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Projected Iterative Algorithms With Application to Multicomponent Transport

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ABSTRACT

We investigate projected iterative algorithms for solving constrained symmetric singular linear systems. We discuss the symmetry of generalized inverses and investigate projected standard iterative methods as well as projected conjugate-gradient algorithms. Using a generalization of Stein's theorem for singular matrices, we obtain a new proof of Keller's theorem. We also strengthen a result from Neumann and Plemmons about the spectrum of iteration matrices. As an application, we consider the linear systems arising from the kinetic theory of gases and providing transport coefficients in multicomponent gas mixtures. We obtain low-cost accurate approximate expressions for the transport coefficients that can be used in multicomponent flow models. Typical examples for the species diffusion coefficients and the volume viscosity are presented. © *Elsevier Science Inc., 1997*

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1. INTRODUCTION

1.1. Transport Linear Systems

In multicomponent gas mixtures, the evaluation of transport coefficients —such as the species diffusion coefficients or the viscosity—requires solving linear systems derived from the kinetic theory of dilute gases. These linear systems arise from variational procedures used to solve approximately linear integral equations. These integral equations are, in turn, obtained from the Enskog-Chapman expansion and involve a linearized Boltzmann integral collision operator. For more details about the derivation of the transport linear systems, we refer to [3, 6, 5]. These systems are constrained singular systems in the form

$$\begin{aligned} G\alpha &= \beta, \\ \alpha &\in \mathscr{C}, \end{aligned} \tag{1.1}$$

where $G \in \mathbb{R}^{\omega, \omega}$ is a symmetric positive semidefinite matrix, $\alpha, \beta \in \mathbb{R}^{\omega}$ are vectors, and $\mathscr{C}$ is a linear subspace of $\mathbb{R}^{\omega}$. In some applications, there are ω 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 $\alpha \in \mathscr{C}$ 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 unique transport coefficient associated with the system (1.1), which is usually given by the scalar product

$$\mu = \langle \alpha, \beta \rangle. \tag{1.2}$$

This situation occurs with the volume viscosity coefficient for instance and will be referred to as the *scalar case*. In this situation the constraint is not strictly necessary, because any solution x of $Gx = \beta$ is such that $x - \alpha \in N(G)$ and thus yields the same transport coefficient $\mu = \langle x, \beta \rangle$, thanks to $\beta \in R(G) = N(G)^{\perp}$. However, if for practical purposes the expression (1.2) is replaced by $\mu = \langle \alpha, \beta' \rangle$, where $\beta' - \beta \in \mathscr{C}^{\perp}$, then the constraint on α is again required.

The authors have developed a theory of iterative algorithms for solving the linear systems arising from multicomponent transport [5]. A first step was to derive the mathematical structure and the properties of the linear systems directly from those of the original integral equations. Once these properties were obtained, it was then possible to use iterative techniques to obtain convergent iterative algorithms. As a result, the authors were able to expand the transport coefficients as convergent series. By truncating these series, rigorously derived, analytic approximations have been obtained for all the transport coefficients [5].

In this paper, we generalize the mathematical tools that have been used to investigate the constrained linear systems of multicomponent transport. We first relate the solution of (1.1) to generalized inverses naturally associated with the problem and investigate their symmetry. We then study the convergence of projected standard iterative methods and projected conjugate-gradient methods for solving the constrained singular system (1.1). The conjugate-gradient methods usually have better convergence behavior and should generally be preferred. However, as opposed to standard methods, they do not yield a linear dependence between the iterates and the second members, and this linear dependence turns out to be of fundamental importance in some applications, as for instance with the species diffusion coefficients. Thus, when this linear dependence is needed, only standard iterative methods can be used.

In some applications also, there exists a block structure of the transport linear systems such that the lower right block is diagonal and nonsingular. In this case, it is possible to consider the Schur complement of this lower right block and to use an iterative algorithm to solve the associated linear system of smaller size. Indeed, keeping in mind that each iteration mainly requires to form the product of the Schur complement with a vector, the corresponding computational costs are identical to those associated with the original system, thanks to the diagonal structure of the lower right block. As a consequence, we also investigate iterative techniques for Schur complements. Note, however, that the analysis of convergence is still valid when the lower right block is not diagonal.

We then present typical applications associated with the species diffusion coefficients and the volume viscosity in multicomponent mixtures. We also present numerical results concerning these coefficients for a mixture associated with metal-organic chemical vapor deposition reactors.

After some mathematical preliminaries in Section 1, we investigate in Section 2 the properties of generalized inverses. In Section 3, we then study the convergence of projected iterative algorithms. Finally, in Section 4, we present the applications together with the numerical results.

1.2. Notation and Preliminaries

We denote by $\mathbb{R}^{\omega}$ the ω-dimensional real space and by $\mathbb{R}^{\omega_1, \omega_2}$ the set of matrices with ω_1 rows and ω_2 columns. For a vector $x \in \mathbb{R}^{\omega}$, we denote by $x = (x_1, \dots, x_\omega)$ its components and by $\mathbb{R}x$ the subspace span(x). For $x, y \in \mathbb{R}^{\omega}$, $\langle x, y \rangle$ denotes the scalar product $\langle x, y \rangle = \sum_{k \in [1, \omega]} x_k y_k$ and

$\|x\| = \langle x, x\rangle^{1/2}$ the Euclidean norm of x. For a subspace S of $\mathbb{R}^{\omega}$, we denote by $S^{\perp}$ its orthogonal complement. If S_1 and S_2 are two complementary subspaces of $\mathbb{R}^{\omega}$, i.e., $S_1 \oplus S_2 = \mathbb{R}^{\omega}$, we denote by P_{S_1, S_2} the oblique projector onto the subspace S_1 along the subspace S_2. For $A \in \mathbb{R}^{\omega_1, \omega_2}$, we write

$$A = (A_{kl})_{k \in [1, \omega_1], l \in [1, \omega_2]}$$

for the entries of the matrix A, and A^t for 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 rank A. For $x, y \in \mathbb{R}^{\omega}$, $x \otimes y \in \mathbb{R}^{\omega, \omega}$ denotes the tensor-product matrix $x \otimes y = (x_k y_l)_{k, l \in [1, \omega]}$. The identity matrix is denoted by I, and $\mathrm{diag}(\lambda_1, \dots, \lambda_\omega)$ is the diagonal matrix with diagonal elements $\lambda_1, \dots, \lambda_\omega$. For a matrix $A \in \mathbb{R}^{\omega_1, \omega_2}$, we define

$$\mathrm{diag}(A) = (A_{kl}\delta_{kl})_{k \in [1, \omega_1], l \in [1, \omega_2]},$$

where δ_{kl} is the Kronecker symbol, and we denote by $\|A\|$ its Frobenius norm

$$\|A\| = \left(\sum_{k \in [1, \omega_1], l \in [1, \omega_2]} A_{kl}^2 \right)^{1/2}.$$

Finally, for a matrix $A \in \mathbb{R}^{\omega, \omega}$, we denote by Π_A the characteristic polynomial of A.

The following propositions can be found in [1, 2] and characterize generalized inverses with prescribed range and nullspace as well as group inverses.

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

PROPOSITION 1.2. *Let $G \in \mathbb{R}^{\omega, \omega}$ be a matrix such that $N(G) \oplus R(G) = \mathbb{R}^{\omega}$. Then there exists a unique matrix Z such that $GZG = G$, $ZGZ = Z$, and $GZ = ZG$. The matrix Z is called the group inverse of G and is denoted by $G^{\#}$. The group inverse is also the generalized inverse with prescribed range $R(G)$ and nullspace $N(G)$ and is also such that $GZ = ZG = P_{R(G), N(G)}$.*

For a matrix $T \in \mathbb{R}^{\omega,\omega}$, $\sigma(T)$ and $\rho(T)$ denote respectively the spectrum and the spectral radius of T, and we also define $\gamma(T) = \max\{|\lambda|; \lambda \in \sigma(T), \lambda \neq 1\}$. A matrix T is said to be convergent when $\lim_{i\to\infty} T^i$ exists, not necessarily being zero. This corresponds to the terminology of Neumann and Plemmons [13] as opposed to the more conventional terminology, where a matrix T is said to be convergent when $\lim_{i\to\infty} T^i = 0$. The following result [14, 13] characterizes convergent matrices.

PROPOSITION 1.3. *A matrix $T \in \mathbb{R}^{\omega,\omega}$ is convergent if and only if either $\rho(T) < 1$ or $\rho(T) = 1$, $1 \in \sigma(T)$, $\gamma(T) < 1$, and $(I - T)^{\#}$ exists, i.e., T has only elementary divisors corresponding to the eigenvalue* 1.

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

$$G = M - W \tag{1.3}$$

is a splitting if the matrix M is invertible. Following Ortega [15], this splitting is said to be P-regular if the matrix $M + W$ is positive definite. In order to solve the linear system

$$G\alpha = \beta, \tag{1.4}$$

where $\beta \in \mathbb{R}^{\omega}$, the splitting (1.3) induces the iterative scheme

$$x_{i+1} = Tx_i + M^{-1}\beta, \qquad i \geqslant 0, \tag{1.5}$$

where $T = M^{-1}W$. Assuming that $\beta \in R(G)$, we have $M^{-1}\beta \in R(I - T)$, and the behavior of the sequences of iterates (1.5) is given in Lemma 1.4, which can be found in [12, 2] except for misprints in the matrix E corrected in the recent version of [2].

LEMMA 1.4. *Let $T \in \mathbb{R}^{\omega,\omega}$, and let $z \in \mathbb{R}^{\omega}$ such that $z \in R(I - T)$. Then the iterative scheme $x_{i+1} = Tx_i + z$, $i \geqslant 0$, converges for any $x_0 \in \mathbb{R}^{\omega}$ if and only if T is convergent. In this situation, the limit $\lim_{i\to\infty} x_i = x_\infty$ is given by $x_\infty = (I - T)^{\#}z + Ex_0$, where $E = I - (I - T)(I - T)^{\#}$.*

2. CONSTRAINED SINGULAR SYSTEMS

2.1. *Well-Posedness*

We first investigate the 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 $G \in \mathbb{R}^{\omega,\omega}$ be a matrix, and let $\mathscr{C}$ be a subspace of $\mathbb{R}^{\omega}$. Then the constrained linear system* (1.1) *is well posed, i.e., admits a unique solution α for any $\beta \in R(G)$, if and only if $N(G) \oplus \mathscr{C} = \mathbb{R}^{\omega}$. In this situation, for any subspace S such that $R(G) \oplus S = \mathbb{R}^{\omega}$, the solution α can be written $\alpha = Z\beta$, where Z is the generalized inverse of G with prescribed range $\mathscr{C}$ and nullspace S.*

Proof. The proof is straightforward and is omitted. ∎

2.2. Symmetric Generalized Inverse

By using the symmetry property of the matrix G, it is possible to select a symmetric generalized inverse of G with prescribed range $\mathscr{C}$.

PROPOSITION 2.2. *Let $G \in \mathbb{R}^{\omega,\omega}$ be a singular symmetric positive semidefinite matrix, let $\mathscr{C}$ be a subspace of $\mathbb{R}^{\omega}$, and assume that $N(G) \oplus \mathscr{C} = \mathbb{R}^{\omega}$. Let Z be the generalized inverse of G with prescribed nullspace $N(Z) = \mathscr{C}^{\perp}$ and range $R(Z) = \mathscr{C}$. Then the matrix Z is symmetric, positive semidefinite, and positive definite on the subspace $R(G)$. It is the unique symmetric generalized inverse of G with range $\mathscr{C}$, that is, the unique symmetric matrix L such that $LGL = L$, $GLG = G$, and $R(L) = \mathscr{C}$. Furthermore, denoting by $u_1, \dots, u_p$ a basis of $N(G)$, where $p = \dim N(G) \geqslant 1$, there exist vectors $v_1, \dots, v_p$ spanning $\mathscr{C}^{\perp}$ such that $\langle v_i, u_j \rangle = \delta_{ij}$, $1 \leqslant i, j \leqslant p$, and for any positive numbers a_i, b_i, $1 \leqslant i \leqslant p$, such that $a_i b_i = 1$, $1 \leqslant i \leqslant p$, we have*

$$Z = \left(G + \sum_{i=1}^{p} a_i v_i \otimes v_i \right)^{-1} - \sum_{i=1}^{p} b_i u_i \otimes u_i, \tag{2.1}$$

where the matrix $G + \sum_{i=1}^{p} a_i v_i \otimes v_i$ is symmetric positive definite. Furthermore, for $\beta \in R(G)$, the solution α of (1.1) *obtained from Proposition* 2.1 *also satisfies the system*

$$\left(G + \sum_{i=1}^{p} a_i v_i \otimes v_i \right) \alpha = \beta, \tag{2.2}$$

and we also have

$$P_{\mathscr{C}, N(G)} = I - \sum_{i=1}^{p} u_i \otimes v_i. \tag{2.3}$$

Proof. From $N(G) \oplus \mathscr{C} = \mathbb{R}^{\omega}$ it is straightforward to obtain that $N(G)^{\perp} \oplus \mathscr{C}^{\perp} = \mathbb{R}^{\omega}$, so that $R(G) \oplus \mathscr{C}^{\perp} = \mathbb{R}^{\omega}$, since G is symmetric. The generalized inverse of G with prescribed range $\mathscr{C}$ and prescribed nullspace $\mathscr{C}^{\perp}$ is therefore well defined. Furthermore, from $GZG = G$, $ZGZ = Z$, $N(Z) = \mathscr{C}^{\perp}$, $R(Z) = \mathscr{C}$, and $G^t = G$, we first deduce that $GZ^tG = G$, $Z^tGZ^t = Z^t$, $N(Z^t) = \mathscr{C}^{\perp}$, and $R(Z^t) = \mathscr{C}$, since $R(Z^t) = N(Z)^{\perp}$ and $N(Z^t) = R(Z)^{\perp}$. From the uniqueness of the generalized inverse with prescribed range and nullspace, we deduce that $Z = Z^t$, i.e., Z is symmetric. Moreover, Z is positive semidefinite, since for $y \in \mathbb{R}^{\omega}$, we have $\langle y, Zy \rangle = \langle Zy, GZy \rangle \geqslant 0$ because $Z = ZGZ$, Z is symmetric, and G is positive semidefinite. We then deduce that Z is positive definite on $R(G)$, since this subspace is complementary to $N(Z)$. Any symmetric matrix L such that $LGL = L$, $GLG = G$, and $R(L) = \mathscr{C}$ also satisfies $N(L) = \mathscr{C}^{\perp}$ by symmetry and therefore coincides with Z. The vectors v_i, $1 \leqslant i \leqslant p$, with $p = \dim N(G)$ are then easily obtained by selecting for v_i a nonzero element in the one-dimensional subspace

$$\left[\operatorname{span}(u_1, \ldots, u_{i-1}, u_{i+1}, \ldots, u_p)\right]^{\perp} \cap \mathscr{C}^{\perp},$$

and by normalizing it. It is then easily shown that $P_{R(Z), N(G)} = I - \sum_{i=1}^{p} u_i \otimes v_i$ and $P_{R(G), N(Z)} = I - \sum_{i=1}^{p} v_i \otimes u_i$, which yields (2.3) and implies that $GZ = I - \sum_{i=1}^{p} v_i \otimes u_i$, and the formula (2.1) directly follows. The equation (2.2) is then a direct consequence of (2.1), since $\beta \in [N(G)]^{\perp}$. ■

2.3. *Schur Complements*

In some applications, there exists a block structure of the transport linear systems such that the lower right block is nonsingular. In that case, it is possible to consider the Schur complement of this lower right block and to use an iterative algorithm to solve the associated linear system of smaller size. This strategy is computationally interesting when the lower right block is diagonal, as discussed in Section 3.2.

Therefore, we assume in this section that $\mathbb{R}^{\omega} = \mathbb{R}^{\omega_1} \times \mathbb{R}^{\omega_2}$ with $\omega = \omega_1 + \omega_2$, and we consider the associated block decomposition of the symmetric matrix $G \in \mathbb{R}^{\omega, \omega}$

$$G = \begin{bmatrix} G^{11} & G^{12} \\ G^{21} & G^{22} \end{bmatrix}, \tag{2.4}$$

where $G^{11} \in \mathbb{R}^{\omega_1, \omega_1}$, $G^{12} \in \mathbb{R}^{\omega_1, \omega_2}$, $G^{21} \in \mathbb{R}^{\omega_2, \omega_1}$, $G^{22} \in \mathbb{R}^{\omega_2, \omega_2}$. Each vector $x \in \mathbb{R}^{\omega}$ is correspondingly decomposed into $x = (x^1, x^2)$, $x^1 \in \mathbb{R}^{\omega_1}$,

$x^2 \in \mathbb{R}^{\omega_2}$. Finally, we assume that the submatrix G^{22} is nonsingular, and we denote by $G_{[s]} \in \mathbb{R}^{\omega_1, \omega_1}$ its Schur complement

$$G_{[s]} = G^{11} - G^{12}(G^{22})^{-1}G^{21}. \tag{2.5}$$

LEMMA 2.3. *Let $G \in \mathbb{R}^{\omega,\omega}$ be a singular symmetric positive semidefinite matrix, and let $\beta \in R(G)$. Let $\mathscr{C}$ be a subspace of $\mathbb{R}^{\omega}$ such that $N(G) \oplus \mathscr{C} = \mathbb{R}^{\omega}$, and denote by $v_1, \ldots, v_p$ a basis of $\mathscr{C}^{\perp}$ where $p =$ dim $N(G) \geqslant 1$. Define next $v_{[s]i} = v_i^1 - G^{12}(G^{22})^{-1}v_i^2$, $1 \leqslant i \leqslant p$, $\mathscr{C}_{[s]} =$ [span$(v_{[s]1}, \ldots, v_{[s]p})]^{\perp}$, and $\beta_{[s]} = \beta^1 - G^{12}(G^{22})^{-1}\beta^2$. Then the matrix $G_{[s]}$ is singular symmetric positive semidefinite, and the constrained linear system*

$$\begin{aligned} G_{[s]}\alpha_{[s]} &= \beta_{[s]}, \\ \alpha_{[s]} &\in \mathscr{C}_{[s]} \end{aligned} \tag{2.6}$$

is well posed, that is, $\beta_{[s]} \in R(G_{[s]})$ and $N(G_{[s]}) \oplus \mathscr{C}_{[s]} = \mathbb{R}^{\omega_1}$. Moreover, denoting by $\alpha_{[s]}$ and α the unique solutions of (2.6) *and* (1.1), *respectively, we have $\alpha^1 - \alpha_{[s]} \in N(G_{[s]})$, so that we have*

$$\mu = \langle \alpha_{[s]}, \beta_{[s]} \rangle + \left\langle (G^{22})^{-1}\beta^2, \beta^2 \right\rangle, \tag{2.7}$$

where $\mu = \langle \alpha, \beta \rangle$.

Proof. The proof—lengthy but straightforward—is omitted. ∎

3. PROJECTED ITERATIVE ALGORITHMS

3.1. Generalized Inverses and 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 will be important for some of our applications, in particular for the matrix of species diffusion coefficients.

For a given splitting $G = M - W$ and for $\beta \in R(G)$, assuming that the iteration matrix $T = M^{-1}W$ is convergent, the iterates (1.5) will converge for any x_0. When the matrix G is singular, we have $\rho(T) = 1$, since $Tx = x$ for $x \in N(G)$, and neither the iterates $\{x_i;\ i \geqslant 0\}$ nor the limit x_∞ are guaranteed to be in the constraint space $\mathscr{C}$. In order to overcome these difficulties, we investigate a projected iterative scheme in the form

$$y_{i+1} = PTy_i + PM^{-1}\beta, \qquad i \geqslant 0, \tag{3.1}$$

where $P = P_{\mathscr{C}, N(G)}$ is the projector onto the subspace $\mathscr{C}$ along $N(G)$. This algorithm and its iteration matrix PT provide very useful tools for investigating the convergence properties of (1.5) and of its iteration matrix T. In addition all the corresponding iterates $\{y_i;\ i \geqslant 0\}$ 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. The projected iterative algorithms are thus interesting from both a theoretical and a practical point of view. These schemes were introduced in [7] when studying convergent iterative methods for multicomponent diffusion coefficients.

For the transport linear system (1.1), assuming that the splitting $G = M - W$ is P-regular, the convergence of the matrix T is obtained from Keller's theorem [10].

THEOREM 3.1 (Keller). *Let $G \in \mathbb{R}^{\omega, \omega}$ be a symmetric matrix, and let $G = M - W$ be a P-regular splitting. Then $T = M^{-1}W$ is convergent if and only if G is positive semidefinite.*

The spectral radius of the iteration matrix PT can then be estimated by using a result from Neumann and Plemmons [13].

THEOREM 3.2 (Neumann and Plemmons). *Let T be a matrix such that $(I - T)^{\#}$ exists, i.e., such that $R(I - T) \cap N(I - T) = \{0\}$. Let $\mathscr{C}$ be a subspace complementary to $N(I - T)$, i.e., such that $N(I - T) \oplus \mathscr{C} = \mathbb{R}^{\omega}$, and let P be the oblique projector onto the subspace $\mathscr{C}$ along $N(I - T)$. Then we have the relation*

$$\rho(PT) = \gamma(T). \tag{3.2}$$

Proof. Since $R(I - T) \cap N(I - T) = \{0\}$, the root subspace of T associated with the eigenvalue 1 is $N(I - T)$. Let P' denote the projection onto the join of all root subspaces of T associated with the eigenvalues other than 1 along the eigenspace of T associated with the eigenvalue 1. By definition of $\gamma(T)$, we have the relation $\gamma(T) = \rho(TP')$, and it is well known that P' commutes with T. One may also easily check that $PP' = P$ and $P'P = P'$, since $N(P) = N(P') = N(I - T)$. Keeping in mind that $\rho(AB) = \rho(BA)$

for any $A, B \in \mathbb{R}^{\omega,\omega}$, we now obtain that

$$\gamma(T) = \rho(TP') = \rho(TP'P) = \rho(PTP') = \rho(PP'T) = \rho(PT),$$

so that $\rho(PT) = \gamma(T)$. ∎

In this paper, we give new proofs of Theorems 3.1–3.2, and we strengthen (3.2) by establishing that the spectra of T and PT are essentially the same.

THEOREM 3.3. *Keep the assumptions of Theorem 3.2. Then*

$$\sigma(PT) = \begin{cases} [\sigma(T) \setminus \{1\}] \cup \{0\} & \text{if } N(I-T) \neq \{0\}, \\ \sigma(T) & \text{if } N(I-T) = \{0\}. \end{cases} \tag{3.3}$$

Furthermore, the matrices T and P satisfy the relation $PT = PTP$.

Our proof of Theorem 3.1 will use a generalization of Stein's theorem [16] to the case of singular matrices.

THEOREM 3.4. *A matrix T is convergent if and only if there exist two symmetric positive semidefinite matrices A and B such that $B = A - T^tAT$ and $N(A) = N(B) = N(I-T)$.*

We will first establish Theorem 3.3, then Theorem 3.4, and finally Theorem 3.1.

Proof of Theorem 3.3. We first note that $PTP = PT$, since for $z \in \mathscr{E}$ we have $Pz = z$, and for $z \in N(I-T)$ we obtain $Tz = z$ and $Pz = 0$, so that PTP and PT coincide on $\mathscr{E}$ and $N(I-T)$ and hence on $\mathbb{R}^{\omega} = N(I-T) \oplus \mathscr{E}$. In the rest of the proof, we only consider the nontrivial case $P \neq I$, that is, the case $N(I-T) \neq \{0\}$.

Let now $\lambda \in \sigma(T)$ and $u \neq 0$ be such that $Tu = \lambda u$. Applying the projector P then yields $PTu = \lambda Pu$ and thus $PTv = \lambda v$ with $v = Pu$, thanks to $PTP = PT$. If $\lambda \neq 1$ then $v \neq 0$, since $v = 0$ implies $u \in N(P) = N(I - T)$, which yields $\lambda = 1$. We have thus shown that $\sigma(T) \setminus \{1\} \subset \sigma(PT)$ and we also have $0 \in \sigma(PT)$ because rank $PT \leqslant$ rank $P < \omega$, so that finally $[\sigma(T) \setminus \{1\}] \cup \{0\} \subset \sigma(PT)$.

Conversely, let $\lambda \in \sigma(PT)$ and $u \neq 0$ be such that $PTu = \lambda u$. All we have to show is that if $\lambda \neq 0$ then $\lambda \in \sigma(T)$ and $\lambda \neq 1$. Assuming that

$\lambda \neq 0$, we first obtain that $u = (1/\lambda)PTu \in \mathscr{C}$. Since $u \in \mathscr{C}$, we have $u = Pu$ and thus $PTu = \lambda Pu$, which yields $P(Tu - \lambda u) = 0$. As a consequence, we obtain that $Tu - \lambda u \in N(I - T)$, so that $(I - T)(T - \lambda I)u = 0$ and hence $(T - \lambda I)v = 0$ where $v = (I - T)u$.

We then note that $v = (I - T)u \neq 0$, since $v = 0$ yields $u \in N(I - T)$ and thus $u \in \mathscr{C} \cap N(I - T) = \{0\}$, contradicting $u \neq 0$. In addition, if $\lambda = 1$, then $v \in R(I - T) \cap N(I - T)$ and thus $v = 0$, since $(I - T)^{\#}$ exists, contradicting $v \neq 0$. Therefore, we have $v \neq 0$, $\lambda \neq 1$, and $(T - \lambda I)v = 0$, so that $\lambda \in \sigma(T) \setminus \{1\}$, and the proof is complete. ∎

REMARK 3.5. It is also possible to relate the characteristic polynomials of T and PT. More specifically, let w_i, $1 \leqslant i \leqslant \omega$, be a basis of $\mathbb{R}^\omega$ such that w_i, $1 \leqslant i \leqslant \omega - p$, is a basis $\mathscr{C}$ and w_i, $\omega - p + 1 \leqslant i \leqslant \omega$, is a basis of $N(I - T) = N(P)$ with $p = \dim[N(I - T)]$, and let $\mathscr{O}$ be the associated transformation matrix. Then the matrices $\mathscr{O}^{-1}T\mathscr{O}$ and $\mathscr{O}^{-1}PT\mathscr{O}$ admit the following block decompositions:

$$\mathscr{O}^{-1}T\mathscr{O} = \begin{pmatrix} \mathscr{T} & 0 \\ \mathscr{S} & I \end{pmatrix}, \qquad \mathscr{O}^{-1}PT\mathscr{O} = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \mathscr{T} & 0 \\ \mathscr{S} & I \end{pmatrix} = \begin{pmatrix} \mathscr{T} & 0 \\ 0 & 0 \end{pmatrix}.$$

which implies that $\Pi_T(\lambda) = \Pi_{\mathscr{T}}(\lambda)(1 - \lambda)^p$ and $\Pi_{PT}(\lambda) = \Pi_{\mathscr{T}}(\lambda)(-\lambda)^p$. We also note that $\Pi_{\mathscr{T}}(1) \neq 0$, since $(I - T)^{\#}$ exists.

Proof of Theorem 3.4. Assume first that there exist two symmetric positive semidefinite matrices A and B such that $B = A - T^tAT$ and $N(A) = N(B) = N(I - T)$. Consider any complementary space $\mathscr{C}$ to $N(I - T)$, and let P be the oblique projector onto the subspace $\mathscr{C}$ along $N(I - T)$. We then have $N(P) = N(I - T) = N(A) = N(B)$, so that in particular $A = AP = P^TA$, keeping in mind that A is symmetric, and thus we have $B = A - T^tAT = A - (PT)^tA(PT)$. Defining then $A' = A + (I - P)^t(I - P)$ and $B' = B + (I - P)^t(I - P)$, we obtain that $B' = A' - (PT)^tA'(PT)$ thanks to $(I - P)P = 0$. We remark now that both A' and B' are positive definite, since A, B and $(I - P)^t(I - P)$ are positive semidefinite, and since $N(I - P) = \mathscr{C}$ and $N(I - T) \cap \mathscr{C} = \{0\}$. Applying now the nonsingular version of Stein's theorem [16], we deduce that $\rho(PT) < 1$.

When $P = I$, that is, when $I - T$ is regular, we get $\rho(T) = \rho(PT) < 1$ and T is thus convergent. In the strictly singular case, where $N(I - T)$ is nonzero, all we need to show is that $(I - T)^{\#}$ exists. Indeed, from Theorem 3.2 and $\rho(PT) < 1$, we will get that $\gamma(T) = \rho(PT) < 1$, and, using Proposition 1.3, this will prove that T is convergent. We have thus to establish that $N(I - T) \cap R(I - T) = \{0\}$. Arguing by contradiction, we assume that there exist $u \neq 0$ and $v \neq 0$ such that $Tv = v + u$ and $Tu = u$. Since $v \notin N(I - T)$, we note that $\langle Bv, v \rangle > 0$, since $N(B) = N(I - T)$, and that $u \in N(I - T)$ yields $Au = 0$. Furthermore, $\langle Bv, v \rangle = \langle Av, v \rangle - \langle ATv, Tv \rangle$, and using $Tv = v + u$, $Au = 0$, and the symmetry of A yields that $\langle ATv, Tv \rangle = \langle Av, v \rangle$, so that $\langle Bv, v \rangle = 0$, an obvious contradiction, and we have thus shown that T is convergent.

Conversely, assume now that T is convergent. Consider any complementary space $\mathscr{E}$ to $N(I - T)$, and let P be the oblique projector onto the subspace $\mathscr{E}$ along $N(I - T)$. Since T is convergent, we know from Theorems 3.2 and 3.3 that $\rho(PT) < 1$. From the nonsingular version of Stein's theorem, we know that there exist two symmetric positive definite matrices A' and B' such that $B' = A' - (PT)^t A'(PT)$. We now let $A = P^t A' P$ and $B = P^t B' P$, and we have $B = A - T^t AT$ thanks to $PT = PTP$ from Theorem 3.3. Finally, A and B are symmetric positive semidefinite, and we have $N(A) = N(B) = N(P) = N(I - T)$, and the proof is complete. ∎

Proof of Theorem 3.1. Assume first that G is positive semidefinite. Consider any complementary space $\mathscr{E}$ to $N(I - T) = N(G)$, and let P be the oblique projector onto the subspace $\mathscr{E}$ along $N(I - T)$. Defining then $A = G$ and $B = A - T^t AT$, we note that A and B are symmetric and that A is positive semidefinite. On the other hand, since $T = I - M^{-1}G$, we also get after some algebra

$$B = (M^{-1}G)^t (M^t + W)(M^{-1}G).$$

Noting that $M^t + W$ is positive definite with $M + W$, we see that the matrix in the right-hand side is positive semidefinite and A and B have kernel $N(A) = N(B) = N(G) = N(I - T)$. Applying Theorem 3.4, we conclude that T is convergent.

Conversely, assuming now that T is convergent, we have to show that G is positive semidefinite. Proceeding as in the first part of the proof, we introduce a complementary space $\mathscr{E}$ to $N(I - T)$ and the corresponding projector P. Using Theorems 3.2 and 3.3, we then have $\rho(PT) < 1$. Defining again $B = G - T^t GT$, we still have $GP = P^t G = G$, so that $B = G - (PT)^t G(PT)$. On the other hand, from $T = I - M^{-1}G$ we again have $B = (M^{-1}G)^t (M^t + W)(M^{-1}G)$, and thus $B = G - (PT)^t G(PT)$ is positive semidefinite. An easy induction then yields that $G - [(PT)^m]^t G(PT)^m$ is positive semidefinite for all $m \geqslant 0$. Using now $\rho(PT) < 1$, which implies that $\lim_{m \to \infty} (PT)^m = 0$, and passing to the limit $m \to \infty$, we get that G is positive semidefinite, as was to be shown, and the proof is complete. ∎

We now investigate the convergence and properties of projected iterative algorithms.

THEOREM 3.6. *Let $G \in \mathbb{R}^{\omega,\omega}$ be a singular symmetric positive semidefinite matrix, and let $\mathscr{C}$ be a subspace complementary to $N(G)$, i.e., $N(G) \oplus \mathscr{C} = \mathbb{R}^{\omega}$. Consider a P-regular splitting $G = M - W$, assume that M is symmetric, and define $T = M^{-1}W$. Let P be the oblique projector onto the subspace $\mathscr{C}$ along $N(G)$. Let also $\beta \in R(G)$, $x_0 \in \mathbb{R}^{\omega}$, $y_0 = Px_0$, and consider for $i \geqslant 0$ the iterates $x_{i+1} = Tx_i + M^{-1}\beta$ as in* (1.5) *and $y_{i+1} = PTy_i + PM^{-1}\beta$ as in* (3.1). *Then $y_i = Px_i$ for all $i \geqslant 0$, the matrices T and PT are convergent, $\rho(T) = 1$, $\rho(PT) = \gamma(T) < 1$, and we have the following limits:*

$$\lim_{i\to\infty} y_i = P\Big(\lim_{i\to\infty} x_i\Big) = \alpha, \tag{3.4}$$

where α is the unique solution of (1.1). *Moreover, for all $i \geqslant 0$, each partial sum*

$$Z_i = \sum_{j=0}^{i} (PT)^j PM^{-1}P^t \tag{3.5}$$

is symmetric, is positive semidefinite, is positive definite on $R(G)$, and admits nullspace $N(Z_i) = \mathscr{C}^{\perp}$ and range $R(Z_i) = \mathscr{C}$. In addition, we have

$$Z = \sum_{j=0}^{\infty} (PT)^j PM^{-1}P^t, \tag{3.6}$$

where Z is the symmetric generalized inverse of G with prescribed nullspace $N(Z) = \mathscr{C}^{\perp}$ and range $R(Z) = \mathscr{C}$. Furthermore, the quantities $\mu_{[i]} = \langle Z_i\beta, \beta\rangle$ are positive for $i \geqslant 0$ if $\beta \neq 0$, and we have

$$\lim_{i\to\infty} \mu_{[i]} = \langle Z\beta, \beta\rangle = \langle \alpha, \beta\rangle = \mu. \tag{3.7}$$

Proof. From Theorems 3.1 and 3.3 we first obtain that T is convergent and that $\rho(PT) = \gamma(T) < 1$. Furthermore, from $\beta \in R(G)$, we deduce that $M^{-1}\beta \in R(I - T)$, and since T is convergent, the sequence $\{x_i;\ i \geqslant 0\}$ is then convergent by Lemma 1.4. In addition, since $\rho(PT) < 1$, we deduce that the sequence $\{y_i;\ i \geqslant 0\}$ is also convergent. From Theorem 3.3 we also have $PTP = PT$, and we then deduce by induction that $y_i = Px_i$ for all $i \geqslant 0$. Consequently, we have $\lim_{i\to\infty} y_i = P(\lim_{i\to\infty} x_i)$, and denoting by α this limit, we have $\alpha \in \mathscr{E}$. Moreover, from the relation $GP = G$ and (1.5), we easily deduce that $G\alpha = G(\lim_{i\to\infty} x_i) = \beta$, and therefore α is the unique solution of (1.1). Furthermore, since $\beta \in R(G)$, we obtain by induction that $y_{i+1} = Z_i\beta$ for the particular choice $y_0 = 0$, and from Proposition 2.1 we also deduce that $\alpha = Z\beta$, where Z is the generalized inverse of G with prescribed nullspace $N(Z) = \mathscr{E}^\perp$ and range $R(Z) = \mathscr{E}$. Since $\lim_{i\to\infty} y_i = \alpha$, we obtain $\alpha = Z\beta = \sum_{j=0}^{\infty}(PT)^jPM^{-1}P^t\beta$. The matrices Z and $\sum_{j=0}^{\infty}(PT)^jPM^{-1}P^t$ therefore coincide on $R(G)$. Furthermore, they trivially coincide on $\mathscr{E}^\perp$, and hence (3.6) is proven, since $R(G) \oplus \mathscr{E}^\perp = \mathbb{R}^\omega$.

Furthermore, from the relation $PTP = PT$, one can easily show by induction that $(PT)^jP = PT^j$ for all $j \geqslant 0$, and we also have $(T^jM^{-1})^t = T^jM^{-1}$ for all $j \geqslant 0$. Therefore, we can write $Z_i = \sum_{j=0}^{i} PT^jM^{-1}P^t$ and Z_i is thus symmetric. In addition, we have the relations

$$\langle PT^{2j}M^{-1}P^tz, z\rangle = \langle MT^jw, T^jw\rangle$$

for any $z \in \mathbb{R}^\omega$, where $w = M^{-1}P^tz$, and

$$\langle PT^{2j+1}M^{-1}P^tz, z\rangle + \langle PT^{2j}M^{-1}P^tz, z\rangle = \big\langle (M+W)T^jw, T^jw\big\rangle.$$

Thanks to the positive definiteness of M and $M + W$, these relations imply that for any $i \geqslant 1$ and $z \in \mathbb{R}^\omega$ we have

$$\langle Z_{2i}z, z\rangle \geqslant \langle Z_{2i-1}z, z\rangle,$$

and

$$\langle Z_{2i+1}z, z\rangle \geqslant \langle Z_{2i-1}z, z\rangle \geqslant \cdots \geqslant \langle Z_1z, z\rangle.$$

Since $\langle Z_1z, z\rangle = \langle (M+W)w, w\rangle$ and $\langle Z_0z, z\rangle = \langle Mw, w\rangle$ with $w = M^{-1}P^tz$, all the matrices Z_i, $i \geqslant 0$, are positive semidefinite. In addition, we have $\langle Z_iz, z\rangle = 0$ if an only if $w = 0$, which in turn is equivalent to $z \in \mathscr{E}^\perp$. This implies that $N(Z_i) = \mathscr{E}^\perp$ and that Z_i is positive definite on $R(G)$, since $R(G) \oplus \mathscr{E}^\perp = \mathbb{R}^\omega$. From the symmetry of Z_i, we next deduce that $R(Z_i) = \mathscr{E}$. In addition, the quantities$\langle Z_i\beta, \beta\rangle$, $i \geqslant 0$, are then positive if $\beta \neq 0$, since $\beta \in R(G)$. Finally, the limit (3.7) results from (3.6), since $\mu = \langle Z\beta, \beta\rangle$. ∎

REMARK 3.7. The projector P is needed for the convergence of the series (3.6). Indeed, although the partial sums Z_i in (3.5) can be rewritten in the form

$$Z_i = P\left(\sum_{j=0}^{i} T^j M^{-1}\right) P^t,$$

the series $\sum_{j=0}^{i} T^j M^{-1}$ has no limit, since $\sum_{j=0}^{i} T^j M^{-1}(Mu) = (i+1)u$ for $u \in N(G)$. Furthermore, in the vector case where all the components of the vector α are transport coefficients, any satisfactory approximation for these coefficients must also satisfy the physical constraint, so that the most interesting approximations are given by the projected iterates (3.1). On the other hand, note also that we have $Tz = z$ for $z \in N(G)$ and $M^{-1}\beta \in R(I-T)$, since $\beta \in R(G)$, so that $P_{N(G), R(I-T)} x_i = P_{N(G), R(I-T)} x_0$ for all $i \geqslant 0$.

REMARK 3.8. Assuming that the splitting matrix M is diagonal, or more generally such that forming the product of M^{-1} with a given vector only costs $O(\omega)$ flops, each iteration of the scheme (1.5) costs $\omega^2 + O(\omega)$ flops. Similarly, each iteration of (3.1) requires the same cost, thanks to the decomposition $P_{\mathscr{C}, N(G)} = I - \sum_{i=1}^{p} u_i \otimes v_i$ obtained in Proposition 2.2.

REMARK 3.9. Iterative methods applied to the regular formulation (2.2) usually converge more slowly than those applied to the singular formulation (1.1) [5]. Moreover, the corresponding iterates do not generally satisfy the constraint at each step, so that they cannot be used satisfactorily as approximate transport coefficients in the vector case.

REMARK 3.10. Various parts of Theorems 3.1 and 3.6 are still valid for nonsymmetric systems [5]. Indeed, let $G \in \mathbb{R}^{\omega,\omega}$ be a nonsymmetric matrix, let $G = M - W$ be a splitting, and assume that the matrix $T = M^{-1}W$ is convergent. Assume also that the subspaces $\mathscr{C}$ and S are such that $N(G) \oplus \mathscr{C} = \mathbb{R}^{\omega}$ and $R(G) \oplus S = \mathbb{R}^{\omega}$, and denote by P the oblique projector onto the subspace $\mathscr{C}$ along $N(G)$, and by Q the oblique projector onto $R(G)$ along the subspace S. Then we still have (3.2) and $Z = \sum_{j=0}^{\infty}(PT)^j PM^{-1}Q$, where Z is the generalized inverse of G with prescribed range $\mathscr{C}$ and nullspace S. In addition, if we denote by Z_i the partial sum $Z_i = \sum_{j=0}^{i}(PT)^j PM^{-1}Q$, then Z_i admits nullspace $N(Z_i) = S$ and range $R(Z_i) = \mathscr{C}$.

3.2. Schur Complements

We now investigate iterative methods for Schur complements of lower right diagonal nonsingular blocks. Consider a splitting matrix $M_{[s]}$ for the Schur complement $G_{[s]} = G^{11} - G^{12}(G^{22})^{-1}G^{21}$, which is diagonal or such that forming the product of $M_{[s]}^{-1}$ with a given vector only costs $O(\omega^1)$ flops. Then, an iteration for the Schur complement—projected or not—costs $\omega_1^2 + 2\omega_1\omega_2 + O(\omega) = \omega^2 - \omega_2^2 + O(\omega)$. This is exactly the cost of an iteration for the full matrix, as discussed in Remark 3.8, making use of the diagonal structure of the lower right block. As a consequence, it is also interesting to consider iterative methods for the Schur complement.

The convergence Theorem 3.1 can readily be applied to the system (3.6) associated $G_{[s]}$. In the next proposition, we relate the convergence properties of a splitting of the Schur complement to those of a special splitting of the original system (1.1). This splitting yields more zeros in the residual matrix and may thus lead to higher convergence rates. Note that this proposition does not require the lower right block G^{22} to be diagonal.

PROPOSITION 3.11. *Let $G \in \mathbb{R}^{\omega,\omega}$ be a symmetric positive semidefinite matrix; assume that G admits the block decomposition (2.4), and that the matrix G^{22} is nonsingular. Let $M_{[s]} \in \mathbb{R}^{\omega_1,\omega_1}$ be a symmetric positive definite matrix, and consider the splittings $G_{[s]} = M_{[s]} - W_{[s]}$ and $G = M - W$, where*

$$M = \begin{bmatrix} M_{[s]} & 0 \\ G^{21} & G^{22} \end{bmatrix}, \tag{3.8}$$

and the corresponding iteration matrices $T_{[s]} = (M_{[s]})^{-1}W_{[s]}$ and $T = M^{-1}W$. Then T is convergent if and only if $T_{[s]}$ is convergent, and $\rho(T_{[s]}) = \rho(T)$. In particular, if $2M_{[s]} - G^{11}$ is positive definite, then $T_{[s]}$ and T are convergent. Furthermore, consider the auxiliary system $Gz = \zeta$ with $\zeta^1 = \beta_{[s]}$ and $\zeta^2 = 0$, and the corresponding iterates $x_{[s]i} \in \mathbb{R}^{\omega_1}$ and $z_i \in \mathbb{R}^{\omega}$, $i \geqslant 0$, defined by $x_{[s]i+1} = T_{[s]}x_{[s]i} + (M_{[s]})^{-1}\beta_{[s]}$ and $z_{i+1} = Tz_i + M^{-1}\zeta$. Then for all $i \geqslant 0$, we have the relations $z_i^1 = x_{[s]i}$ and $z_i^2 = \Pi z_i^1$ where $\Pi = -(G^{22})^{-1}G^{21}$.

Proof. We denote by $\mathscr{H}$ the subspace of $\mathbb{R}^{\omega}$ defined by

$$\mathscr{H} = \{x \in \mathbb{R}^{\omega},\, x^2 = \Pi x^1\},$$

and by ϕ the application $\phi:\mathscr{H}\to\mathbb{R}^{\omega_1}$ such that $\phi(x)=x^1$. Notice that ϕ is an isomorphism and that $\phi^{-1}(x^1)=(x^1,\Pi x^1)$. On the other hand, a direct calculation yields that

$$M^{-1}W=\begin{bmatrix}(M_{[s]})^{-1}(M_{[s]}-G^{11}) & -(M_{[s]})^{-1}G^{12}\\ \Pi(M_{[s]})^{-1}(M_{[s]}-G^{11}) & -\Pi(M_{[s]})^{-1}G^{12}\end{bmatrix},$$

which implies—after some algebra—that $\phi T\phi^{-1}=T_{[s]}$. This shows that $T_{[s]}$ is convergent if and only if $\phi T\phi^{-1}$ is convergent. In addition, it is readily seen that $R(T)\subset\mathscr{H}$, so that we also have $\phi^{-1}\phi T=T$. As a consequence, we have $T^i=\phi^{-1}(\phi T\phi^{-1})^i\phi T$, and $\phi T\phi^{-1}$ is convergent if and only if T is convergent. In addition, since $R(T)\subset\mathscr{H}$, it is easily shown that T has the same spectral radius as its restriction to $\mathscr{H}$, and since $\phi T\phi^{-1}=T_{[s]}$, we obtain that $\rho(T)=\rho(T_{[s]})$. An easy calculation then yields that the matrix $M+W^t$ admits the block decomposition

$$M+W^t=\begin{bmatrix}2M_{[s]}-G^{11} & 0\\ 0 & G^{22}\end{bmatrix},$$

which shows that if $2M_{[s]}-G^{11}$ is positive definite, then $M+W^t$ is positive definite and thus $M+W$ also, and therefore T and $T_{[s]}$ are convergent from Theorem 3.1. Finally, considering the iterates for the Schur complement $\{x_{[s]i};\ i\geqslant 0\}$ and for the auxiliary system $\{z_i;\ i\geqslant 0\}$, the relations $z_i^1=x_{[s]i}$ and $z_i^2=\Pi z_i^1$ are easily established by induction. ■

3.3. *Conjugate-Gradient Methods for Constrained Systems*

In this section we introduce a projected conjugate-gradient method for positive semidefinite systems which extends the results of Lewis and Rehm [11]. This projected conjugate-gradient method usually has better convergence behavior than the projected standard method and should generally be preferred. However, the corresponding iterates depend nonlinearly on the right member β because of the quadratic nature of the conjugate-gradient algorithm. This prevents its use in some special situations, as for instance with the species diffusion coefficients.

THEOREM 3.12. *Let $G\in\mathbb{R}^{\omega,\omega}$ be a symmetric positive semidefinite matrix, and let $M\in\mathbb{R}^{\omega,\omega}$ be a symmetric positive definite matrix. Let $\mathscr{C}$ be a subspace complementary to $N(G)$, i.e., $N(G)\oplus\mathscr{C}=\mathbb{R}^{\omega}$; let P be the* *oblique projector onto the subspace $\mathscr{C}$ along $N(G)$; and let $\beta \in R(G)$. Let also $x_0 \in \mathbb{R}^\omega$, $y_0 = Px_0$, $r_0 = \beta - Gx_0$, $p_0 = 0$, $t_0 = 0$, and consider for $i \geqslant 0$ the iterates*

$$\begin{aligned} p_{i+1} &= M^{-1}r_i + t_i p_i, \\ s_{i+1} &= \langle r_i, M^{-1}r_i \rangle / \langle p_{i+1}, Gp_{i+1} \rangle, \\ x_{i+1} &= x_i + s_{i+1} p_{i+1}, \\ y_{i+1} &= y_i + P(s_{i+1} p_{i+1}), \\ r_{i+1} &= r_i - s_{i+1} G p_{i+1}, \\ t_{i+1} &= \langle r_{i+1}, M^{-1} r_{i+1} \rangle / \langle r_i, M^{-1} r_i \rangle. \end{aligned} \tag{3.9}$$

Then $y_i = Px_i$ for all $i \geqslant 0$, and the sequence of iterates y_i converges towards the unique solution of (1.1) *in at most* rank G *steps. Furthermore, if $x_0 = 0$ and $\beta \neq 0$, the quantities $\mu_{[i]} = \langle y_i, \beta \rangle = \langle x_i, \beta \rangle$ are positive for all $i \geqslant 1$ and converge towards $\mu = \langle \alpha, \beta \rangle$ in at most* rank G *steps.*

Proof. First, we can easily show by induction that we have $y_i = Px_i$ and that $r_i = \beta - Gy_i = \beta - Gx_i$, $i \geqslant 0$, since $GP = G$. One can also prove by induction that the orthogonality relations [9, 8]

$$\begin{aligned} \langle M^{-1}r_i, r_j \rangle &= 0, \qquad i \neq j, \\ \langle p_i, Gp_j \rangle &= 0, \qquad i \neq j, \\ \langle r_i, p_j \rangle &= 0, \qquad i \geqslant j, \end{aligned} \tag{3.10}$$

are still valid when G is positive semidefinite. From these relations, we can deduce that the iterates y_i converge towards α in at most rank G steps, since the vectors r_i are all in $R(G)$. Furthermore, we have $\langle y_i, \beta \rangle = \langle x_i, \beta \rangle$, since $y_i = Px_i$ and $P^t\beta = \beta$. Assuming then that $x_0 = 0$ and $\beta \neq 0$, we have

$$\mu_{[1]} = \frac{\langle M^{-1}\beta, \beta \rangle^2}{\langle M^{-1}\beta, GM^{-1}\beta \rangle} > 0,$$

since G and M are positive definite. For $i \geqslant 1$, we also obtain $\mu_{[i+1]} = \mu_{[i]} + s_{i+1}\langle p_{i+1}, \beta \rangle$ and $\langle p_{i+1}, \beta \rangle = \langle p_{i+1}, r_0 \rangle = t_i \langle p_i, \beta \rangle$, using the relation $\langle M^{-1}r_i, r_0\rangle = 0$ valid for $i \geqslant 1$. Finally, since $\langle p_1, \beta\rangle \geqslant 0$, we get by induction that $\langle p_{i+1}, \beta\rangle \geqslant 0$ for $i \geqslant 1$, which implies that $\mu_{[i]} \geqslant \cdots \geqslant \mu_{[1]} > 0$ for all $i \geqslant 1$. ∎

REMARK 3.13. A breakdown in (3.9) can only occur if convergence is already achieved. Indeed, assuming that $\langle p_{i+1}, Gp_{i+1}\rangle = 0$, We first obtain that $p_{i+1} \in N(G)$, but, on the other hand, we deduce from the relations $p_{j+1} = M^{-1}r_j + t_j p_j$, valid for $j = 0, \dots, i$, that $Mp_{i+1} \in R(G)$. This yields $\langle p_{i+1}, Mp_{i+1}\rangle = 0$, since $N(G) = R(G)^{\perp}$; and since M is positive definite, we obtain that $p_{i+1} = 0$. We then deduce from the last orthogonality property in (3.10) and $p_{i+1} = 0$ that $\langle r_i, M^{-1}r_i\rangle = 0$, i.e., $r_i = 0$, as was to be shown.

REMARK 3.14. The conjugate-gradient algorithm (3.9) can also be applied to Schur complements of lower right diagonal nonsingular blocks. In this situation, the computational costs associated with the two systems are identical, but the size of the Schur complement is smaller and may thus lead to faster convergence, as illustrated in Section 4.

4. APPLICATION TO MULTICOMPONENT TRANSPORT

4.1. *Transport Coefficients in Multicomponent Gas Mixtures*

The equations governing multicomponent gas laminar flows are derived from the kinetic theory of dilute gases and express the conservation of mass, momentum, and energy. These equations contain the terms for transport fluxes, that is, the pressure tensor, the species diffusion velocities, and the heat flux vector [3, 6, 5]. In this paper, we will only consider the pressure tensor $\mathscr{P}$ and the species diffusion velocities V_k, $k \in [1, n] = \{1, \dots, n\}$, where n is the number of species in the mixture. These fluxes can be written in the form

$$\mathscr{P} = \bar{p}I - \left(\kappa - \tfrac{2}{3}\eta\right)(\nabla \cdot v)I - \eta\left[\nabla v + (\nabla v)^t\right], \tag{4.1}$$

$$V_k = -\sum_{l \in [1, n]} D_{kl}\left[\nabla X_l + (X_l - Y_l)\nabla \log \bar{p} + \chi_l \nabla \log \bar{T}\right], \tag{4.2}$$

where $\bar{p}$ is the thermodynamic pressure, I the identity matrix, κ the volume viscosity, η the shear viscosity, ∇ the space derivative operator, v the flow velocity, $D = (D_{kl})_{k,l \in [1,n]}$ the diffusion matrix, X_k the mole fraction of the kth species, Y_k the mass fraction of the kth species, $\chi = (\chi_k)_{k \in [1,n]}$ the thermal diffusion ratios, and $\overline{T}$ the absolute temperature. The transport coefficients, that is, the volume viscosity κ, the shear viscosity η, the diffusion matrix D, and the thermal diffusion ratios χ, are functions of the state variables $(\overline{T}, \overline{p}, Y_1, \dots, Y_n)$.

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 [3, 6, 5]. On the other hand, solving these linear systems by direct methods may become computationally expensive, since their size can be large and since transport properties have to be evaluated at each computational cell in space and time. Consequently, the authors have developed a mathematical and numerical theory of iterative algorithms for solving the transport linear systems [5]. This theory has led to new cost-effective algorithms with which to evaluate transport properties in practical applications.

In the next sections, we discuss, in particular, the evaluation of the diffusion matrix and of the volume viscosity in a multicomponent gas mixture of n components. We assume in the following that $n \geqslant 3$ and that the state variables $(\overline{T}, \overline{p}, Y_1, \dots, Y_n)$ are given positive quantities. We also assume that the mass fractions satisfy the natural normalization condition $\sum_{k=1}^{n} Y_k = 1$.

4.2. *Application to the Diffusion Matrix*

The transport linear systems associated with the evaluation of the diffusion matrix D are the following n systems of size $\omega = n$ indexed by l, $1 \leqslant l \leqslant n$:

$$\begin{aligned} \Delta \alpha^{D_l} &= \beta^{D_l}, \\ \alpha^{D_l} &\in Y^{\perp}, \end{aligned} \tag{4.3}$$

where $\Delta \in \mathbb{R}^{n,n}$ and $\alpha^{D_l}, \beta^{D_l}, Y \in \mathbb{R}^n$ [5].

The coefficients of the transport linear systems are functions of the state variables $(\overline{T}, \overline{p}, Y_1, \dots, Y_n)$ which usually have complex expressions. In the particular case of the diffusion matrix, these expressions remain fairly simple and the matrix Δ is given by

$$\begin{aligned} \Delta_{kk} &= \sum_{\substack{l \in [1,n] \\ l \neq k}} \frac{X_k X_l}{\mathscr{D}_{kl}}, \qquad && k \in [1, n], \\ \Delta_{kl} &= -\frac{X_k X_l}{\mathscr{D}_{kl}}, && k, l \in [1, n], \quad k \neq l, \end{aligned} \tag{4.4}$$

where $\mathscr{D}_{kl}$ denotes the binary diffusion coefficient for the species pair (k, l), which only depends on temperature and pressure: $\mathscr{D}_{kl} = \mathscr{D}_{kl}(\overline{T}, \overline{p})$. The mole fractions can be expressed in terms of the mass fractions by the formulas

$$X_k = \frac{Y_k}{W_k}\left(\sum_{l\in[1,n]} \frac{Y_l}{W_l}\right)^{-1}, \qquad k \in [1, n], \tag{4.5}$$

where W_k, $k \in [1, n]$, are the species molecular weights, which are positive constants. The right members β^{D_l}, $l \in [1, n]$, are given by

$$\beta_k^{D_l} = \delta_{kl} - Y_k, \qquad k \in [1, n], \tag{4.6}$$

and the vector $Y \in \mathbb{R}^n$ is given by $Y = (Y_1, \ldots, Y_n)$. Finally, the diffusion coefficients D_{kl}, $k, l \in [1, n]$, are given by

$$D_{kl} = \alpha_k^{D_l}, \qquad k, l \in [1, n]. \tag{4.7}$$

The vectors α^{D_l}, $l \in [1, n]$, are therefore the column vectors of the diffusion matrix D, and we are exactly in the vector case for each column vector of D.

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 matrix Δ and the vectors Y and β^{D_l}, $l \in [1, n]$, when $n \geqslant 3$ [5]:

(Δ1) Δ is symmetric positive semidefinite and positive definite on $Y^{\perp}$.
(Δ2) $N(\Delta) = \mathbb{R}U$, where $U = (1, \ldots, 1)$.
(Δ3) $\langle Y, U\rangle \neq 0$.
(Δ4) $\beta^{D_l} \in R(\Delta)$, $l \in [1, n]$.
(Δ5) $2\,\mathrm{diag}(\Delta) - \Delta$ is symmetric positive definite.
(Δ6) $\mathrm{diag}(\Delta)$ is symmetric positive definite.

In our particular case, however, since the expressions for the linear system coefficients are fairly simple, these properties can also be obtained directly [7].

PROPOSITION 4.1. *Let W_k, $k \in [1, n]$, be positive numbers, let $\mathscr{D}_{kl}$ be positive numbers defined for $k, l \in [1, n]$, $k \neq l$, and symmetric, and assume that the mass fractions are positive. Then the matrix Δ and the vectors Y and β^{D_l}, $l \in [1, n]$, defined as in* (4.4)–(4.6) *satisfy properties* (Δ1)–(Δ6).

As an application of generalized inverses, we have the following characterization of the multicomponent diffusion matrix D.

PROPOSITION 4.2. *Assume that the matrix Δ and the vectors Y and β^{D_l}, $l \in [1, n]$, satisfy properties $(\Delta 1)$–$(\Delta 4)$. Then the n systems (4.3) are well posed. In addition, assume that the vectors β^{D_l} are given by (4.6). Then the matrix D defined by (4.7) is the generalized inverse of Δ with prescribed range $Y^{\perp}$ and prescribed nullspace $\mathbb{R}Y$. The matrix D is symmetric positive semidefinite and positive definite on $U^{\perp}$.*

Proof. From the properties of Δ it is easily seen that for each $l \in [1, n]$ the system (4.3) satisfies the assumptions of Proposition 2.1 and is well posed. From Proposition 2.2 the generalized inverse Z of Δ with prescribed range $Y^{\perp}$ and nullspace $\mathbb{R}Y$ is symmetric and positive definite on $U^{\perp}$. Assume now that the vectors β^{D_l}, $l \in [1, n]$, are given by (4.6). The column vectors $Z_{\cdot l} = (Z_{1l}, \dots, Z_{nl})$, $l \in [1, n]$, of Z are then easily seen to satisfy the system (4.3), since $\Delta Z = P_{U^{\perp}, \mathbb{R}Y}$. As a consequence, we have $Z_{\cdot l} = \alpha^{D_l}$, $l \in [1, n]$, and thus $Z_{kl} = \alpha_k^{D_l}$, $k, l \in [1, n]$, so that $D_{kl} = Z_{kl} = Z_{lk}$, $k, l \in [1, n]$, and the proof is complete. ∎

REMARK 4.3. The constraints in (4.3) imply that $\sum_{k=1}^{n} Y_k D_{kl} = 0$, $l \in [1, n]$, and thus that $\sum_{k=1}^{n} Y_k V_k = 0$, which is a mass conservation constraint for the species diffusion velocities [6, 7, 5]. The positive definiteness of D on $U^{\perp}$ also corresponds to the positiveness of the entropy-production quadratic form $d \to (\overline{p}/\overline{T})\langle Dd, d\rangle$ on the hyperplane of driving forces $U^{\perp}$ keeping in mind that for $d = (d_1, \dots, d_n)$ and $d_k = \nabla X_k + (X_k - Y_k)\nabla \log \overline{p} + \chi_k \nabla \log \overline{T}$, we have $d \in U^{\perp}$ thanks to $\sum_{k \in [1,n]} X_k = 1$, $\sum_{k \in [1,n]} Y_k = 1$, and $\sum_{k \in [1,n]} \chi_k = 0$ [6, 7, 5].

By applying now Theorem 3.6 to the multicomponent diffusion problem (4.3), and by using the linear properties of standard iterative techniques, we obtain an asymptotic expansion for the diffusion matrix D.

THEOREM 4.4. *Let $\Delta \in \mathbb{R}^{n,n}$ be a matrix satisfying properties $(\Delta 1)$–$(\Delta 6)$, and let $M = \operatorname{diag}(M_1, \dots, M_n)$ be such that $M_k \geqslant \Delta_{kk}$, $k \in [1, n]$. Consider the splitting $\Delta = M - W$ and the iteration matrix $T = M^{-1}W$, and let $P = I - U \otimes Y/\langle U, Y\rangle$ denote the oblique projector onto $Y^{\perp}$ along $\mathbb{R}U$. Let $x_0^l \in \mathbb{R}^n$, $y_0^l = Px_0^l$, and consider for $i \geqslant 0$ and $l \in [1, n]$*

the iterates $x_{i+1}^l = Tx_i^l + M^{-1}\beta^{D_l}$ *and* $y_{i+1}^l = PTy_i^l + PM^{-1}\beta^{D_l}$. *Then* $y_i^l = Px_i^l$ *for all* $i \geqslant 0$, *the matrices* T *and* PT *are convergent*, $\rho(T) = 1$, $\rho(PT) < 1$, *and we have the following limits*:

$$\lim_{i \to \infty} y_i^l = P\Big(\lim_{i \to \infty} x_i^l\Big) = \alpha^{D_l}, \qquad l \in [1, n], \tag{4.8}$$

where α^{D_l} *is the unique solution of* (4.3). *Moreover, for all* $i \geqslant 1$, *each partial sum*

$$D_{[i]} = \sum_{j=0}^{i-1} (PT)^j PM^{-1}P^t \tag{4.9}$$

is symmetric, is positive semidefinite, is positive definite on the hyperplane $U^\perp$, *and admits nullspace* $N(D_{[i]}) = \mathbb{R}Y$ *and range* $R(D_{[i]}) = Y^\perp$. *Finally, we have*

$$D = \lim_{i \to \infty} D_{[i]} = \sum_{j=0}^{\infty} (PT)^j PM^{-1}P^t. \tag{4.10}$$

REMARK 4.5. Note that each matrix iterate $D_{[i]}$ is symmetric, satisfies the mass conservation constraints $\sum_{k=1}^n Y_k D_{[i]kl} = 0$, $l \in [1, n]$, and yields a positive entropy-production quadratic form $d \to (\overline{p}/\overline{T})\langle D_{[i]}d, d\rangle$ on the hyperplane of driving forces $U^\perp$, as previously discussed for D in Remark 4.3.

REMARK 4.6. By using conjugate-gradient techniques, the resulting approximate diffusion matrices are not guaranteed to be symmetric or to yield a positive entropy production on the hyperplane of zero-sum driving forces, unless convergence is already achieved.

4.3. *Application to the Volume Viscosity*

The transport linear system associated with the evaluation of the volume viscosity is the system of size $\omega = n + p$

$$\begin{aligned} K\alpha^\kappa &= \beta^\kappa, \\ \alpha^\kappa &\in \mathscr{K}^\perp, \end{aligned} \tag{4.11}$$

where $K \in \mathbb{R}^{n+p,n+p}$, $\alpha^\kappa, \beta^\kappa, \mathscr{K} \in \mathbb{R}^{n+p}$, and p is the number of polyatomic species in the mixture [5]. In this section, we assume that $p \geqslant 1$, since the volume viscosity vanishes otherwise [6].

The coefficients of the matrix K and of the vectors $\mathscr{K}$ and β^{κ} are complex functions of the state variables involving collision integrals and will be omitted [5]. On the other hand, the volume viscosity is given by

$$\kappa = \langle \alpha^{\kappa}, \beta^{\kappa} \rangle, \tag{4.12}$$

which can be simplified into the relation

$$\kappa = \sum_{k \in [1, n]} X_k \alpha_k^{\kappa} \tag{4.13}$$

by explicitly using the constraint in (4.11).

Furthermore, there exists a natural block structure of the system (4.11) associated with the decomposition $\mathbb{R}^{\omega} = \mathbb{R}^{n} \times \mathbb{R}^{p}$, and we denote it by

$$K = \begin{bmatrix} K^{11} & K^{12} \\ K^{21} & K^{22} \end{bmatrix}. \tag{4.14}$$

We will also need the matrix $\mathrm{db}(K)$ constituted by the diagonals of the blocks of K,

$$\mathrm{db}(K) = \begin{bmatrix} \mathrm{diag}(K^{11}) & \mathrm{diag}(K^{12}) \\ \mathrm{diag}(K^{21}) & \mathrm{diag}(K^{22}) \end{bmatrix}. \tag{4.15}$$

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 matrix K and the vectors $\mathscr{K}$ and β^{κ} when $n \geqslant 3$ [5]:

($K1$) K is symmetric positive semidefinite and positive definite on $\mathscr{K}^{\perp}$.
($K2$) $N(K) = \mathbb{R}\mathscr{Y}$, where $\mathscr{Y} = (1, \dots, 1)$.
($K3$) $\langle \mathscr{K}, \mathscr{Y} \rangle \neq 0$.
($K4$) $\beta^{\kappa} \in R(K)$ and $\beta^{\kappa} \neq 0$.
($K5$) $2\,\mathrm{db}(K) - K$ is symmetric positive definite.
($K6$) $\mathrm{db}(K)$ is symmetric positive definite.

As a direct application of Proposition 2.1, we first obtain the following result.

PROPOSITION 4.6. *Let $K \in \mathbb{R}^{n+p,\,n+p}$ be a matrix satisfying properties ($K1$)–($K4$). Then the constrained linear system (4.11) admits a unique solution α^{κ}, and the quantity κ is positive.*

We now investigate the linear system of size n associated with the Schur complement $K_{[s]} = K^{11} - K^{12}(K^{22})^{-1}K^{21}$ of K^{22}. We will freely use the notation introduced in Section 2.3 and Section 3.2. We have in particular $\omega_1 = n$, $\omega_2 = p$, and we define $\mathscr{V}_{[s]} = \mathscr{V}^1$, $\mathscr{K}_{[s]} = \mathscr{K}^1 - K^{12}(K^{22})^{-1}\mathscr{K}^2$, and $\beta^{\kappa}_{[s]} = \beta^{\kappa 1} - K^{12}(K^{22})^{-1}\beta^{\kappa 2}$. In the following theorem, as a direct application of Lemma 2.3 and Proposition 3.11, we obtain a new expansion of the volume viscosity κ for multicomponent mixtures.

THEOREM 4.7. *Let $K \in \mathbb{R}^{n+p,n+p}$ be a matrix satisfying properties* $(K1)$–$(K6)$. *Let $M_{[s]} \in \mathbb{R}^{n,n}$ be the matrix $M_{[s]} = \operatorname{diag}(M_1, \dots, M_n)$ with $M_k \geq K^{11}_{kk}$, $k \in [1, n]$. Consider the splitting $K_{[s]} = M_{[s]} - W_{[s]}$ with the iteration matrix $T_{[s]} = (M_{[s]})^{-1}W_{[s]}$, and let $P_{[s]} = I - \mathscr{V}_{[s]} \otimes \mathscr{K}_{[s]}/\langle \mathscr{V}_{[s]}, \mathscr{K}_{[s]}\rangle$ denote the oblique projector onto $\mathscr{K}^{\perp}_{[s]}$ along $\mathbb{R}\mathscr{V}_{[s]}$. Then we have the expansion*

$$\kappa = \left\langle \sum_{j=0}^{\infty} (P_{[s]}T_{[s]})^j P_{[s]}(M_{[s]})^{-1}\beta^{\kappa}_{[s]}, \beta^{\kappa}_{[s]} \right\rangle + \left\langle (K^{22})^{-1}\beta^{\kappa 2}, \beta^{\kappa 2}\right\rangle. \quad (4.16)$$

4.4. Numerical Experiments

In this section we perform numerical experiments illustrating the convergence results established in the previous sections. Numerical tests are performed for a 22-species mixture associated with gallium arsenide chemical vapor deposition reactors, at temperature $\overline{T} = 1000$ K and pressure $\overline{p} = 1$ atm [4]. The mixture is constituted by the $n = 22$ species AsH_3, AsH_2, AsH, As, As_2, $Ga(CH_3)_3$, $Ga(CH_3)_2$, $GaCH_3$, Ga, CH_4, CH_3, CH_2, CH, C, H_2, H, C_2H_6, C_2H_5, C_2H_4, C_2H_3, C_2H_2, C_2H, and is taken in the equimolar state $X_k = 1/n$, $k \in [1, n]$. The linear system coefficients are complicated expressions in the state variables and involve molecular parameters describing the interaction between species pairs, which for brevity are not given [5].

We first considered the systems (4.3) associated with the evaluation of the species diffusion matrix. We evaluated the first matrix iterates (4.9) obtained by using the diagonal splitting $M = \operatorname{diag}(M_1, \dots, M_n)$ with $M_k = \Delta_{kk}/(1 - Y_k)$. This splitting is suggested by writing that $M^{-1}\Delta \approx D\Delta = P$ and by identifying the diagonal coefficients. The corresponding reduced errors $\|D - D_{[i]}\|/\|D\|$, for $i = 1, \dots, 10$, are given in Table 1, in the column labeled D, SM. These errors clearly indicate very good convergence behavior of the iterative scheme (3.1) for the diffusion matrix problem and the mixture considered. It is interesting to note, in particular, that the second iterate $D_{[2]}$ 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.

TABLE 1

REDUCED ERRORS FOR ITERATES IN COMPUTING DIFFUSION COEFFICIENTS AND VOLUME VISCOSITIES: GALLIUM ARSENIDE MIXTURE IN EQUIMOLAR STATE

i	D, SM	κ, SM	κ, CG	$\kappa_{[s]}$, CG
1	2.67E − 2	6.57E − 2	1.13E − 1	8.56E − 2
2	2.12E − 3	2.45E − 2	4.05E − 2	1.19E − 3
3	2.47E − 4	5.65E − 3	8.74E − 4	2.38E − 5
4	3.74E − 5	2.11E − 3	7.77E − 6	5.51E − 7
5	6.95E − 6	6.58E − 4	4.07E − 7	6.06E − 9
6	1.45E − 6	3.96E − 4	1.82E − 8	1.47E − 10
7	3.21E − 7	4.94E − 5	5.86E − 10	5.00E − 12
8	7.28E − 8	1.73E − 5	4.41E − 12	2.58E − 13
9	1.66E − 8	4.76E − 6	1.02E − 13	2.45E − 13
10	3.81E − 9	1.62E − 6	3.46E − 14	2.45E − 13

We then considered the system associated with the volume viscosity of the mixture. We evaluated the first iterates of the projected standard iterative method using the splitting $M = \mathrm{db}(K)$ and those of the projected conjugate-gradient method with the preconditioner $M = \mathrm{db}(K)$, starting with $x_0 = 0$. The corresponding reduced errors $\|\alpha^{\kappa} - y_i\|/\|\alpha^{\kappa}\|$, for $i = 1, \dots, 10$, are given in Table 1, in the columns labeled κ, SM and κ, CG, respectively. These reduced errors reveal the better convergence behavior of the conjugate-gradient algorithm. The corresponding accuracies for the volume viscosity are about the same as those for the vector iterates. Finally, we considered the Schur complement of the lower right block K^{22}, as described in Section 4.3. We have evaluated the first iterates of the projected conjugate-gradient method with the preconditioner $M = \mathrm{diag}(K_{[s]})$. The corresponding reduced errors $\|\alpha^{\kappa}_{[s]} - y_i\|/\|\alpha^{\kappa}_{[s]}\|$, for $i = 1, \dots, 10$, are given in Table 1, in the column labeled $\kappa_{[s]}$, CG. These reduced errors also indicate an excellent convergence rate. The accuracy of the iterates is also higher than that obtained with the full matrix.

REMARK 4.8. Similar results can be obtained for hydrogen and methane mixtures associated with combustion applications [5].

REMARK 4.9. The numerical tests only concern the multicomponent transport linear systems. In these applications, the size of the systems is not very large, but these systems have to be solved at each computational cell in space and time in numerical models of multicomponent flows. As a consequence, iterative methods provide a low-cost alternative to direct methods.

However, because of the modest size of these linear systems, the numerical experiments cannot be extrapolated to other applications involving much larger matrices. In addition, no attempts have been made to investigate error propagation due to numerical roundoff in the projected algorithms.

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