u_i$, which yields (2.4) and implies that $\mathcal{G}\mathcal{Z} = I - \sum_{1 \leq i \leq p} v_i \otimes u_i$ and the formula

(2.2) directly follows. Equation (2.3) is then a direct consequence of (2.2) since $\beta \in R(\mathcal{G}) = N(G)^\perp + iN(G)^\perp$. \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 $\mathcal{G} + \sum_{1 \leq i \leq p} a_i v_i \otimes v_i$ with a positive definite real part $G + \sum_{1 \leq i \leq p} a_i v_i \otimes v_i$ 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 arising from magnetized multicomponent transport. Cholesky decomposition may also be used for large full systems arising from discretized integral equations [2].

Theorem 2.4. *Let \mathcal{A} be a complex symmetric matrix such that all principal minors Δ_i , $1 \leq i \leq \omega$, are nonzero. There exists an upper triangular matrix \mathcal{L} with diagonal coefficient unity such that*

$$\mathcal{A} = \mathcal{L}^t \mathcal{D} \mathcal{L}, \quad (2.6)$$

where \mathcal{D} is the diagonal matrix $\mathcal{D} = \text{diag}(\Delta_1, \Delta_2/\Delta_1, \dots, \Delta_\omega/\Delta_{\omega-1})$.

Proof. We denote by e_1, \dots, e_ω the canonical basis of \mathbb{C}^ω . The matrix \mathcal{A} is associated with a bilinear form denoted by φ so that $\varphi(a, b) = (\mathcal{A}a, b) = \langle \mathcal{A}a, \bar{b} \rangle$, $a, b \in \mathbb{C}^\omega$, and $\mathcal{A}_{ij} = \varphi(e_i, e_j)$, for $1 \leq i, j \leq \omega$. Denoting by $\mathcal{A}^{[k]}$ the submatrix $\mathcal{A}^{[k]} = (\mathcal{A}_{ij})_{1 \leq i, j \leq k}$, we know by assumption that $\mathcal{A}^{[k]}$ is invertible and that $\Delta_k = \det(\mathcal{A}^{[k]})$. We will denote by a_{ik} the cofactor of $\varphi(e_i, e_k) = \mathcal{A}_{ik}$ in $\mathcal{A}^{[k]}$ and we have in particular $a_{kk} = \Delta_{k-1}$ for $2 \leq k \leq \omega$.

We then define $f_1 = e_1$ and

$$f_k = \frac{1}{a_{kk}} \sum_{1 \leq i \leq k} a_{ik} e_i = e_k + \frac{1}{a_{kk}} \sum_{1 \leq i \leq k-1} a_{ik} e_i, \quad 2 \leq k \leq \omega. \quad (2.7)$$

Since $a_{kk}\varphi(f_k, e_j) = \sum_{1 \leq i \leq k} a_{ik}\varphi(e_i, e_j)$ corresponds to the expansion of the determinant according to the k th column of the matrix obtained from $\mathcal{A}^{[k]}$ by replacing the k th column by the j th column, we obtain that $\varphi(f_k, e_j) = 0$ whenever $1 \leq j \leq k-1$ and $\Delta_{k-1}\varphi(f_k, e_k) = \Delta_k$. As a consequence, the family f_1, \dots, f_ω is an orthogonal family for φ , and denoting by \mathcal{L} the matrix composed by the components of f_1, \dots, f_ω with respect to e_1, \dots, e_ω , the matrix \mathcal{L} is upper triangular with diagonal coefficients equal to unity. The family f_1, \dots, f_ω is thus a basis of \mathbb{C}^ω and $\text{span}(f_1, \dots, f_k) = \text{span}(e_1, \dots, e_k)$ for $1 \leq k \leq \omega$.

On the other hand, we have $\varphi(f_1, f_1) = \Delta_1$ and from $\varphi(f_k, f_k) = \varphi(f_k, e_k)$, we deduce that $\varphi(f_k, f_k) = \Delta_k/\Delta_{k-1}$, $2 \leq k \leq \omega$. Finally, the matrix of the bilinear form φ with respect to the basis f_1, \dots, f_ω is the diagonal $\mathcal{D} = \text{diag}(\Delta_1, \Delta_2/\Delta_1, \dots, \Delta_\omega/\Delta_{\omega-1})$ and we have $\mathcal{A} = \mathcal{L}^t \mathcal{D} \mathcal{L}$. \square

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 $\mathcal{G} + \sum_{1 \leq i \leq p} a_i v_i \otimes v_i$ can be decomposed in the form $\mathcal{L}^t \mathcal{D} \mathcal{L}$ where \mathcal{L} is an upper triangular matrix with diagonal coefficients unity and \mathcal{D} is a diagonal matrix whose diagonal coefficients have a positive real part.*

Proof. Denoting $\mathcal{A} = \mathcal{G} + \sum_{1 \leq i \leq p} a_i v_i \otimes v_i$ we have to check that $\mathcal{A}^{[k]}$ is invertible. Assume that $\mathcal{A}^{[k]} z^{[k]} = 0$ where $z^{[k]} \in \mathbb{C}^k$ and define $z_i = z_i^{[k]}$ if $1 \leq i \leq k$ and $z_i = 0$ otherwise. Then $\langle \mathcal{A}z, z \rangle = 0$ and from symmetry $\langle \mathcal{A}z, z \rangle = \langle \mathcal{A}z, z \rangle + i\langle G^B z, z \rangle$ where $A = G + \sum_{1 \leq i \leq p} a_i v_i \otimes v_i$ is positive definite. Upon decomposing $z = x + iy$, $x, y \in \mathbb{R}^\omega$, we also have $\langle \mathcal{A}z, z \rangle = \langle Ax, x \rangle + \langle Ay, y \rangle$ in such a way that $z = 0$ and $\mathcal{A}^{[k]}$ is invertible. Moreover, we have obtained in the proof of Theorem 2.4 that $\varphi(f_1, f_1) = \mathcal{D}_{11} = \Delta_1$ and $\varphi(f_k, f_k) = \mathcal{D}_{kk} = \Delta_k/\Delta_{k-1}$ for $2 \leq k \leq \omega$.

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 otherwise

$$\bar{f}_k = e_k + \frac{1}{\bar{a}_{kk}} \sum_{1 \leq i \leq k-1} \bar{a}_{ik} e_i, \quad 2 \leq k \leq \omega. \quad (2.8)$$

The proof is then complete then since $\varphi(f_k, \bar{f}_k) = (Af_k, \bar{f}_k) = \langle Af_k, f_k \rangle = \langle Af_k, f_k \rangle + i \langle G^B f_k, f_k \rangle$ so that $\mathcal{D}_{kk} = \langle Af_k, f_k \rangle + i \langle G^B f_k, f_k \rangle$ and A is positive definite. \square

3 Standard Iterative Algorithms

3.1 Convergence of projected iterative algorithms

We are now interested in solving the constrained singular system (1.1) by standard iterative techniques. These techniques provide iterates which depend linearly on the right member β , and this property is important for some applications, in particular for the matrices of species diffusion coefficients.

For a given splitting $\mathcal{G} = \mathcal{M} - \mathcal{W}$ and for $\beta \in R(\mathcal{G})$, assuming that the iteration matrix $\mathcal{T} = \mathcal{M}^{-1}\mathcal{W}$ is convergent, the iterates (1.4) will converge for any z_0 . When the matrix \mathcal{G} is singular, we have $\rho(\mathcal{T}) = 1$ since $\mathcal{T}z = z$ for $z \in N(\mathcal{G})$, and neither the iterates $\{z_i; i \geq 0\}$ nor the limit z_∞ are guaranteed to be in the constrained space \mathcal{C} . In order to overcome these difficulties, we will use a projected iterative scheme [16, 8]

$$z'_{i+1} = \mathcal{P}\mathcal{T}z'_i + \mathcal{P}\mathcal{M}^{-1}\beta, \quad i \geq 0, \quad (3.1)$$

where $\mathcal{P} = P_{\mathcal{C}, N(\mathcal{G})}$ is the projector matrix onto the subspace \mathcal{C} along $N(\mathcal{G})$. All the corresponding iterates $\{z'_i; i \geq 0\}$ satisfy the constraint which is important in “the vector case” in order to obtain satisfactory approximate transport coefficients, keeping in mind that the constraint is typically associated with a conservation property. Moreover, in order to obtain an iterative scheme with convergence properties valid for all magnetic fields, that is for small as well as large values of the matrix G^B proportional to the norm of the magnetic field, we will include the full imaginary part iG^B of \mathcal{G} in the splitting matrix \mathcal{M} . We will thus use splitting matrices in the form

$$\mathcal{M} = M + iG^B, \quad (3.2)$$

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

The spectral radius of the iteration matrix $\mathcal{P}\mathcal{T}$ associated with (3.1) can be estimated by using the following result of Neumann and Plemmons [25].

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

$$\rho(\mathcal{P}\mathcal{T}) = \gamma(\mathcal{T}). \quad (3.3)$$

This result (3.3) has also been strengthened and the spectra of \mathcal{T} and $\mathcal{P}\mathcal{T}$ are essentially the same [8]. Although the proof in [8] 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,*

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

Furthermore, the matrices \mathcal{T} and \mathcal{P} satisfy the relation $\mathcal{PT} = \mathcal{PTP}$.

We now investigate the convergence and properties of the projected iterative algorithms (3.1) when applied to the complex symmetric constrained singular systems associated with magnetized transport. Note that Keller's theorem [23] cannot be applied directly as in the unmagnetized case [8] since \mathcal{G} is not Hermitian when G^B is nonzero.

Theorem 3.3. *Let $\mathcal{G} = G + iG^B$ where G, G^B are real symmetric matrices, G is positive semi-definite and $G^B N(G) = 0$. Let $\mathcal{C} \subset \mathbb{R}^\omega$ 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 $\mathcal{M} = M + iG^B$, $\mathcal{G} = \mathcal{M} - W$, so that $W = W$, and $\mathcal{T} = \mathcal{M}^{-1}W$, $T = M^{-1}W$. Let $\mathcal{P} = P$ be the oblique projector matrix onto the subspace \mathcal{C} along $N(G)$. Let also $\beta \in R(\mathcal{G})$, $z_0 \in \mathbb{C}^\omega$, $z'_0 = \mathcal{P}z_0$, and consider for $i \geq 0$ the iterates $z_{i+1} = \mathcal{T}z_i + M^{-1}\beta$ as in (1.4) and $z'_{i+1} = \mathcal{PT}z'_i + \mathcal{P}M^{-1}\beta$ as in (3.1). Then $z'_i = \mathcal{P}z_i$ for all $i \geq 0$, the matrices \mathcal{T} , \mathcal{PT} , T , and PT are convergent, $\rho(T) = \rho(\mathcal{T}) = 1$ when $\dim(N(G)) \geq 1$, $\rho(\mathcal{PT}) = \gamma(\mathcal{T}) < 1$, $\rho(PT) = \gamma(T) < 1$, and*

$$\gamma(\mathcal{T}) \leq \gamma(T), \quad (3.4)$$

so that the convergence rate is always better in the magnetized case, and we have the following limits

$$\lim_{i \rightarrow \infty} z'_i = \mathcal{P}(\lim_{i \rightarrow \infty} z_i) = \alpha, \quad (3.5)$$

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

$$\mathcal{Z}_i = \sum_{0 \leq j \leq i-1} (\mathcal{PT})^j \mathcal{P}M^{-1}\mathcal{P}^t, \quad (3.6)$$

is symmetric and $\lim_{i \rightarrow \infty} \mathcal{Z}_i = \mathcal{Z}$ where

$$\mathcal{Z} = \sum_{0 \leq j < \infty} (\mathcal{PT})^j \mathcal{P}M^{-1}\mathcal{P}^t, \quad (3.7)$$

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

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*

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

Proof. By applying Keller's theorem [23, 8] 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 $\dim(N(G)) \geq 1$.

With respect to \mathcal{T} , we first note that $1 \in \sigma(\mathcal{T})$ when $\dim(N(G)) \geq 1$ since then \mathcal{G} is singular, $N(\mathcal{G}) = N(G) + iN(G)$, and $\mathcal{T}z = z$ for any $z \in N(\mathcal{G})$. Let now $\lambda \in \sigma(\mathcal{T})$, $\lambda \neq 1$, so that

there exists $z \neq 0$ with $\mathcal{T}z = \lambda z$ and $z \notin N(\mathcal{G})$. Upon writing $z = x + iy$, $x, y \in \mathbb{R}^\omega$, 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 $z \in N(\mathcal{G})$. Since $z \notin N(\mathcal{G})$ 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 $\mathcal{T}z = \lambda z$, upon multiplying by \mathcal{M} this identity we obtain that $Wz = \lambda \mathcal{M}z = \lambda(M + iG^B)z$. Taking the scalar product with z we obtain

$$\lambda = \frac{\langle Wz, z \rangle}{\langle Mz, z \rangle + i\langle G^B z, z \rangle}, \quad (3.9)$$

and

$$|\lambda| \leq \frac{|\langle Wz, z \rangle|}{\langle Mz, z \rangle} < 1 \quad (3.10)$$

thanks to $\langle Mz, z \rangle \leq |\langle Mz, z \rangle + i\langle G^B z, z \rangle|$ and we have established that $\gamma(\mathcal{T}) < 1$.

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

$$\langle Wz', z \rangle = \langle (M + iG^B)(z' + z), z \rangle = \langle M(z' + z), z \rangle, \quad (3.11)$$

since $\langle G^B(z' + z), z \rangle = \langle G^B z', z \rangle = \langle z', G^B z \rangle = 0$ thanks to $G^B z = 0$. Therefore (3.11) implies

$$\langle Mz', z \rangle + \langle Mz, z \rangle = \langle z', Wz \rangle = \langle z', Mz \rangle = \langle Mz', z \rangle,$$

and this yields $\langle Mz, z \rangle = 0$ which in turns implies $z = 0$ and this contradicts $z \neq 0$, and we have established that \mathcal{T} is convergent.

In order to compare the values of $\gamma(T)$ and $\gamma(\mathcal{T})$ we now make use of Lemma 3.4. If $z \in \mathbb{C}^\omega$, $z \neq 0$ is such that $\mathcal{T}z = \lambda z$ with $\lambda \neq 1$, and if $u \in \mathbb{R}^\omega$ is such that $u \in N(G)$ we have $Wz = \lambda(M + iG^B)z$ and $Wu = Mu$. Therefore, $\langle Wz, u \rangle = \lambda \langle (M + iG^B)z, u \rangle = \lambda \langle Mz, u \rangle$ since $G^B u = 0$. 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 $z = x + iy$, $x, y \in \mathbb{R}^\omega$, we deduce that $\langle Mx, u \rangle + i\langle My, u \rangle = 0$ so that finally $\langle Mx, u \rangle = \langle My, u \rangle = 0$ for any $u \in N(G)$. We can now write from (3.10)

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

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

Since the matrices \mathcal{T} and $\mathcal{P}\mathcal{T}$ are convergent, we know that both sequences $\{z_i; i \geq 0\}$ and $\{z'_i; i \geq 0\}$ are convergent. Denoting by z_∞ and z'_∞ the corresponding limits, we deduce from the relation $z_{i+1} = \mathcal{T}z_i + M^{-1}\beta$ that $z_\infty = \mathcal{T}z_\infty + \mathcal{M}^{-1}\beta$. This shows that $\mathcal{G}z_\infty = \beta$ and since $\mathcal{P}\mathcal{T} = \mathcal{P}\mathcal{T}\mathcal{P}$ it is easily established by induction that $z'_i = \mathcal{P}z_i$, for any $i \geq 0$. Therefore, $\mathcal{P}z_\infty = z'_\infty$ and since $\mathcal{G}\mathcal{P} = \mathcal{G}$ we obtain that $\mathcal{G}z'_\infty = \mathcal{G}z_\infty = \beta$. Finally, since $z'_\infty = \mathcal{P}z'_\infty$ we have $z'_\infty \in \mathcal{C}$ 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 $z'_i = \mathcal{Z}_i\beta$ for any $i \geq 1$. We indeed have $z'_1 = \mathcal{P}\mathcal{M}^{-1}\beta = \mathcal{Z}_1\beta$, and assuming by induction that $z'_i = \mathcal{Z}_i\beta$ we obtain that

$$z'_{i+1} = \mathcal{P}\mathcal{T}z'_i + \mathcal{P}\mathcal{M}^{-1}\beta = (\mathcal{P}\mathcal{T}\mathcal{Z}_i + \mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t)\beta = \mathcal{Z}_{i+1}\beta,$$

since $\mathcal{Z}_{i+1} = \mathcal{P}\mathcal{T}\mathcal{Z}_i + \mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t$. Passing to the limit $i \rightarrow \infty$ and thanks to Proposition 2.1 we obtain that for any $\beta \in R(\mathcal{G})$

$$\mathcal{Z}\beta = \sum_{i \geq 0} (\mathcal{P}\mathcal{T})^i \mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t\beta,$$

so that \mathcal{Z} and $\sum_{i \geq 0} (\mathcal{P}\mathcal{J})^i \mathcal{P}\mathcal{M}^{-1} \mathcal{P}^t$ coincide over $R(\mathcal{G})$ and $\mathcal{C}^\perp + i\mathcal{C}^\perp$ and therefore over \mathbb{C}^ω . Finally, in order to establish that \mathcal{Z}_i is symmetric, it is sufficient to establish that each term $(\mathcal{P}\mathcal{J})^j \mathcal{P}\mathcal{M}^{-1} \mathcal{P}^t$ in the series (3.6) is symmetric. However, from the relation $\mathcal{P}\mathcal{J} = \mathcal{P}\mathcal{J}\mathcal{P}$ we obtain $(\mathcal{P}\mathcal{J})^j \mathcal{P}\mathcal{M}^{-1} \mathcal{P}^t = \mathcal{P}\mathcal{J}^j \mathcal{M}^{-1} \mathcal{P}^t$ which is symmetric since $\mathcal{J} = \mathcal{M}^{-1} \mathcal{W}$ and \mathcal{M} and \mathcal{W} are symmetric. \square

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

Remark 3.6. Upon writing $\mathcal{Z}_i = Z_i + iZ_i^B$, where $Z_i, Z_i^B \in \mathbb{R}^{\omega, \omega}$, we have established that Z_i and Z_i^B are symmetric and it should be true that Z_i is positive semi-definite, $Z_i^B N(Z_i) = 0$, and $N(Z_i) = \mathcal{C}^\perp$. This can indeed be established for the first iterates $\mathcal{Z}_1 = \mathcal{P}\mathcal{M}^{-1} \mathcal{P}^t$ and $\mathcal{Z}_2 = \mathcal{P}\mathcal{M}^{-1}(\mathcal{M} + \mathcal{W})\mathcal{M}^{-1} \mathcal{P}^t$. More specifically, we first note that if $\mathcal{M}^{-1} = A + iA^B$, $A, A^B \in \mathbb{R}^{\omega, \omega}$, then we have $AM - A^B G^B = I$ and $AG^B + A^B M = 0$ so that $AMA + A^B M A^B = A$ and A is positive definite since $A = (M + G^B M^{-1} G^B)^{-1}$. We then obtain after some algebra that $Z_1 = PAP^t$ and $Z_2 = P(A + AWA - A^B W A^B)P^t$ so that $Z_2 = P(A(M + W)A + A^B(M - W)A^B)P^t$ and Z_1 and Z_2 are positive semi-definite with nullspace \mathcal{C}^\perp . Since by construction $Z_1^B \mathcal{C}^\perp = 0$ and $Z_2^B \mathcal{C}^\perp = 0$ we get that $Z_1^B N(Z_1) = 0$ and $Z_2^B N(Z_2) = 0$. On the other hand, the next iterates Z_i , $i \geq 3$, are intricated expressions involving A , A^B , 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 $\langle\langle \cdot, \cdot \rangle\rangle$ the scalar product $\langle\langle x, y \rangle\rangle = \langle Mx, y \rangle$, $x, y \in \mathbb{R}^\omega$. 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 $\langle\langle \cdot, \cdot \rangle\rangle$. In addition, the eigenspace associated with the eigenvalue 1 is the eigenspace $N(I - T) = N(G)$, so that

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

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 $\mathcal{M} = M + iG^B$ can easily be evaluated. In practical applications, even though the matrix G^B may not be sparse, it generally has the special structure [18, 19]

$$G^B = P^t M^B P, \tag{3.12}$$

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

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

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

$$G^B = (I - Y \otimes U) M^B (I - U \otimes Y),$$

where $Y, U \in \mathbb{R}^\omega$, $\langle Y, U \rangle = 1$, and $M^B \in \mathbb{R}^{\omega,\omega}$ is a symmetric matrix. The matrices $M + iM^B$ and $M + iG^B$ are invertible, $\langle (M + iM^B)^{-1}Y, Y \rangle \neq 0$, and we define the matrix \mathcal{E} by

$$\mathcal{E} = (M + iM^B)^{-1} - \frac{(M + iM^B)^{-1}Y \otimes (M + iM^B)^{-1}Y}{\langle (M + iM^B)^{-1}Y, Y \rangle}. \quad (3.13)$$

Then $\langle (M - M\mathcal{E}M)U, U \rangle \neq 0$ and the inverse of $M + iG^B$ is given by

$$(M + iG^B)^{-1} = \mathcal{E} + \frac{(I - \mathcal{E}M)U \otimes (I - \mathcal{E}M)U}{\langle (M - M\mathcal{E}M)U, U \rangle}. \quad (3.14)$$

Proof. We introduce for convenience the compact notation $P = I - U \otimes Y$ and $Q = I - Y \otimes U$ in such a way that $G^B = QM^BP$. It is first easily checked that $M + iM^B$ and $M + iG^B$ are invertible since M is symmetric positive definite and M^B and G^B are symmetric. Moreover, defining $z = (M + iM^B)^{-1}Y$ we have $\langle (M + iM^B)^{-1}Y, Y \rangle = \langle z, (M + iM^B)z \rangle = \langle (M - iM^B)z, z \rangle$, and upon decomposing $z = x + iy$, the real part of $\langle (M - iM^B)z, z \rangle$ 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 $\langle (M + iM^B)^{-1}Y, Y \rangle \neq 0$.

The matrix \mathcal{E} is thus well defined and denoting $\mathcal{F} = Q(M + iM^B)P = QMP + iG^B$, \mathcal{E} is the generalized inverse of \mathcal{F} with nullspace $\mathbb{C}Y$ and range $Y^\perp + iY^\perp$, since it is easily checked that $\mathcal{E}\mathcal{F} = I - U \otimes Y$ and $\mathcal{F}\mathcal{E} = I - Y \otimes U$.

We introduce $U' = (M + iG^B)(U - \mathcal{E}MU)$ and U' is nonzero since $M + iG^B$ is invertible and $U - \mathcal{E}MU$ is nonzero because $R(\mathcal{E}) = Y^\perp + iY^\perp$ and $U \notin Y^\perp$. We now establish that $U' = \langle (M - M\mathcal{E}M)U, U \rangle Y$. Indeed, we first have $U' = MU - M\mathcal{E}MU - iQM^B\mathcal{E}MU$ since $PU = 0$ and $P\mathcal{E} = \mathcal{E}$ thanks to $\mathcal{E} = \mathcal{E}^t$ and $\mathcal{E}Y = 0$. This yields $U' = MU - Q(M + iM^B)\mathcal{E}MU - (I - Q)M\mathcal{E}MU$, and thus

$$U' = MU - Q \left(I - \frac{Y \otimes (M + iM^B)^{-1}Y}{\langle (M + iM^B)^{-1}Y, Y \rangle} \right) MU - (I - Q)M\mathcal{E}MU.$$

Since $QY = 0$ we get $U' = MU - QMU - (I - Q)M\mathcal{E}MU = (I - Q)(MU - M\mathcal{E}MU)$, and thus $U' = Y \otimes U (MU - M\mathcal{E}MU) = \langle (M - M\mathcal{E}M)U, U \rangle Y$ and this shows that $\langle (M - M\mathcal{E}M)U, U \rangle \neq 0$ since U' is nonzero.

We now decompose $M + iG^B = M + iQM^BP = M - QMP + Q(M + iM^B)P$ and evaluate the product of $M + iG^B$ by the right member of (3.14) by forming

$$\left(\mathcal{E} + \frac{(I - \mathcal{E}M)U \otimes (I - \mathcal{E}M)U}{\langle (M - M\mathcal{E}M)U, U \rangle} \right) (M - QMP + Q(M + iM^B)P). \quad (3.15)$$

The first contribution simplifies into $\mathcal{E}(M - QMP) = \mathcal{E}(M - MP) = \mathcal{E}M(I - P) = \mathcal{E}MU \otimes Y$ since $\mathcal{E}Q = \mathcal{E}$ thanks to $Q = I - Y \otimes U$ and $\mathcal{E}Y = 0$. Moreover

$$\mathcal{E}Q(M + iM^B)P = \mathcal{E}(M + iM^B)P = \left(I - \frac{(M + iM^B)^{-1}Y \otimes Y}{\langle (M + iM^B)^{-1}Y, Y \rangle} \right) P = P,$$

since $a \otimes YP = a \otimes (P^tY) = a \otimes (QY) = 0$, and the whole contribution $\mathcal{E}(M + iG^B)$ finally sum up to $\mathcal{E}MU \otimes Y + I - U \otimes Y = I - (U - \mathcal{E}MU) \otimes Y$. We now form the product

$$(I - \mathcal{E}M)U \otimes (I - \mathcal{E}M)U (M + iG^B) = (I - \mathcal{E}M)U \otimes ((M + iG^B)(I - \mathcal{E}M)U),$$

and $U' = (M + iG^B)(U - \mathcal{E}MU) = \langle (M - M\mathcal{E}M)U, U \rangle Y$ so that gathering all terms of the product (3.15) we obtain $I - (U - \mathcal{E}MU) \otimes Y + (U - \mathcal{E}MU) \otimes Y = I$ and the proof is complete. \square

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

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

$$G^B = \left(I - \sum_{1 \leq i \leq p} v_i \otimes u_i\right) M^B \left(I - \sum_{1 \leq i \leq p} u_i \otimes v_i\right), \quad (3.16)$$

where $p \geq 1$, u_1, \dots, u_p are real independent vectors, v_1, \dots, v_p are real independent vectors, $\langle v_i, u_j \rangle = \delta_{ij}$, $1 \leq i, j \leq p$, and $M^B \in \mathbb{R}^{\omega,\omega}$ is a symmetric matrix. The matrices $M + iM^B$ and $M + iG^B$ are invertible, and the matrix $\left(\langle (M + iM^B)^{-1}v_i, v_j \rangle\right)_{1 \leq i, j \leq p}$ is invertible. Upon denoting by $(\gamma_{ij})_{1 \leq i, j \leq p}$ its inverse, we define the matrix \mathcal{E} by

$$\mathcal{E} = (M + iM^B)^{-1} - \sum_{1 \leq i, j \leq p} \gamma_{ij} (M + iM^B)^{-1} v_i \otimes (M + iM^B)^{-1} v_j. \quad (3.17)$$

Then the matrix $\left(\langle (M - M\mathcal{E}M)u_i, u_j \rangle\right)_{1 \leq i, j \leq p}$ is invertible, and denoting by $(\mu_{ij})_{1 \leq i, j \leq p}$ its inverse, the inverse of $M + iG^B$ is given by

$$(M + iG^B)^{-1} = \mathcal{E} + \sum_{1 \leq i, j \leq p} \mu_{ij} (I - \mathcal{E}M)u_i \otimes (I - \mathcal{E}M)u_j. \quad (3.18)$$

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

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

$$(M + iQM^BP)(u_i - \mathcal{E}Mu_i) = \sum_{1 \leq j \leq p} \langle (M - M\mathcal{E}M)u_i, u_j \rangle v_j, \quad 1 \leq i \leq p. \quad (3.19)$$

The vectors $u_i - \mathcal{E}Mu_i$, $1 \leq i \leq p$, are linearly independent since if there exists a linear relation $\sum_{1 \leq i \leq p} \theta_i (u_i - \mathcal{E}Mu_i) = 0$, we obtain upon taking the scalar product with v_j that $\theta_j = 0$ since $\langle u_i, v_j \rangle = \delta_{ij}$, $R(\mathcal{E}) \subset \mathcal{C} + i\mathcal{C}$, and v_j , $1 \leq j \leq p$, form a basis of \mathcal{C}^\perp . As a consequence, the vectors $(M + iQM^BP)(u_i - \mathcal{E}Mu_i)$, $1 \leq i \leq p$, are independent, and from the relations (3.19) we deduce that $\left(\langle (M - M\mathcal{E}M)u_i, u_j \rangle\right)_{1 \leq i, j \leq p}$ is invertible. Finally, a direct calculation shows that the right member of (3.18) is the inverse of $M + iQM^BP$. \square

Remark 3.10. Assume that the splitting matrix M is diagonal and that G^B is in the form (3.16) where the matrix M^B is diagonal. Then each iteration of the scheme (1.4) costs $\omega^2 + O(\omega)$ (complex) flops thanks to the expression of (3.18) of $(M + iQM^BP)^{-1}$. The main costs are associated with the ω^2 operations required by the multiplication of W by a complex vector. Similarly, each iteration of (3.1) requires approximately the same cost thanks to the decomposition $P_{\mathcal{C}, N(G)} = I - \sum_{1 \leq i \leq p} u_i \otimes v_i$ 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 [22, 28, 20]. Projected conjugate gradients methods have been introduced in particular to solve the symmetric constrained singular systems associated with nonmagnetized transport [6, 8]. 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 hermitian properties [10]. Examples of short recurrence algorithms are CGS or BiCGStab whereas GMRES [30] corresponds to a global error minimisation over the Krylov subspaces.

Complex symmetric systems have received much less attention than real systems even though symmetric complex systems arise in electromagnetic applications [11, 13, 14, 2]. Special systems with diagonal positive imaginary parts have been investigated by Freund [13] as well as the Lanczos recursion and related algorithms [14]. Freund has also shown that it is generally more efficient to solve the systems in their complex form rather than in their real equivalent form [14].

We investigate in this section projected orthogonal residuals methods for solving the complex symmetric constrained singular systems arising from magnetized transport. Orthogonal residual methods are a natural generalization of conjugate gradient algorithms associated with Arnoldi algorithm [30] as well as with orthogonal errors methods introduced by Faber and Manteuffel [11]. Orthogonal residuals methods seems natural in the context of multicomponent transport since they make use of the positivity properties of the real symmetric part—associated with entropy production—and they exactly correspond to previously introduced projected algorithms in the absence of magnetic fields [8].

The projected orthogonal residuals method usually has a better convergence behavior than the projected standard method introduced in the previous section and should generally be preferred as in the nonmagnetized case. However, the corresponding iterates depend nonlinearly on the right member β because of the quadratic nature of conjugate gradients type algorithms. This prevents its use in some special situations as for instance with the species diffusion matrices.

4.1 A projected orthogonal residuals algorithm

In this section we investigate a projected orthogonal residuals method for the constrained singular linear systems arising from the kinetic theory of magnetized ionized mixtures. 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 [11].

Theorem 4.1. *Let $\mathcal{G} = G + iG^B$ where G, G^B are real symmetric matrices, G is positive semi-definite and $G^B N(G) = 0$. Let $\mathcal{C} \subset \mathbb{R}^\omega$ be complementary to $N(G)$ and let \mathcal{C} be the complexification of \mathcal{C} . Let $z_0 \in \mathbb{C}^\omega$, $r_0 = \beta - \mathcal{G}z_0$, $p_0 = r_0$ and consider the following algorithm. If $\langle \mathcal{G}p_0, p_0 \rangle = 0$ then $r_0 = 0$ and we stop at step 0, and if $\langle \mathcal{G}p_0, p_0 \rangle \neq 0$ we set $\sigma_0 = \langle r_0, p_0 \rangle / \langle \mathcal{G}p_0, p_0 \rangle$, $\nu_{00} = \langle \mathcal{G}^2 p_0, p_0 \rangle / \langle \mathcal{G}p_0, p_0 \rangle$, and we define $p_1 = \mathcal{G}p_0 - \nu_{00}p_0$, $z_1 = z_0 + \sigma_0 p_0$, and $r_1 = r_0 - \sigma_0 \mathcal{G}p_0$. Assume now by induction that for $k \geq 1$ we have defined $\{p_i\}_{0 \leq i \leq k}$, $\{z_i\}_{0 \leq i \leq k}$, $\{r_i\}_{0 \leq i \leq k}$, with $\prod_{0 \leq i \leq k-1} \langle \mathcal{G}p_i, p_i \rangle \neq 0$, $r_i = \beta - \mathcal{G}z_i$, $0 \leq i \leq k$, and*

$$\langle r_i, r_j \rangle = 0, \quad 0 \leq j < i \leq k, \quad (4.1)$$

$$\langle \mathcal{G}p_i, p_j \rangle = 0, \quad 0 \leq j < i \leq k, \quad (4.2)$$

$$\langle r_i, p_j \rangle = 0, \quad 0 \leq j < i \leq k, \quad (4.3)$$

$$\mathcal{K}_i = \text{span}(p_0, \dots, p_i) = \text{span}(r_0, \dots, r_i) = \text{span}(r_0, \dots, \mathcal{G}^i r_0), \quad 0 \leq i \leq k, \quad (4.4)$$

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

solving the linear system

$$\begin{pmatrix} \langle \mathcal{G}p_0, p_0 \rangle \\ \langle \mathcal{G}p_0, p_1 \rangle & \langle \mathcal{G}p_1, p_1 \rangle \\ \vdots & \vdots & \ddots \\ \langle \mathcal{G}p_0, p_k \rangle & \langle \mathcal{G}p_1, p_k \rangle & \cdots & \langle \mathcal{G}p_k, p_k \rangle \end{pmatrix} \begin{pmatrix} \nu_{k0} \\ \nu_{k1} \\ \vdots \\ \nu_{kk} \end{pmatrix} = \begin{pmatrix} \langle \mathcal{G}^2 p_k, p_0 \rangle \\ \langle \mathcal{G}^2 p_k, p_1 \rangle \\ \vdots \\ \langle \mathcal{G}^2 p_k, p_k \rangle \end{pmatrix}, \quad (4.5)$$

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

$$p_{k+1} = \mathcal{G}p_k - \sum_{0 \leq j \leq k} \nu_{kj} p_j, \quad z_{k+1} = z_k + \sigma_k p_k, \quad r_{k+1} = r_k - \sigma_k \mathcal{G}p_k. \quad (4.6)$$

Then the algorithm is well defined and converges in at most $\text{rank}(\mathcal{G})$ steps towards the unique solution z of $\mathcal{G}z = \beta$ and $z \in R(\mathcal{G})$.

Consider now the projected algorithm defined similarly by using projected directions. More specifically, we set $z'_0 = \mathcal{P}z_0$, $p'_0 = \mathcal{P}p_0$, $r'_0 = \beta - \mathcal{G}z'_0$, and if $\langle \mathcal{G}p'_0, p'_0 \rangle = 0$ we stop at step 0, whereas if $\langle \mathcal{G}p'_0, p'_0 \rangle \neq 0$ we define $\sigma'_0 = \langle r'_0, p'_0 \rangle / \langle \mathcal{G}p'_0, p'_0 \rangle$, $\nu'_{00} = \langle \mathcal{G}^2 p'_0, p'_0 \rangle / \langle \mathcal{G}p'_0, p'_0 \rangle$, and $p'_1 = \mathcal{P}\mathcal{G}p'_0 - \nu'_{00} p'_0$, $z'_1 = z'_0 + \sigma'_0 p'_0$, and $r'_1 = r'_0 - \sigma'_0 \mathcal{G}p'_0$. Assume now by induction that for $k \geq 1$ we have defined $\{p'_i\}_{0 \leq i \leq k}$, $\{z'_i\}_{0 \leq i \leq k}$, $\{r'_i\}_{0 \leq i \leq k}$, with $\prod_{0 \leq i \leq k-1} \langle \mathcal{G}p'_i, p'_i \rangle \neq 0$ and $r'_i = \beta - \mathcal{G}z'_i$, $0 \leq i \leq k$. Then $\langle \mathcal{G}p'_k, p'_k \rangle = 0$ if and only if $r'_k = 0$ and in this situation we stop at step k . On the other hand if $\langle \mathcal{G}p'_k, p'_k \rangle \neq 0$ we introduce the solution $\nu'_{k0}, \dots, \nu'_{kk}$ of the linear system similar to (4.5) but using the directions $\{p'_i\}_{0 \leq i \leq k}$ instead of $\{p_i\}_{0 \leq i \leq k}$ to form the system coefficients, we define as well $\sigma'_k = \langle r'_k, p'_k \rangle / \langle \mathcal{G}p'_k, p'_k \rangle$ and we set

$$p'_{k+1} = \mathcal{P}\mathcal{G}p'_k - \sum_{0 \leq j \leq k} \nu'_{kj} p'_j, \quad z'_{k+1} = z'_k + \sigma'_k p'_k, \quad r'_{k+1} = r'_k - \sigma'_k \mathcal{G}p'_k. \quad (4.7)$$

Then the algorithm is well defined and converges in at most $\text{rank}(\mathcal{G})$ steps towards the unique solution α of $\mathcal{G}\alpha = \beta$ and $\alpha \in \mathcal{C}$. Moreover, at each step k , we have $r'_k = r_k$, $z'_k = \mathcal{P}z_k$, $p'_k = \mathcal{P}p_k$, $\sigma'_k = \sigma_k$, as well as $\langle \mathcal{G}p'_k, p'_j \rangle = \langle \mathcal{G}p_k, p_j \rangle$, $\langle r'_k, p'_j \rangle = \langle r_k, p_j \rangle$, and $\nu'_{ki} = \nu_{ki}$, for $0 \leq i \leq k$. Finally, we have at step k

$$\mathcal{K}'_i = \text{span}(p'_0, \dots, p'_i) = \mathcal{P}\mathcal{K}_i, \quad \mathcal{K}_i = \mathcal{H}\mathcal{K}'_i, \quad 0 \leq i \leq k, \quad (4.8)$$

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

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

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

Suppose now that $\langle \mathcal{G}p_k, p_k \rangle \neq 0$, 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 $p_k \in \text{span}(r_0, \dots, r_k)$ we obtain $p_k \in \text{span}(r_0, \dots, r_{k-1})$ and $p_k \in \text{span}(p_0, \dots, p_{k-1})$ in such a way that $\langle \mathcal{G}p_k, p_k \rangle = 0$. We next have $\langle \mathcal{G}p_{k+1}, p_i \rangle = 0$, $0 \leq i \leq k$, 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)(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 $r_{k+1} = \beta - \mathcal{G}z_k - \sigma_k \mathcal{G}p_k = \beta - \mathcal{G}(z_k + \sigma_k p_k) = \beta - \mathcal{G}z_{k+1}$.

From $r_{k+1} = r_k - \sigma \mathcal{G}p_k$ we first obtain $r_{k+1} \in \text{span}(r_0, \dots, \mathcal{G}^{k+1}r_0)$ since $p_k \in \mathcal{K}_k$ so that $\text{span}(r_0, \dots, r_{k+1}) \subset \text{span}(r_0, \dots, \mathcal{G}^{k+1}r_0)$. Conversely, since $\sigma_k \neq 0$, we have $\mathcal{G}p_k \in \text{span}(r_0, \dots, r_{k+1})$ and if $0 \leq i \leq k-1$, $\mathcal{G}p_i \in \mathcal{G}\mathcal{K}_{k-1} \subset \mathcal{K}_k$. This shows $\mathcal{G}\mathcal{K}_k \subset \text{span}(r_0, \dots, r_{k+1})$ so that $\text{span}(r_0, \dots, \mathcal{G}^{k+1}r_0) \subset \text{span}(r_0, \dots, r_{k+1})$. Similarly, from $p_{k+1} = \mathcal{G}p_k - \sum_{0 \leq j \leq k} \nu_{kj} p_j$, we have $\mathcal{G}p_k \in \text{span}(p_0, \dots, p_{k+1})$ and if $0 \leq i \leq k-1$, $\mathcal{G}p_i \in \mathcal{G}\mathcal{K}_{k-1} \subset \mathcal{K}_k$, so that $\mathcal{G}\mathcal{K}_k \subset \text{span}(p_0, \dots, p_{k+1})$ and $\text{span}(r_0, \dots, \mathcal{G}^{k+1}r_0) \subset \text{span}(p_0, \dots, p_{k+1})$. Conversely, since $p_i \in \mathcal{K}_k$ if $0 \leq i \leq k$, $\text{span}(p_0, \dots, p_{k+1}) \subset \text{span}(r_0, \dots, \mathcal{G}^{k+1}r_0)$ and we have established (4.4) for $k+1$. Finally, we also have $\dim(\mathcal{K}_k) = k+1$ 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 $p'_k = \mathcal{P}p_k$, $z'_k = \mathcal{P}z_k$ and $r'_k = r_k$ at each step. We first note the relations $\mathcal{G} = \mathcal{G}\mathcal{P} = \mathcal{P}^t\mathcal{G}$ which imply in particular that for any $a, b \in \mathcal{C}^\omega$, $a' = \mathcal{P}a$, $b' = \mathcal{P}b$, we have $\langle \mathcal{G}a, b \rangle = \langle \mathcal{G}a', b' \rangle = \langle \mathcal{G}a, b' \rangle = \langle \mathcal{G}a', b \rangle$, and similarly that $\langle \mathcal{G}^2 a, b \rangle = \langle \mathcal{G}^2 a', b' \rangle$. Now for $k=0$ we know by assumption that $p'_0 = \mathcal{P}p_0$ and $z'_0 = \mathcal{P}z_0$ so that $r'_0 = \beta - \mathcal{G}z'_0 = \beta - \mathcal{G}z_0 = r_0$ and $\langle \mathcal{G}p_0, p_0 \rangle = \langle \mathcal{G}p'_0, p'_0 \rangle$. Therefore $\langle \mathcal{G}p'_0, p'_0 \rangle = 0$ if and only if $r'_0 = 0$ and then we stop at step 0. When $\langle \mathcal{G}p_0, p_0 \rangle \neq 0$ then it is easily checked that $\nu'_{00} = \nu_{00}$ and $\sigma'_0 = \sigma_0$. Since $p'_1 = \mathcal{P}\mathcal{G}p'_0 - \nu'_{00}p'_0$, and $z'_1 = z'_0 + \sigma'_0 p'_0$, we obtain that $p'_1 = \mathcal{P}(\mathcal{G}p'_0 - \nu_{00}p_0) = \mathcal{P}p_1$ and $z'_1 = \mathcal{P}(z_0 + \sigma_0 p_0) = \mathcal{P}z_1$ and thus $r'_1 = \beta - \mathcal{G}\mathcal{P}z_1 = r_1$. Assume now by induction that for $k \geq 1$ we have defined $\{p'_i\}_{0 \leq i \leq k}$, $\{z'_i\}_{0 \leq i \leq k}$, $\{r'_i\}_{0 \leq i \leq k}$, with $\prod_{0 \leq i \leq k-1} \langle \mathcal{G}p'_i, p'_i \rangle \neq 0$, and that $p'_i = \mathcal{P}p_i$, $z'_i = \mathcal{P}z_i$ and $r'_i = r_i$ for $0 \leq i \leq k$. Since $\langle \mathcal{G}p_k, p_k \rangle = \langle \mathcal{G}p'_k, p'_k \rangle$ and $r'_k = r_k$, $\langle \mathcal{G}p'_k, p'_k \rangle = 0$ if and only if $r'_k = 0$. On the other hand, when $\langle \mathcal{G}p'_k, p'_k \rangle \neq 0$ we define the coefficients ν'_{kj} , $0 \leq j \leq k$, by solving the linear system

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

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

$$\begin{cases} \mathcal{B}^{-1} \mathcal{G} \mathcal{B}^{-*} (\mathcal{B}^* \alpha) = \mathcal{B}^{-1} \beta, \\ \mathcal{B}^* \alpha \in \mathcal{B}^* \mathcal{C}, \end{cases} \quad (4.10)$$

where \mathcal{B} is an invertible matrix, \mathcal{B}^* its adjoint and \mathcal{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 $\mathcal{B}^{-1}\mathcal{G}\mathcal{B}^{-*}$, the new second member $\mathcal{B}^{-1}\beta$, the new unknown $\mathcal{B}^*\alpha$, with the directions \mathcal{B}^*p_i and residuals $\mathcal{B}^{-1}r_i$, and finally by reformulating back the resulting algorithm in terms of the original system with the help of the hermitian matrix $M = \mathcal{B}\mathcal{B}^*$. The form (4.10) seems natural since $\langle \mathcal{B}^{-1}\mathcal{G}\mathcal{B}^{-*}z, z \rangle = \langle \mathcal{G}\mathcal{B}^{-*}z, \mathcal{B}^{-*}z \rangle$ in such a way that the positivity properties of the matrix \mathcal{G} associated with (1.1) are maintained with the matrix $\mathcal{B}^{-1}\mathcal{G}\mathcal{B}^{-*}$ associated with (4.10).

Theorem 4.2. *Let $\mathcal{G} = G + iG^B$ where G, G^B are real symmetric matrices, G is positive semi-definite and $G^B N(G) = 0$. Let $\mathcal{C} \subset \mathbb{R}^\omega$ be complementary to $N(G)$ and let \mathcal{C} be the complexification of \mathcal{C} . Assume that M is an hermitian positive definite matrix. Let $z_0 \in \mathbb{C}^\omega$, $r_0 = \beta - \mathcal{G}z_0$, $p_0 = M^{-1}r_0$ and consider the following algorithm. If $\langle \mathcal{G}p_0, p_0 \rangle = 0$ then $r_0 = 0$ and we stop at step 0, and if $\langle \mathcal{G}p_0, p_0 \rangle \neq 0$ we set $\sigma_0 = \langle r_0, p_0 \rangle / \langle \mathcal{G}p_0, p_0 \rangle$, $\nu_{00} = \langle \mathcal{G}M^{-1}\mathcal{G}p_0, p_0 \rangle / \langle \mathcal{G}p_0, p_0 \rangle$, and we define $p_1 = M^{-1}\mathcal{G}p_0 - \nu_{00}p_0$, $z_1 = z_0 + \sigma_0 p_0$, and $r_1 = r_0 - \sigma_0 \mathcal{G}p_0$. Assume now by induction that for $k \geq 1$ we have defined $\{p_i\}_{0 \leq i \leq k}$, $\{z_i\}_{0 \leq i \leq k}$, $\{r_i\}_{0 \leq i \leq k}$, with $\prod_{0 \leq i \leq k-1} \langle \mathcal{G}p_i, p_i \rangle \neq 0$, $r_i = \beta - \mathcal{G}z_i$, $0 \leq i \leq k$, and*

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

$$\langle \mathcal{G}p_i, p_j \rangle = 0, \quad 0 \leq j < i \leq k, \quad (4.12)$$

$$\langle r_i, p_j \rangle = 0, \quad 0 \leq j < i \leq k, \quad (4.13)$$

$$\mathcal{K}_i = M \text{span}(p_0, \dots, p_i) = \text{span}(r_0, \dots, r_i) = \text{span}(r_0, \dots, (\mathcal{G}M^{-1})^i r_0), \quad 0 \leq i \leq k, \quad (4.14)$$

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

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

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

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

Then the algorithm is well defined and converges in at most $\text{rank}(\mathcal{G})$ steps towards the unique solution z of $\mathcal{G}z = \beta$ and $z \in R(\mathcal{G})$.

Consider now the projected algorithm defined similarly by using projected directions. More specifically, we set $z'_0 = \mathcal{P}z_0$, $p'_0 = \mathcal{P}M^{-1}p_0$, $r'_0 = \beta - \mathcal{G}z'_0$, and if $\langle \mathcal{G}p'_0, p'_0 \rangle = 0$ we stop at step 0, whereas if $\langle \mathcal{G}p'_0, p'_0 \rangle \neq 0$ we define $\sigma'_0 = \langle r'_0, p'_0 \rangle / \langle \mathcal{G}p'_0, p'_0 \rangle$, $\nu'_{00} = \langle \mathcal{G}M^{-1}\mathcal{G}p'_0, p'_0 \rangle / \langle \mathcal{G}p'_0, p'_0 \rangle$, and $p'_1 = \mathcal{P}M^{-1}\mathcal{G}p'_0 - \nu'_{00}p'_0$, $z'_1 = z'_0 + \sigma'_0 p'_0$, and $r'_1 = r'_0 - \sigma'_0 \mathcal{G}p'_0$. Assume now by induction that for $k \geq 1$ we have defined $\{p'_i\}_{0 \leq i \leq k}$, $\{z'_i\}_{0 \leq i \leq k}$, $\{r'_i\}_{0 \leq i \leq k}$, with $\prod_{0 \leq i \leq k-1} \langle \mathcal{G}p'_i, p'_i \rangle \neq 0$ and $r'_i = \beta - \mathcal{G}z'_i$, $0 \leq i \leq k$. Then $\langle \mathcal{G}p'_k, p'_k \rangle = 0$ if and only if $r'_k = 0$ and in this situation we stop at step k . On the other hand if $\langle \mathcal{G}p'_k, p'_k \rangle \neq 0$ we introduce the solution $\nu'_{k0}, \dots, \nu'_{kk}$ of the linear systems similar to (4.15) but using the directions $\{p'_i\}_{0 \leq i \leq k}$ instead of $\{p_i\}_{0 \leq i \leq k}$ to form the system coefficients, as well as $\sigma'_k = \langle r'_k, p'_k \rangle / \langle \mathcal{G}p'_k, p'_k \rangle$ and we set

$$p'_{k+1} = \mathcal{P}M^{-1}\mathcal{G}p'_k - \sum_{0 \leq j \leq k} \nu'_{kj} p'_j, \quad z'_{k+1} = z'_k + \sigma'_k p'_k, \quad r'_{k+1} = r'_k - \sigma'_k \mathcal{G}p'_k. \quad (4.17)$$

Then the algorithm is well defined and converges in at most $\text{rank}(\mathcal{G})$ steps towards the unique solution α of $\mathcal{G}\alpha = \beta$ and $\alpha \in \mathcal{C}$. Moreover, at each step k , we have $r'_k = r_k$, $z'_k = \mathcal{P}z_k$, $p'_k = \mathcal{P}p_k$,

$\sigma'_k = \sigma_k$, as well as $\langle \mathcal{G}p'_k, p'_j \rangle = \langle \mathcal{G}p_k, p_j \rangle$, $\langle r'_k, p'_j \rangle = \langle r_k, p_j \rangle$, and $\nu'_{ki} = \nu_{ki}$, for $0 \leq i \leq k$. Finally, we have

$$\mathcal{K}'_i = \text{span}(p'_0, \dots, p'_i) = \mathcal{P}M^{-1}\mathcal{K}_i, \quad \mathcal{K}_i = \mathcal{H}\mathcal{K}'_i, \quad 0 \leq i \leq k, \quad (4.18)$$

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

Proof. The proof is similar to that of the unpreconditioned algorithm. \square

Remark 4.3. In order to precondition the orthogonal residuals algorithm one may also consider the following reformulation of (1.1)

$$\begin{cases} \mathcal{B}^{-1} \mathcal{G} \mathcal{B}^{-1} (\mathcal{B} \alpha) = \mathcal{B}^{-1} \beta, \\ \mathcal{B} \alpha \in \mathcal{B} \mathcal{C}, \end{cases} \quad (4.19)$$

where \mathcal{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 $M = \mathcal{B} \mathcal{B}^*$, $\tilde{M} = \mathcal{B} \mathcal{B}$ and $\tilde{O} = \mathcal{B} \mathcal{B}^{-*}$. The coefficient of the linear system are $\langle \tilde{O}^{-1} \mathcal{G} p_k, p_j \rangle$ and the right members $\langle \tilde{O}^{-1} \mathcal{G} \tilde{M}^{-1} \mathcal{G} p_k, p_j \rangle$. At step k the orthogonal relations are $\langle M^{-1} r_i, r_j \rangle = 0$, $\langle \tilde{O}^{-1} \mathcal{G} p_i, p_j \rangle = 0$, $\langle \tilde{O}^{-1} r_i, p_j \rangle = 0$, for $0 \leq j < i \leq k$. The new directions are defined from the relations $p_{k+1} = \tilde{M}^{-1} \mathcal{G} p_k - \sum_{0 \leq j \leq k} \nu_{kj} p_j$. This algorithm is not guarantee to converge unless \mathcal{B} is such that $\langle \tilde{O}^{-1} \mathcal{G} z, z \rangle = 0$ implies that $z \in N(\mathcal{G})$ and $\langle \tilde{M}^{-1} z, z \rangle = 0$ 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 \mathcal{B} is hermitian, we have $\tilde{O} = I$, $\tilde{M} = M$ and we recover the simpler algorithm introduced in Theorem 4.2.

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 [5, 12, 18, 19]. These equations contain the terms for transport fluxes, that is, the viscous tensor, the species diffusion velocities, and the heat flux vector, which are nonisotropic under the influence of the magnetic field. In this paper, we discuss the species diffusion velocities \mathbf{V}_k , $1 \leq k \leq n$, where n is the number of species in the mixture, and the heat flux \mathbf{q} , which are vectors of \mathbb{R}^3 .

In order to express the nonisotropy of transport fluxes induced by the magnetic field we introduce some convenient notation. We denote by \mathbf{B} the magnetic field, assumed to be nonzero, by $B = \|\mathbf{B}\|$ its norm and by \mathcal{B} the corresponding unitary vector $\mathcal{B} = \mathbf{B}/B$. Then for any vector $\boldsymbol{\xi} \in \mathbb{R}^3$, we define

$$\boldsymbol{\xi}^{\parallel} = \langle \boldsymbol{\xi}, \mathcal{B} \rangle \mathcal{B}, \quad \boldsymbol{\xi}^{\perp} = \boldsymbol{\xi} - \boldsymbol{\xi}^{\parallel}, \quad \boldsymbol{\xi}^{\odot} = \mathcal{B} \wedge \boldsymbol{\xi},$$

where $\mathbf{a} \wedge \mathbf{b}$ denotes the vector product of $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$. Upon neglecting thermal diffusion—for the sake of simplicity—the species diffusion velocities and the heat flux can be written in the form [5, 12, 18, 19]

$$\mathbf{V}_i = - \sum_{1 \leq j \leq n} (D_{ij}^{\parallel} \mathbf{d}_j^{\parallel} + D_{ij}^{\perp} \mathbf{d}_j^{\perp} + D_{ij}^{\odot} \mathbf{d}_j^{\odot}), \quad 1 \leq i \leq n, \quad (5.1)$$

$$\mathbf{q} = -(\lambda^{\parallel} (\nabla \bar{T})^{\parallel} + \lambda^{\perp} (\nabla \bar{T})^{\perp} + \lambda^{\odot} (\nabla \bar{T})^{\odot}) + \sum_{1 \leq i \leq n} h_i \rho_i \mathbf{V}_i, \quad (5.2)$$

where \mathbf{d}_j is the diffusion driving force of the j th species

$$\mathbf{d}_j = (\nabla p_j - \rho_j \mathbf{g} - \rho_j \zeta_j (\mathbf{E} + \mathbf{v} \wedge \mathbf{B})) / \bar{p}. \quad (5.3)$$

In these expressions, $D^{\parallel} = (D_{ij}^{\parallel})_{1 \leq i, j \leq n}$, $D^{\perp} = (D_{ij}^{\perp})_{1 \leq i, j \leq n}$ and $D^{\odot} = (D_{ij}^{\odot})_{1 \leq i, j \leq n}$ are the diffusion matrices parallel, perpendicular and transverse to the magnetic field, λ^{\parallel} , λ^{\perp} and λ^{\odot} the thermal conductivities parallel, perpendicular and transverse to the magnetic field, ∇ the space derivative operator, \bar{T} the absolute temperature, \bar{p} the pressure, p_j the partial pressure of the j th species, $\bar{\rho}$ the mass density, $\rho_j = \bar{\rho} Y_j$ the partial density of the j th species, h_j the specific enthalpy of the j th species, \mathbf{g} the gravity, ζ_j the charge per unit mass of the j th species, \mathbf{E} the electric field, \mathbf{v} the mixture velocity, and \mathbf{B} the magnetic field.

The transport coefficients, that is, the diffusion matrices D^{\parallel} , D^{\perp} , D^{\odot} , and the thermal conductivities λ^{\parallel} , λ^{\perp} , and λ^{\odot} , are functions of the state variables $(\bar{T}, \bar{p}, Y_1, \dots, Y_n)$. 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 [5, 12, 18, 4, 19]. The size of these systems is typically $\omega \approx rn$ where $r \in \{1, 2, 3\}$ and the number of species in the mixture n is generally in the range $10 \leq n \leq 100$ —although very large chemical mechanisms involving several of hundreds of reactive species $100 \leq n \leq 1000$ are sometimes encountered. The resulting size of the transport linear systems is thus between $10 \leq \omega \leq 300$ 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, 8, 9] has been generalized to the situation of ionized mixtures in strong magnetic fields [18, 19].

In the next sections, we discuss, in particular, the evaluation of the first order diffusion matrices and of the thermal conductivities in a multicomponent gas mixture of n components. It is also possible to introduce higher order transport coefficients associated with transport linear systems of larger size but the mathematical and numerical behavior of the algorithms associated with the larger systems is essentially analogous to that of the linear systems considered in the next sections [19]. We assume in the following that $n \geq 3$ and that the state variables $(\bar{T}, \bar{p}, Y_1, \dots, Y_n)$ are given positive quantities. We also assume that the mass fractions satisfy the natural normalization condition $\sum_{1 \leq k \leq n} Y_k = 1$. The charge per unit mass ζ_k , $1 \leq k \leq n$, are real parameters and we assume that the total charge per unit volume vanishes $\sum_{1 \leq k \leq n} \rho_k \zeta_k = 0$.

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 systems of size $\omega = n$ indexed by l , $1 \leq l \leq n$,

$$\begin{cases} \Delta \alpha^{D_l(1)} = \beta^{D_l}, \\ \alpha^{D_l(1)} \in Y^{\perp}, \end{cases} \quad \begin{cases} (\Delta + i\Delta^B) \alpha^{D_l(2)} = \beta^{D_l}, \\ \alpha^{D_l(2)} \in Y^{\perp} + iY^{\perp}, \end{cases} \quad (5.4)$$

where $\Delta, \Delta^B \in \mathbb{R}^{n,n}$ and $\alpha^{D_l(1)}, \beta^{D_l}, Y \in \mathbb{R}^n$ and $\alpha^{D_l(2)} \in \mathbb{C}^n$ [19]. The coefficients of the transport linear systems are functions of the state variables $(\bar{T}, \bar{p}, Y_1, \dots, Y_n)$ which usually have complex expressions. In the case of first-order diffusion matrices, however, these expressions remain fairly simple and the matrix Δ can be written

$$\Delta_{kk} = \sum_{\substack{1 \leq l \leq n \\ l \neq k}} \frac{X_k X_l}{\mathcal{D}_{kl}}, \quad 1 \leq k \leq n, \quad \Delta_{kl} = -\frac{X_k X_l}{\mathcal{D}_{kl}}, \quad 1 \leq k, l \leq n, \quad k \neq l, \quad (5.5)$$

where \mathcal{D}_{kl} denotes the binary diffusion coefficient for the species pair (k, l) which only depends on temperature, pressure, and electron mole fraction $\mathcal{D}_{kl} = \mathcal{D}_{kl}(\bar{T}, \bar{p}, X_E)$ [5, 12, 31]. The mole fractions can be expressed in terms of the mass fractions $X_k = Y_k m / m_k$, $1 \leq k \leq n$, where m_k , $1 \leq k \leq n$, the species molar masses, are positive constants and where $1/m = \sum_{1 \leq l \leq n} Y_l / m_l$. The constraint vector is $Y = (Y_1, \dots, Y_n)$ where Y_k is the mass fraction of the k th species. The right members $\beta^{D_l} = (\beta_1^{D_l}, \dots, \beta_n^{D_l})$, $1 \leq l \leq n$, are given by

$$\beta_k^{D_l} = \delta_{lk} - Y_k, \quad 1 \leq k, l \leq n, \quad (5.6)$$

where δ_{kl} denotes the Kronecker symbol and finally the matrix Δ^B is given by

$$\Delta^B = (I - Y \otimes U) \mathcal{D}^B (I - U \otimes Y), \quad (5.7)$$

where \mathcal{D}^B is the diagonal matrix $\mathcal{D}_{kl}^B = \delta_{kl} \rho_k \zeta_k B / \bar{p}$ and $U = (1, \dots, 1) \in \mathbb{R}^n$. Once the solutions of the transport linear systems (5.4) are obtained, the diffusion coefficients are evaluated from

$$D_{kl}^{\parallel} = \alpha_k^{D_l(1)}, \quad D_{kl}^{\perp} + iD_{kl}^{\odot} = \alpha_k^{D_l(2)}. \quad (5.8)$$

The vectors $\alpha^{D_l(1)}$, $1 \leq l \leq n$, are therefore the column vectors of the diffusion matrix D^{\parallel} , and the vectors $\alpha^{D_l(2)}$, $1 \leq l \leq n$, are the column vectors of the diffusion matrix $D^{\perp} + iD^{\odot}$.

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 Δ , Δ^B , and the vectors Y , U , and β^{D_l} , $1 \leq l \leq n$, when $n \geq 3$ [6, 19] :

- ($\Delta 1$) Δ is symmetric positive semi-definite.
- ($\Delta 2$) $N(\Delta) = \mathbb{R}U$ where $U = (1, \dots, 1)$.
- ($\Delta 3$) $\langle Y, U \rangle = 1$.
- ($\Delta 4$) $\beta_k^{D_l} = \delta_{lk} - Y_k$, $1 \leq k, l \leq n$.
- ($\Delta 5$) $2\text{diag}(\Delta) - \Delta$ is symmetric positive definite.
- ($\Delta 6$) Δ^B is symmetric.
- ($\Delta 7$) $\Delta^B N(\Delta) = 0$.

In the situation of first order diffusion matrices, however, the properties ($\Delta 1$)–($\Delta 7$) can directly be deduced from the special structure of Δ , Δ^B , and of the vectors Y , U , and β^{D_l} , $1 \leq l \leq n$, and the matrix Δ is a singular M-Matrix [6, 8, 26]. The proof is essentially similar to that of the unmagnetized case and we refer to [8] for more details. From the properties ($\Delta 1$)–($\Delta 7$) 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 Δ , Δ^B , and the vectors Y , U , and β^{D_l} , $1 \leq l \leq n$, satisfy the properties ($\Delta 1$)–($\Delta 7$). Then the n systems (5.4) are well posed, the matrix D^{\parallel} is symmetric and is the generalized inverse of Δ with prescribed range Y^{\perp} and prescribed nullspace $\mathbb{R}Y$, whereas the matrix $D^{\perp} + iD^{\odot}$ is symmetric and is the generalized inverse of $\Delta + i\Delta^B$ with prescribed range $Y^{\perp} + iY^{\perp}$ and nullspace $Y + iY$. The matrices D^{\parallel} and D^{\perp} are symmetric positive semi-definite and $N(D^{\parallel}) = N(D^{\perp}) = \mathbb{R}Y$. In addition, the diffusion matrices can be evaluated from $D^{\parallel} = (\Delta + aY \otimes Y)^{-1} - (1/a)U \otimes U$ and $D^{\perp} + iD^{\odot} = (\Delta + i\Delta^B + aY \otimes Y)^{-1} - (1/a)U \otimes U$ where $a > 0$ is arbitrary.*

Proof. The proof is similar to that of the unmagnetized case thanks to Propositions 2.3 and 2.1 and since $\beta^{D_l} \in R(\Delta) = U^{\perp}$ and we refer to [8] for more details. \square

A natural question arising from the decomposition (5.1), defined in terms of the unitary vector $\mathbf{B} = \mathbf{B}/B$, is the smoothness of the diffusion velocities as the magnetic field goes to zero. Upon introducing the tensorial transport coefficients D_{ij} , $1 \leq i, j \leq n$, defined by

$$D_{ij} = D_{ij}^{\parallel} \mathbf{B} \otimes \mathbf{B} + D_{ij}^{\perp} (\mathbf{I} - \mathbf{B} \otimes \mathbf{B}) + D_{ij}^{\circ} \mathbf{R}(\mathbf{B}), \quad (5.9)$$

where $\mathbf{R}(\boldsymbol{\zeta})$ is the rotation matrix associated with the vector $\boldsymbol{\zeta}$, that is, $\mathbf{R}(\boldsymbol{\zeta})\boldsymbol{\xi} = \boldsymbol{\zeta} \wedge \boldsymbol{\xi}$, we obtain a compact formulation for the diffusion velocities

$$\mathbf{V}_i = - \sum_{1 \leq j \leq n} D_{ij} \mathbf{d}_j, \quad 1 \leq i \leq n, \quad (5.10)$$

and we have to investigate the smoothness of the 3×3 matrices D_{ij} . However, for any set of coefficients μ^{\parallel} , μ^{\perp} , and μ° , such that μ^{\parallel} is independent of B , $\mu^{\perp} - \mu^{\parallel} = B^2 \psi_{\mu}^{\perp}(B^2)$ and $\mu^{\circ} = B \psi_{\mu}^{\circ}(B^2)$, where the functions ψ_{μ}^{\perp} and ψ_{μ}° are smooth, we directly obtain that

$$\mu^{\parallel} \mathbf{B} \otimes \mathbf{B} + \mu^{\perp} (\mathbf{I} - \mathbf{B} \otimes \mathbf{B}) + \mu^{\circ} \mathbf{R}(\mathbf{B}) = \mu^{\parallel} \mathbf{I} + \psi_{\mu}^{\perp}(B^2) (B^2 \mathbf{I} - \mathbf{B} \otimes \mathbf{B}) + \psi_{\mu}^{\circ}(B^2) \mathbf{R}(\mathbf{B}),$$

since $\mathbf{B} = B \mathbf{B}$ so that $\mu^{\parallel} \mathbf{B} \otimes \mathbf{B} + \mu^{\perp} (\mathbf{I} - \mathbf{B} \otimes \mathbf{B}) + \mu^{\circ} \mathbf{R}(\mathbf{B})$ is smooth for any \mathbf{B} and converges towards $\mu^{\parallel} \mathbf{I}$ as $\mathbf{B} \rightarrow 0$. As a consequence, the smoothness of the species diffusion velocities as functions of the magnetic field \mathbf{B} is a consequence of the following Proposition.

Proposition 5.2. *Let D^{\parallel} , D^{\perp} , and D° , be defined from (5.8) where $\alpha^{D_l(1)}, \alpha^{D_l(2)}$, $1 \leq l \leq n$, are the solutions of the transport linear systems (5.4). Assume that only Δ^B depends on the magnetic field, being simply proportional to $B = \|\mathbf{B}\|$. Then D^{\parallel} is independent of B , $D^{\perp} - D^{\parallel} = B^2 \psi_D^{\perp}(B^2)$ and $D^{\circ} = B \psi_D^{\circ}(B^2)$ where the functions ψ_D^{\perp} and ψ_D° are smooth over $[0, \infty)$.*

Proof. We write $\Delta^B = B \widehat{\Delta}^B$ where $\widehat{\Delta}^B$ is independent of B and expand the diffusion matrices in series of B . Since $D^{\perp} + iD^{\circ} = (\Delta + i\Delta^B + Y \otimes Y)^{-1} - U \otimes U$ we can write

$$D^{\perp} + iD^{\circ} = (I + iB(\Delta + Y \otimes Y)^{-1} \widehat{\Delta}^B)^{-1} (\Delta + Y \otimes Y)^{-1} - U \otimes U.$$

Upon defining $H = -(\Delta + Y \otimes Y)^{-1} \widehat{\Delta}^B$ we deduce that for $B\|H\| < 1$ we have

$$D^{\perp} + iD^{\circ} = \sum_{0 \leq j < \infty} i^j B^j H^j (\Delta + Y \otimes Y)^{-1} - U \otimes U.$$

Since the zeroth-order term $(\Delta + Y \otimes Y)^{-1} - U \otimes U$ is precisely D^{\parallel} , we obtain that

$$D^{\perp} - D^{\parallel} = \sum_{1 \leq l < \infty} (-1)^l B^{2l} H^{2l} (\Delta + Y \otimes Y)^{-1}, \quad D^{\circ} = \sum_{0 \leq l < \infty} (-1)^l B^{2l+1} H^{2l+1} (\Delta + Y \otimes Y)^{-1}.$$

We may thus define for $s \in [0, 1/\|H\|^2)$

$$\psi_D^{\perp}(s) = \sum_{1 \leq l < \infty} (-1)^l s^{l-1} H^{2l} (\Delta + Y \otimes Y)^{-1}, \quad \psi_D^{\circ}(s) = \sum_{0 \leq l < \infty} (-1)^l s^l H^{2l+1} (\Delta + Y \otimes Y)^{-1},$$

and then D^{\parallel} is independent of B , $D^{\perp} - D^{\parallel} = B^2 \psi_D^{\perp}(B^2)$, $D^{\circ} = B \psi_D^{\circ}(B^2)$, and the functions ψ_D^{\perp} and ψ_D° are smooth over $[0, 1/\|H\|^2)$. Furthermore, whenever $B\|H\| \geq 1/2$ we may directly define $\psi_D^{\perp}(B^2) = (D^{\perp} - D^{\parallel})/B^2$ and $\psi_D^{\circ}(B^2) = D^{\circ}/B$ and the resulting functions ψ_D^{\perp} and ψ_D° are smooth over $[0, \infty)$ thanks to $D^{\perp} + iD^{\circ} = (\Delta + i\Delta^B + aY \otimes Y)^{-1} - (1/a)U \otimes U$ and the smoothness of $A \rightarrow A^{-1}$ over the open set of invertible matrices. \square

Projected standard iterative techniques as well as projected orthogonal residuals methods can be used to solve the constrained singular systems associated with the diffusion coefficients (5.4). Iterative techniques for the real transport linear systems associated with D^{\parallel} are similar to that of nonionized mixtures and have been investigated comprehensively [16, 6]. We thus only discuss in the following the evaluation by iterative techniques of the complex matrix $D^{\perp} + iD^{\circ}$ by solving the corresponding constrained linear systems (5.4). As a direct application of Theorem 3.3 we obtain indeed an asymptotic expansion for $D^{\perp} + iD^{\circ}$.

Theorem 5.3. Let $\Delta, \Delta^B \in \mathbb{R}^{n,n}$ be matrices, and $Y, U \in \mathbb{R}^n$, $\beta^{D_l} \in \mathbb{R}^n$, $1 \leq l \leq n$, be vectors satisfying the properties $(\Delta 1)$ – $(\Delta 7)$ and let $M = \text{diag}(M_1, \dots, M_n)$ be such that $M_k \geq \Delta_{kk}$, $1 \leq k \leq n$. Consider the splittings $\Delta = M - W$ and $\Delta + i\Delta^B = \mathcal{M} - \mathcal{W}$, where $\mathcal{M} = M + i\Delta^B$, the iteration matrices $T = M^{-1}W$, and $\mathcal{T} = \mathcal{M}^{-1}\mathcal{W}$, and let $\mathcal{P} = P = I - U \otimes Y$ denote the oblique projector matrix onto Y^\perp along $\mathbb{R}U$. Let $z_0^l \in \mathbb{R}^n$, $z_0^l = \mathcal{P}z_0^l$, and consider for $i \geq 0$ and $1 \leq l \leq n$ the iterates $z_{i+1}^l = \mathcal{T}z_i^l + M^{-1}\beta^{D_l}$ and $z_{i+1}^l = \mathcal{P}\mathcal{T}z_i^l + \mathcal{P}\mathcal{M}^{-1}\beta^{D_l}$. Then $z_i^l = \mathcal{P}z_i^l$ for all $i \geq 0$, the matrices T, \mathcal{T}, PT and $\mathcal{P}\mathcal{T}$ are convergent, $\rho(T) = \rho(\mathcal{T}) = 1$, $\gamma(T) = \rho(PT) < 1$, $\gamma(\mathcal{T}) = \rho(\mathcal{P}\mathcal{T}) < 1$, $\gamma(\mathcal{T}) \leq \gamma(T)$, and we have the following limits

$$\lim_{i \rightarrow \infty} z_i^l = P(\lim_{i \rightarrow \infty} z_i^l) = \alpha^{D_l(2)}, \quad 1 \leq l \leq n, \quad (5.11)$$

where $\alpha^{D_l(2)}$ is the unique solution of the (right) linear system of (5.4). Moreover, for $i \geq 1$, the matrix iterates

$$(D^\perp + iD^\odot)^{[2]} = \sum_{0 \leq j \leq i-1} (\mathcal{P}\mathcal{T})^j \mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t, \quad (5.12)$$

are symmetric, and converge as $i \rightarrow \infty$ towards $D^\perp + iD^\odot$, and we have the convergent asymptotic expansion

$$D^\perp + iD^\odot = \sum_{0 \leq j < \infty} (\mathcal{P}\mathcal{T})^j \mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t.$$

The interest of these algorithms is that they perform well whatever the intensity of the magnetic field since the complete matrix $i\Delta^B$ has been taken into account in the splitting matrix $M = \mathcal{D} + i\Delta^B$. They do not perform well, however, independently of the ionization degree and convergence rates deteriorate as ionization levels increase as investigated by García Muñoz in the unmagnetized case [15, 19]. The first approximation $(D^\perp + iD^\odot)^{[1]} = \mathcal{P}\mathcal{M}^{-1}\mathcal{P}$ generalizes the Hirschfelder-Curtiss approximation with a mass corrector [27, 16, 17] to the magnetized case. Upon using Proposition 3.8 and $\mathcal{P}U = 0$ we obtain the explicit formula

$$(D^\perp + iD^\odot)^{[1]} = \mathcal{E} + \frac{\mathcal{E}MU \otimes \mathcal{E}MU}{\langle (M - M\mathcal{E}M)U, U \rangle}, \quad (5.13)$$

where

$$\mathcal{E} = (M + iM^B)^{-1} - \frac{(M + iM^B)^{-1}Y \otimes (M + iM^B)^{-1}Y}{\langle (M + iM^B)^{-1}Y, Y \rangle}. \quad (5.14)$$

The second order approximation can further be written

$$(D^\perp + iD^\odot)^{[2]} = (D^\perp + iD^\odot)^{[1]} + (D^\perp + iD^\odot)^{[1]}(\mathcal{D} - \Delta)(D^\perp + iD^\odot)^{[1]}, \quad (5.15)$$

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

Remark 5.4. 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 [19]. These generalized complex Stefan-Maxwell equations are easily obtained by multiplying the complex transport linear systems (5.4) by $\mathbf{d}_l^\perp - i\mathbf{d}_l^\odot$ and by summing over $1 \leq l \leq n$. These equations are in the form

$$(\Delta + i\Delta^B)(\mathbf{V}^\perp - i\mathbf{V}^\odot) = \mathbf{d}^\perp - i\mathbf{d}^\odot - Y \sum_{1 \leq l \leq n} (\mathbf{d}_l^\perp - i\mathbf{d}_l^\odot), \quad (5.16)$$

with the constraint $\mathbf{V}^\perp - i\mathbf{V}^\odot \in Y^\perp + iY^\perp$, where $\mathbf{V}^\diamond = (\mathbf{V}_1^\diamond, \dots, \mathbf{V}_n^\diamond)$, $\mathbf{d}^\diamond = (\mathbf{d}_1^\diamond, \dots, \mathbf{d}_n^\diamond)$, $\diamond \in \{\perp, \odot\}$. Only the diffusion velocities are required when an explicit time marching technique is used to compute a multicomponent flow for instance. More generally, when fractional steps are used, the diffusion velocities are also sufficient—that is, the diffusion coefficient matrices are not needed—if the ‘diffusion step’ is taken to be explicit.

5.3 Application to thermal conductivities

The linear systems associated with the thermal conductivities are of size $n + p$ and are in the form

$$\Lambda\alpha^{\lambda(1)} = \beta^\lambda, \quad (\Lambda + i\Lambda^B)\alpha^{\lambda(2)} = \beta^\lambda, \quad (5.17)$$

where $\Lambda, \Lambda^B \in \mathbb{R}^{n+p, n+p}$, $\alpha^{\lambda(1)}, \beta^\lambda \in \mathbb{R}^{n+p}$, $\alpha^{\lambda(2)} \in \mathbb{C}^{n+p}$, and p is the number of polyatomic species. The matrix Λ is symmetric positive definite [6], Λ^B is a diagonal matrix [18, 19], and the thermal conductivities are given by the following scalar products

$$\lambda^\parallel = \frac{\bar{p}}{T} \langle \alpha^{\lambda(1)}, \beta^\lambda \rangle, \quad \lambda^\perp + i\lambda^\odot = \frac{\bar{p}}{T} \langle \alpha^{\lambda(2)}, \beta^\lambda \rangle. \quad (5.18)$$

The coefficients of Λ , Λ^B , and β^λ are intricated expressions involving thermodynamic properties, molecular parameters, collision integrals, and state variables that are omitted for the sake of simplicity [19].

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 Λ, Λ^B and the vector β^λ when $n \geq 3$ [6, 19] :

- ($\Lambda 1$) Λ is symmetric positive definite.
- ($\Lambda 2$) $2\text{diag}(\Lambda) - \Lambda$ is symmetric positive
- ($\Lambda 3$) Λ^B is symmetric.

From these structural assumptions, one easily establishes the following properties.

Proposition 5.5. *Let $\Lambda, \Lambda^B \in \mathbb{R}^{n+p, n+p}$ be matrices satisfying the properties ($\Lambda 1$)–($\Lambda 3$). Then the constrained linear systems (5.17) admits unique solutions $\alpha^{\lambda(1)}$ and $\alpha^{\lambda(2)}$. In addition the quantities λ^\parallel and λ^\perp defined by (5.18) are positive.*

Proof. This directly results from Proposition 2.3. □

The heat flux can be shown to be a smooth function of the magnetic field as for the diffusion velocities [19]. Preconditioned conjugate gradient techniques are especially suited to the solutions of the transport linear systems associated with the thermal conductivities (5.17) using the diagonal as a preconditionner.

5.4 Numerical experiments

In this section we perform numerical experiments illustrating the convergence results established in the previous sections. Numerical tests are performed for an eleven species mixture associated with weakly ionized air, at temperature $\bar{T} = 10000$ K, pressure $\bar{p} = 1$ atm, and magnetic field intensity $B = 10^{-3}$ Tesla [19]. The mixture is constituted by the $n = 11$ species N_2 , O_2 , NO , N , O , N_2^+ , O_2^+ , NO^+ , N^+ , O^+ and E^- , and is taken in the weakly ionized state $X_1 = X_2 = X_3 = X_4 = X_5 = 0.198$, $X_6 = X_7 = X_8 = X_9 = X_{10} = 0.001$, $X_{11} = X_E = 0.005$. The linear system coefficients are complex expressions of the state variables and involve species thermodynamic properties as well as molecular parameters describing the interaction between species pairs which are not given for brevity [6, 19]. For the numerical tests, the collision integrals have been evaluated from [31] and the thermodynamic properties taken from [21]. We have also varied the magnetic field by rescaling the imaginary parts of the transport linear systems (5.4) and (5.17).

We first consider the systems (5.4) of size $n = 11$ associated with the perpendicular and transverse diffusion matrices $D^\perp + iD^\odot$. We have evaluated the matrix iterates (5.12) obtained by using the splitting matrix $\mathcal{M} = \text{diag}(M_1, \dots, M_n) + i\Delta^B$ with $M_k = \Delta_{kk}/(1 - Y_k)$. The

i	$D, \text{SM1}$	$D, \text{SM2}$	V, CG	λ, CG
1	8.13E-3	1.71E-2	1.94E-1	1.74E-1
2	1.85E-3	6.00E-4	5.03E-2	4.45E-3
3	3.47E-4	2.44E-5	3.69E-3	1.24E-4
4	6.59E-5	1.18E-6	3.84E-4	5.80E-6
5	1.25E-5	6.50E-8	5.25E-6	1.35E-7
6	2.37E-6	3.71E-9	3.18E-7	2.76E-9
7	4.50E-7	2.15E-10	2.84E-8	1.87E-10
8	8.54E-8	1.25E-11	7.33E-11	4.43E-13

Table 1: Reduced errors for iterates in computing diffusion matrices and thermal conductivities perpendicular and transverse to the magnetic field in weakly ionized air at 10000K.

corresponding reduced errors $\|D^\perp + iD^\circ - (D^\perp + iD^\circ)^{[i]}\|/\|D^\perp + iD^\circ\|$, for $i = 1, \dots, 8$, are given in Table I, in the column labeled $D, \text{SM1}$. Similar reduced errors are presented in the column labeled $D, \text{SM2}$ for the large value $B = 10^3$ Tesla used in order to illustrate the dependence of the convergence rate on the magnetic field. These errors indicate a very good convergence behavior of the iterative scheme (5.12) for the diffusion matrix problem and the mixture considered. We also observe an improvement of the convergence history for larger values of the intensity of the magnetic field in agreement with Theorem 3.3. The second iterates $(D^\perp + iD^\circ)^{[2]}$ is fairly accurate and has a computational cost which still scales like $O(n^2)$ since no dense matrix multiplications are needed, although n^2 transport coefficients are evaluated. Nevertheless, convergence rates deteriorate as the ionization level X_E increases as was investigated by García Muñoz in the unmagnetized case [15, 19].

We have also tested the convergence of the orthogonal residuals algorithm for solving the generalized Stefan-Maxwell equations (5.16). We have used a typical gradient right member in the form $\beta = (\beta_1, \dots, \beta_n)$ where $\beta_i = \rho_i \zeta_i$, $1 \leq i \leq n$, associated with an applied electric field from the expression of the diffusion driving forces (5.3). The corresponding reduced errors are presented in Table I in the column labeled V, CG . Note that the particular choices used for temperature, pressure or magnetic field do not essentially influences the general behavior of the orthogonal residuals algorithm.

We have next considered the systems (5.17) of size $n+p = 17$ associated with the perpendicular and transverse thermal conductivities of the mixture. We have evaluated the first iterates of the orthogonal residuals method with the preconditioning matrix $M = \text{diag}(m_1, \dots, m_\omega)$ where $m_k = |\Lambda_{kk} + i\Lambda_{kk}^B|$, starting with $z_0 = 0$. The corresponding reduced errors $\|\alpha^\lambda - z_i\|/\|\alpha^\lambda\|$, for $i = 1, \dots, 8$, are given in Table I, in the column labeled λ, CG . These reduced errors reveal the better convergence behavior of the orthogonal residuals algorithm. The corresponding accuracies for the thermal conductivities are about the same as those for the vector iterates in such a way that a few iterates are generally sufficient.

References

- [1] A. Ben-Israel and T. N. E. Greville, Generalized inverses, theory and applications, New York, Wiley, 1974.

- [2] N. Béreux, Fast direct solvers for some complex symmetric block Toeplitz linear systems, *Lin. Alg. and App.*, **404** (2005) 193–222.
- [3] A. Bermann and R. J. Plemmons, Nonnegative matrices in the mathematical science, New York, Academic Press, 1979.
- [4] D. Bruno, C. Catalfamo, A. Laricchiuta, D. Giordano, and M. Capitelli, Convergence of Chapman-Enskog calculation of transport coefficients of magnetized Argon plasma, *Phys. Plasmas*, **13** (2006) 72307.1–72307.9.
- [5] S. Chapman and T. G. Cowling, The mathematical theory of non-uniform gases, Applied Mathematical Sciences, Cambridge University Press, Cambridge 1970.
- [6] A. Ern and V. Giovangigli, Multicomponent Transport Algorithms, Lecture Notes in Physics, New Series Monographs, **m 24**, Heidelberg, Springer-Verlag, 1994.
- [7] A. Ern and V. Giovangigli, Fast and accurate multicomponent transport property evaluation, *J. Comp. Phys.*, **120** (1995) 105–116.
- [8] A. Ern and V. Giovangigli, Projected iterative algorithms with application to multicomponent transport, *Lin. Alg. and App.*, **250** (1997) 289–315.
- [9] A. Ern and V. Giovangigli, EGlib server and User’s manual, <http://www.cmap.polytechnique.fr/www.eglib>.
- [10] V. Faber and T.A. Manteuffel, Necessary and sufficient conditions for the existence of a conjugate gradient method, *SIAM J. Num. Anal.*, **21** (1984) 352–362.
- [11] V. Faber and T.A. Manteuffel, Orthogonal error methods, *SIAM J. Num. Anal.*, **24** (1987) 170–187.
- [12] J. H. Ferziger and H. G. Kaper, Mathematical theory of transport processes in gases, North-Holland, 1972.
- [13] R.W. Freund, On Conjugate gradient type methods and Polynomial Preconditioners for a Class of Complex Non-Hertian Matrices, *Numer. Math.*, **57** (1990) 285–312.
- [14] R.W. Freund, Conjugate gradient type methods for linear systems with complex symmetric coefficient matrices, *SIAM J. Sci. Stat. Comp.*, **13** (1992) 425–448.
- [15] A. García Muñoz, Formulation of molecular diffusion in planetary atmospheres, *Plan. Space Sci.*, **55** (2007) 1414–1425.
- [16] V. Giovangigli, Convergent iterative methods for multicomponent diffusion, *Impact Comput. Sci. Eng.*, **3** (1991) 244–276.
- [17] V. Giovangigli, Multicomponent flow modeling, Birkhäuser, Boston 1999. Erratum at <http://cmap.polytechnique.fr/~giovangi>
- [18] V. Giovangigli and B. Graille, Kinetic theory of partially ionized reactive gas mixtures, *Physica A*, **327** (2003) 313–348.
- [19] V. Giovangigli and B. Graille, Kinetic theory of partially ionized reactive gas mixtures II, Internal Report CMAP 637, (submitted) (2008).
- [20] G.H. Golub and C.F. Van Loan, *Matric computations* The John Hopkins University Press, Baltimore, 1983.

- [21] R.N. Gupta, J.M. Yos, R.A. Thomson, and K. Lee, A review of reaction rates and thermodynamic and transport properties for an 11-Species model for chemical and thermal nonequilibrium calculations to 30000K, *NASA Ref. Pub.*, **1232** (1990).
- [22] M. R. Hestenes and E. Stiefel, Methods of conjugate gradients for solving linear systems, *J. Res. Nat. Bur. Standards*, **49** (1952) 409–436.
- [23] H. B. Keller, On the solution of singular and semidefinite linear systems by iteration, *SIAM J. Numer. Anal.*, **2** (1965) 281–290.
- [24] C. D. Meyer and R. J. Plemmons, Convergent powers of a matrix with applications to iterative methods for singular systems, *SIAM J. Numer. Anal.*, **14** (1977) 699–705.
- [25] M. Neumann and R. J. Plemmons, Convergent nonnegative matrices and iterative methods for consistent linear systems, *Numer. Math.*, **31** (1978) 265–279.
- [26] M. Neumann and R. J. Plemmons, Generalized inverse-positivity and splittings of M-matrices, *Lin. Alg. App.*, **23** (1979) 21–35.
- [27] E. S. Oran and J. P. Boris, Detailed modeling of combustion systems, *Prog. Energy Combust. Sci.*, **7** (1981) 1–72.
- [28] J. G. Lewis and R. R. Rehm, The numerical solution of a nonseparable elliptic partial differential equation by preconditioned conjugate gradients. *J. Res. Nat. Bur. Stand.*, **85** (1980) 367–390.
- [29] R. Oldenburger, Infinite powers of matrices and characteristic roots. *Duke Math J.*, **6** (1940) 357–361.
- [30] Y. Saad, Krylov subspace methods for solving large unsymmetric linear systems. *Math. Comp.*, **37** (1981) 105–126.
- [31] M.J. Wright, D. Bose, G.E. Palmer, and E. Levin, Recommended collision integrals for transport property computations, Part 1: Air species, *AIAA J.*, **43**, (2005) 2558–2564.