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MULTICOMPONENT TRANSPORT ALGORITHMS FOR PARTIALLY IONIZED PLASMAS

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Abstract

We investigate iterative methods for solving transport linear systems of partially ionized plasmas. We consider the situations of weak and strong magnetic fields as well as nonequilibrium and the linear systems are investigated in their natural constrained singular symmetric form. Stationary iterative techniques are considered with a new more singular formulation of the transport linear systems as well as orthogonal error algorithms. The more singular formulation is derived from an expansion of generalized inverses into dyadic products of conjugate directions. Numerical tests are performed with high temperature air and show that iterative techniques lead to fast and accurate evaluation of multicomponent transport coefficients for all ionization levels and magnetic field intensities. We obtain in particular low cost accurate approximations of multicomponent diffusion matrices in partially ionized plasmas.

1 Introduction

Ionized magnetized reactive gas mixtures have many practical applications such as laboratory plasmas, high-speed gas flows, lean flame stabilization or atmospheric phenomena [6, 10, 11, 13, 14, 23, 26, 53]. This motivates kinetic theory investigations and the derivation of macroscopic plasma equations. Applications of the Chapman-Enskog theory to partially ionized mixtures in weak and strong magnetic fields and in a regime where there is only one temperature have been discussed in particular by Chapman and Cowling [11], Ferziger and Kaper [23], Braginsky [6], Kaneko [38], Bruno, Capitelli and Dangola [8], for monatomic species, and Giovangigli and Graille [30, 32] for polyatomic species. Mixtures of monatomic gases at thermodynamic nonequilibrium with multitemperature transport arising from electron/ions mass ratio asymptotics have been investigated by Petit and Darrozes [52], Chmieleski and Ferziger [12], Braginsky [6, 7], Magin and Degrez [43] and a comprehensive multiscale kinetic theory has recently been presented by Graille, Magin and Massot [35].

The conservation equations for partially ionized plasmas derived in these various regimes involve transport fluxes, that is, diffusive mass fluxes, viscous tensors or heat fluxes. These transport fluxes, on the other hand, are expressed in terms of transport coefficients and macroscopic variable gradients. Detailed modeling of multicomponent plasmas thus requires the evaluation of transport coefficients which are functions of the state variables p, T, and $\mathrm{Y}_1, \ldots, \mathrm{Y}_n$ and of the intensity of the magnetic field B.

Evaluation of the transport coefficients, however, requires solving linear systems associated with linearized Boltzmann equations [11, 54, 23, 42, 8, 9, 30, 32, 35, 47]. The corresponding transport linear systems can be obtained in their natural constrained singular symmetric form for all the regimes considered [11, 54, 23, 30, 32, 35]. Since the size of these systems can be relatively large and since transport properties have to be evaluated at each computational cell in space and time, transport property evaluation by direct numerical inversions may become computationally expensive and the use of iterative techniques constitutes an interesting and appealing alternative.

A systematic development of a mathematical and numerical theory of iterative algorithms for evaluating transport coefficients of nonionized polyatomic gas mixtures has been given by Ern and Giovangigli [28, 15, 19]. Various algorithms have been proven to be convergent by using the mathematical properties of linearized Boltzmann collision operators, the structure of usual variational approximation spaces associated with species perturbed distribution functions, and the theory of iterative methods for constrained singular symmetric linear systems [28, 15, 19]. All transport coefficients have been

expressed as convergent series and the resulting algorithms have been found to be efficient especially for numerical simulation of multidimensional reactive flows with complex chemistry [15, 18, 17, 19, 20].

Extensions of these techniques to partially ionized mixtures have further been investigated by Giovangigli and Graille [30, 32, 33] in weak and strong magnetic fields and García Muñoz [26] for nonequilibrium planetary atmospheres. The linear systems in strong magnetic fields are then complex with an imaginary part proportional to the intensity of the magnetic field. Generalized conjugate gradient techniques as well as stationary iterative methods have been discussed [30, 32, 33]. Stationary methods for multicomponent diffusion matrices in multitemperature planetary atmospheres have also been investigated by García Muñoz [26]. The numerical experiments performed by García Muñoz [26] have shown in particular that the convergence rates of stationary iterative methods deteriorate as ionization levels increase. Similar results have been reported by Giovangigli and Graille who investigated transport coefficients in magnetized plasmas [32]. The purpose of this paper is now to derive new transport algorithms which converge rapidly for all ionization levels and magnetic field intensities and to perform comprehensive numerical tests with high temperature air to asses the accuracy of the resulting approximate coefficients.

We first review the mathematical structure of the transport linear systems in various regimes. We consider the situations of weak and strong magnetic fields as well as that of thermodynamic nonequilibrium. We subsequently discuss stationary iterative methods, generalized conjugate gradient techniques, and perform numerical tests with high temperature air.

For stationary methods, we discuss the solution of transport linear systems in terms of generalized inverses with prescribed range and nullspace [2, 4, 27, 28, 15, 19, 33] and present convergence theorems for constrained singular symmetric systems [39, 44, 48, 4, 41, 28, 19, 33]. We next introduce an expansion of symmetric generalized inverses into conjugate directions and recast the transport linear systems into *more singular* formulations. We similarly introduce an expansion of complex symmetric generalized inverses into conjugate directions—spanned by real vectors—and recast the magnetized transport linear systems into more singular formulations. These more singular formulations are then used to define new stationary algorithms. The main idea is that the more singular formulations will yield projected iterative algorithms with better convergence rates.

We next investigate generalized conjugate gradient techniques such as orthogonal residuals algorithms [37, 34, 41, 21, 22, 25, 24, 19, 33] and also discuss the link between the more singular formulations and search directions. It is found that the more singular formulations constrain the first search directions of orthogonal residuals algorithms. The difference between the conjugate expansion of complex symmetric matrices and Hermite type orthogonal residuals algorithms is also addressed.

Numerical experiments are performed with high temperature air for varying ionization levels and magnetic field intensities. The air mixture is constituted by the eleven species N_2, O_2, NO, N, O, N_2^+, O_2^+, NO^+, N^+, O^+, and e. Numerical tests are first conducted for stationary iterative techniques in order to evaluate first order and higher order multicomponent diffusion matrices. Both isotropic and magnetized nonisotropic mixtures are considered. The numerical experiments confirm the fast convergence rates of the new stationary algorithms for all ionization levels and magnetic field intensities. In particular, accurate low cost approximations are obtained for multicomponent diffusion matrices in partially ionized mixtures. Numerical tests are then performed with generalized conjugate gradient algorithms in order to evaluate thermal conductivities and species diffusion velocities for varying ionization levels and magnetic field intensities. The numerical tests confirm the good convergence rate of generalized conjugate gradient techniques independently of ionization levels and magnetic field intensities. The numerical tests with high temperature air thus show that iterative techniques lead to low cost accurate evaluations of multicomnent transport coefficients in partially ionized plasmas.

The transport linear systems and their mathematical structure is investigated in Sections 2 and 3 for isotropic and anisotropic mixtures, respectively, and in Section 4 for thermodynamic nonequilibrium. Stationary iteratives algorithms are investigated in Section 5 and generalized conjugate gradient algorithms in Section 6. Applications to diffusion matrices are presented in Section 7 and applications to thermal conductivities and Stefan-Maxwell equations in Section 8.

2 Transport linear systems in isotropic mixtures

We summarize in this section the transport fluxes and transport linear systems for polyatomic reactive gas mixtures at thermodynamic equilibrium in weak magnetic fields [54, 11, 23, 15, 30].

2.1 Transport fluxes

The transport fluxes derived from the kinetic theory of gases can be written in the form [11, 23, 54, 29]

$$\boldsymbol{\Pi} = -\kappa(\boldsymbol{\nabla}\cdot\boldsymbol{v})\boldsymbol{I} - \eta\big(\boldsymbol{\nabla}\boldsymbol{v} + (\boldsymbol{\nabla}\boldsymbol{v})^t - \tfrac{2}{3}\eta(\boldsymbol{\nabla}\cdot\boldsymbol{v})\boldsymbol{I}\big) \tag{2.1}$$

$$\mathbf{v}_i = -\sum_{j\in\mathcal{S}} D_{ij}\boldsymbol{d}_j - \theta_i\boldsymbol{\nabla}\log T, \qquad i\in\mathcal{S}, \tag{2.2}$$

$$\boldsymbol{q} = -\widehat{\lambda}\boldsymbol{\nabla}T - p\sum_{i\in\mathcal{S}}\theta_i\boldsymbol{d}_i + \sum_{i\in\mathcal{S}}\rho h_i \mathrm{Y}_i\mathbf{v}_i, \tag{2.3}$$

where $\boldsymbol{\Pi}$ denotes the viscous tensor, $\boldsymbol{\nabla} = (\partial_x, \partial_y, \partial_z)^t$ the usual differential operator, $\boldsymbol{I}$ the unit tensor in three dimensions, κ the volume viscosity, η the shear viscosity, $\boldsymbol{v}$ the mass averaged flow velocity, $\mathbf{v}_i$, $i\in\mathcal{S}$, the species diffusion velocities, D_{ij}, $i,j\in\mathcal{S}$, the multicomponent diffusion coefficients, $\boldsymbol{d}_i$, $i\in\mathcal{S}$, the species diffusion driving forces, θ_i, $i\in\mathcal{S}$, the species thermal diffusion coefficients, T the absolute temperature, $\mathcal{S} = \{1,\ldots,n^s\}$ the species indexing set, n^s the number of species, $\boldsymbol{q}$ the heat flux vector, $\widehat{\lambda}$ the partial thermal conductivity, p the pressure, ρ the density, h_i, $i\in\mathcal{S}$, the species enthalpy per unit mass, and Y_i, $i\in\mathcal{S}$, the species mass fractions. Note incidentally that the ratio κ/η is not small for polyatomic gases as taken for granted in most books on fluid dynamics and its impact is investigated in [5]. The vectors $\boldsymbol{d}_i$, $i\in\mathcal{S}$, incorporate the effects of various state variable gradients and external forces and are given by

$$\boldsymbol{d}_i = \frac{\boldsymbol{\nabla}p_i}{p} - \frac{n_i q_i}{p}(\boldsymbol{E} + \boldsymbol{v}\wedge\boldsymbol{B}), \qquad i\in\mathcal{S}, \tag{2.4}$$

where p_i, $i\in\mathcal{S}$, denotes the species partial pressures, n_i, $i\in\mathcal{S}$, the species molar densities, q_i, $i\in\mathcal{S}$, the species molar charges, $\boldsymbol{E}$ the electric field, and $\boldsymbol{B}$ the magnetic field. Alternatively, the diffusion velocities and the heat flux vector may be written in terms of the species thermal diffusion ratios χ_i, $i\in\mathcal{S}$, and the thermal conductivity λ [54]

$$\mathbf{v}_i = -\sum_{j\in\mathcal{S}} D_{ij}(\boldsymbol{d}_j + \chi_j\boldsymbol{\nabla}\log T), \qquad i\in\mathcal{S}, \tag{2.5}$$

$$\boldsymbol{q} = -\lambda\boldsymbol{\nabla}T + p\sum_{i\in\mathcal{S}}\chi_i\mathbf{v}_i + \sum_{i\in\mathcal{S}}\rho h_i\mathrm{Y}_i\mathbf{v}_i. \tag{2.6}$$

The various transport coefficients required in order to evaluate the transport fluxes are thus the volume viscosity κ, the shear viscosity η, the diffusion matrix $D = (D_{ij})_{i,j\in\mathcal{S}}$, and either the thermal diffusion vector $\theta = (\theta_1,\ldots,\theta_{n^s})^t$ and the partial thermal conductivity $\widehat{\lambda}$, or else the thermal diffusion ratios vector $\chi = (\chi_1,\ldots,\chi_{n^s})^t$, and the thermal conductivity λ. The corresponding governing equations expressing the conservation of species mass, momentum and energy are omitted for brevity and we refer to [11, 23, 54, 29] for more details.

2.2 Transport linear systems

The transport linear systems obtained from the kinetic theory take on either the nonsingular form

$$Ga = b, \tag{2.7}$$

or else the constrained singular form

$$\begin{cases} Ga = b, \\ \langle a, \mathrm{g}\rangle = 0, \end{cases} \tag{2.8}$$

where G denotes the system matrix, b the right-hand side, g the constraint vector and $\langle,\rangle$ the Euclidean scalar product [11, 54, 23, 15]. Both systems are typically associated with the evaluation of a transport coefficient $\mu = \langle a, b'\rangle$ where b' is a given vector.

System	Size	Constraint	Evaluation
$Ha^\eta = b^\eta$	n^s	—	$\eta = \langle a^\eta, b^\eta \rangle$
$Ka^\kappa = b^\kappa$	$n^s + n^p$	$\langle a^\kappa, \mathsf{k} \rangle = 0$	$\kappa = \langle a^\kappa, b^\kappa \rangle$
$K_{[01]} a^\kappa_{[01]} = b^\kappa_{[01]}$	n^p	—	$\kappa_{[01]} = \langle a^\kappa_{[01]}, b^\kappa_{[01]} \rangle$
$La^{D_k} = b^{D_k}$	$2n^s + n^p$	$\langle a^{D_k}, \mathcal{Y} \rangle = 0$	$D_{kl} = \langle a^{D_k}, b^{D_l} \rangle$
$L_{[\mathrm{e}]} a^{D_k}_{[\mathrm{e}]} = b^{D_k}_{[\mathrm{e}]}$	$2n^s$	$\langle a^{D_k}_{[\mathrm{e}]}, \mathcal{Y}_{[\mathrm{e}]} \rangle = 0$	$D_{[\mathrm{e}]kl} = \langle a^{D_k}_{[\mathrm{e}]}, b^{D_l}_{[\mathrm{e}]} \rangle$
$\Delta a^{D_k}_{[00]} = b^{D_k}_{[00]}$	n^s	$\langle a^{D_k}_{[00]}, \mathsf{y} \rangle = 0$	$D_{[00]kl} = \langle a^{D_k}_{[00]}, b^{D_l}_{[00]} \rangle$
$La^{\widehat{\lambda}} = b^{\widehat{\lambda}}$	$2n^s + n^p$	$\langle a^{\widehat{\lambda}}, \mathcal{Y} \rangle = 0$	$\widehat{\lambda} = (p/T) \langle a^{\widehat{\lambda}}, b^{\widehat{\lambda}} \rangle$ $\theta_k = -\langle a^{\widehat{\lambda}}, b^{D_k} \rangle$
$\Lambda a^\lambda = b^\lambda$	$n^s + n^p$	—	$\lambda = (p/T) \langle a^\lambda, b^\lambda \rangle$ $\chi = L^{00\lambda} a^\lambda$
$L_{[\mathrm{e}]} a^{\widehat{\lambda}}_{[\mathrm{e}]} = b^{\widehat{\lambda}}_{[\mathrm{e}]}$	$2n^s$	$\langle a^{\widehat{\lambda}}_{[\mathrm{e}]}, \mathcal{Y}_{[\mathrm{e}]} \rangle = 0$	$\widehat{\lambda}_{[\mathrm{e}]} = (p/T) \langle a^{\widehat{\lambda}}_{[\mathrm{e}]}, b^{\widehat{\lambda}}_{[\mathrm{e}]} \rangle$ $\theta_{[\mathrm{e}]k} = -\langle a^{\widehat{\lambda}}_{[\mathrm{e}]}, b^{D_k}_{[\mathrm{e}]} \rangle$
$\Lambda_{[\mathrm{e}]} a^\lambda_{[\mathrm{e}]} = b^\lambda_{[\mathrm{e}]}$	n^s	—	$\lambda_{[\mathrm{e}]} = (p/T) \langle a^\lambda_{[\mathrm{e}]}, b^\lambda_{[\mathrm{e}]} \rangle$ $\chi_{[\mathrm{e}]} = L^{00\lambda}_{[\mathrm{e}]} a^\lambda_{[\mathrm{e}]}$

Table 1: Typical transport linear systems for isotropic gases.

The transport linear systems are derived from a variational procedure used to solve constrained systems of linearized Boltzmann integral equations. For each transport coefficient, various transport linear systems can be considered, corresponding to different choices of the variational approximation space. The standard choices as well as some reduced transport linear systems are presented in Table 1. In this table, the first column contains the system $Ga = b$; the second, the size of the system n where n^s denotes the number of species and n^p denotes the number of polyatomic species in the mixture; the third, the constraint $\langle a, \mathsf{g} \rangle = 0$; and the last, the expression of the associated transport coefficient μ. The transport coefficients corresponding to the largest variational space have been denoted by μ, and the ones associated with a reduced variational space have been denoted by $\mu_{[\mathrm{x}]}$, where x stands for a simple symbol associated with the reduced variational space. The explicit expressions for all of the system matrices, right-hand sides, and constraint vectors can be found in [15].

For nonionized mixtures the reduced systems yield approximations for the transport coefficients which are generally within a few percent accuracy of the transport coefficients obtained with the standard systems [15, 18]. The accuracy of the corresponding coefficients deteriorates for ionized mixtures since the convergence of the Chapman-Enskog expansion is known to be slower [11, 23, 6, 10]. An extreme situation is that of the electrical conductivities which require higher order diffusion coefficients to compensate for the cancellation of significative digits [23, 6, 32].

2.3 Mathematical structure

We introduce some notation associated with the transport linear systems and then define the sparse transport matrix. For $x, y \in \mathbb{R}^n$, $x = (x_1, \ldots, x_n)^t$, $y = (y_1, \ldots, y_n)^t$, the scalar product $\langle x, y \rangle$ is given by $\langle x, y \rangle = \sum_{1 \le k \le n} x_k y_k$. For $x \in \mathbb{R}^n$, $x \neq 0$, we denote $x^\perp = \{\, y \in \mathbb{R}^n ; \langle x, y \rangle = 0 \,\}$. We denote by $\mathbb{R}^{n,n}$ the set of square matrices of size n, and for $G \in \mathbb{R}^{n,n}$, we write G^t the transpose of G, $N(G)$ the nullspace of G, and $R(G)$ the range of G. We denote $\mathbb{I}$ the unit tensor in $\mathbb{R}^{n,n}$ and for $x \in \mathbb{R}^n$, $\mathrm{diag}\big(x_1, \ldots, x_n\big)$ denotes the diagonal matrix of $\mathbb{R}^{n,n}$ whose diagonal elements are x_k, $1 \le k \le n$. For $x, y \in \mathbb{R}^n$, the tensor product matrix $x \otimes y$ is given by $x \otimes y = (x_k y_l)_{1 \le k,l \le n}$.

The sparse transport matrix $db(G)$ is a submatrix formed by diagonals of blocks of G. This matrix has been introduced in [15] and is important from a theoretical as well as practical point of view. It can be used as a splitting matrix for stationary methods as well as a preconditionner for generalized conjugate gradients algorithms. The definition of the matrix $db(G)$ is reminded in Appendix A.

The matrices G and $db(G)$ have a general mathematical structure inherited from the properties of Boltzmann linearized collision operators and the properties of usual variational approximation spaces

associated with the transport linear systems [15]. In order to simplify the presentation, we frequently assume in this paper that the number of species is $n^s \geq 3$. For the nonsingular systems, one can establish that

(G_1) *The matrices G, $2db(G) - G$, and $db(G)$ are symmetric positive definite for $n^s \geq 1$.*

On the other hand, for the singular systems, one can establish that

(G_2) *The matrix G is symmetric positive semi-definite and its nullspace is $N(G) = \mathbb{R}\mathsf{z}$. The nullspace vector z, the constraint vector g and the right member b are such that $\langle \mathsf{z}, \mathsf{g}\rangle \neq 0$ and $\langle \mathsf{z}, b\rangle = 0$. The matrices $2db(G) - G$ and $db(G)$ are symmetric positive definite for $n^s \geq 3$.*

The consequences of (G_1-G_2) are discussed in Section 5, and, in particular, the transport linear systems are well posed. The singular systems can also be recast into the nonsingular form $a = \big(G + \alpha \mathsf{g}\otimes\mathsf{g}\big)^{-1} b$ where $\alpha > 0$ and the matrix $G + \alpha\mathsf{g}\otimes\mathsf{g}$ is symmetric positive definite.

3 Transport linear systems in nonisotropic mixtures

We summarize in this section the transport fluxes and transport linear systems for polyatomic reactive gas mixtures at thermodynamic equilibrium in strong magnetic fields [11, 23, 6, 30, 32].

3.1 Transport fluxes

In the presence of strong magnetic fields, the transport fluxes are not anymore isotropic [11, 23, 6, 30, 32]. In order to express this anisotropy, we introduce some convenient notation. Denoting by $\boldsymbol{B}$ the magnetic field, $B = \|\boldsymbol{B}\|$ the magnetic field intensity, we define the unitary vector $\mathcal{B} = \boldsymbol{B}/B$ and for any three dimensional vector $\mathbf{x}$ the associated vectors

$$\mathbf{x}^{\parallel} = (\mathbf{x}\cdot\mathcal{B})\mathcal{B}, \qquad \mathbf{x}^{\perp} = \mathbf{x} - \mathbf{x}^{\parallel}, \qquad \mathbf{x}^{\odot} = \mathcal{B}\wedge\mathbf{x}.$$

The vectors $\mathbf{x}^{\parallel}$, $\mathbf{x}^{\perp}$ and $\mathbf{x}^{\odot}$ are mutually orthogonal and obtained from $\mathbf{x}$ by applying the linear operators $\mathcal{B}\otimes\mathcal{B}$, $\boldsymbol{I} - \mathcal{B}\otimes\mathcal{B}$ and $\boldsymbol{R}(\mathcal{B})$ where $\boldsymbol{R}(\mathcal{B})$ is the rotation matrix such that $\boldsymbol{R}(\mathcal{B})\mathbf{x} = \mathcal{B}\wedge\mathbf{x}$ for any vector $\mathbf{x}$.

In strong magnetic fields, the viscous tensor $\boldsymbol{\Pi}$ is found in the form

$$\begin{aligned}\boldsymbol{\Pi} \;=\; & -\kappa(\boldsymbol{\nabla}\cdot\boldsymbol{v})\,\boldsymbol{I} - \eta_1\mathbf{S} - \eta_2\big(\boldsymbol{R}(\mathcal{B})\,\mathbf{S} - \mathbf{S}\,\boldsymbol{R}(\mathcal{B})\big) - \eta_3\big(\mathcal{B}^t\mathbf{S}\mathcal{B}\,\mathcal{B}\otimes\mathcal{B} - \boldsymbol{R}(\mathcal{B})\,\mathbf{S}\,\boldsymbol{R}(\mathcal{B})\big)\\ & -\eta_4\big(\mathbf{S}\,\mathcal{B}\otimes\mathcal{B} + \mathcal{B}\otimes\mathcal{B}\,\mathbf{S} - 2\mathcal{B}^t\mathbf{S}\mathcal{B}\,\mathcal{B}\otimes\mathcal{B}\big) - \eta_5\big(\mathcal{B}\otimes\mathcal{B}\,\mathbf{S}\,\boldsymbol{R}(\mathcal{B}) - \boldsymbol{R}(\mathcal{B})\,\mathbf{S}\,\mathcal{B}\otimes\mathcal{B}\big), \qquad (3.1)\end{aligned}$$

where $\mathbf{S} = \boldsymbol{\nabla}\boldsymbol{v} + \boldsymbol{\nabla}\boldsymbol{v}^t - \frac{2}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{v})\,\boldsymbol{I}$, κ is the volume viscosity, and η_j, $1 \leq j \leq 5$, the shear viscosities. The species diffusion velocities $\mathbf{v}_i$, $i \in \mathcal{S}$, are found in the form

$$\mathbf{v}_i \;=\; -\sum_{j\in\mathcal{S}}\big(D_{ij}^{\parallel}\boldsymbol{d}_j^{\parallel} + D_{ij}^{\perp}\boldsymbol{d}_j^{\perp} + D_{ij}^{\odot}\boldsymbol{d}_j^{\odot}\big) - \big(\theta_i^{\parallel}(\boldsymbol{\nabla}\log T)^{\parallel} + \theta_i^{\perp}(\boldsymbol{\nabla}\log T)^{\perp} + \theta_i^{\odot}(\boldsymbol{\nabla}\log T)^{\odot}\big), \quad (3.2)$$

where $D_{ij}^{\parallel}$, $D_{ij}^{\perp}$, and $D_{ij}^{\odot}$, $i,j \in \mathcal{S}$, are the species diffusion coefficients parallel, perpendicular and transverse to the magnetic field, and $\theta_i^{\parallel}$, $\theta_i^{\perp}$, $\theta_i^{\odot}$, $i \in \mathcal{S}$, the species thermal diffusion coefficients parallel, perpendicular and transverse to the magnetic field. The heat flux $\boldsymbol{q}$ can be written similarly in the form

$$\boldsymbol{q} \;=\; -\big(\widehat{\lambda}^{\parallel}(\boldsymbol{\nabla}T)^{\parallel} + \widehat{\lambda}^{\perp}(\boldsymbol{\nabla}T)^{\perp} + \widehat{\lambda}^{\odot}(\boldsymbol{\nabla}T)^{\odot}\big) - p\sum_{i\in\mathcal{S}}\big(\theta_i^{\parallel}\boldsymbol{d}_i^{\parallel} + \theta_i^{\perp}\boldsymbol{d}_i^{\perp} + \theta_i^{\odot}\boldsymbol{d}_i^{\odot}\big) + \sum_{i\in\mathcal{S}}\rho_{\mathrm{Y}i}h_i\mathbf{v}_i, \quad (3.3)$$

where $\widehat{\lambda}^{\parallel}$, $\widehat{\lambda}^{\perp}$, and $\widehat{\lambda}^{\odot}$ are the partial thermal conductivities parallel, perpendicular and transverse to the magnetic field.

Systems	Size	Constraint	Coefficients
$Ha^{\eta 1} = b^{\eta}$ $(H + 2\mathrm{i}H')a^{\eta 2} = b^{\eta}$ $(H + \mathrm{i}H')a^{\eta 3} = b^{\eta}$	n^s	—	$\eta_1 + \mathrm{i}\eta_2 = \frac{1}{2}\langle a^{\eta 1} + a^{\eta 2}, b^{\eta}\rangle$ $\eta_1 + \eta_3 = \langle a^{\eta 1}, b^{\eta}\rangle$ $\eta_4 + \mathrm{i}\eta_5 + \eta_1 + \mathrm{i}\eta_2 = \langle a^{\eta 3}, b^{\eta}\rangle$
$(L + \mathrm{i}L')a^{D_j} = b^{D_j}$	$2n^s + n^p$	$\langle a^{D_j}, \mathscr{y}\rangle = 0$	$D^{\perp}_{ij} + \mathrm{i}D^{\odot}_{ij} = \langle a^{D_j}, b^{D_i}\rangle$
$(\Delta + \mathrm{i}\Delta')a^{D_j}_{[00]} = b^{D_j}_{[00]}$	n^s	$\langle a^{D_j}_{[00]}, \mathsf{y}\rangle = 0$	$D^{\perp}_{[00]ij} + \mathrm{i}D^{\odot}_{[00]ij} = \langle a^{D_j}_{[00]}, b^{D_i}_{[00]}\rangle$
$(L + \mathrm{i}L')a^{\widehat{\lambda}} = b^{\widehat{\lambda}}$	$2n^s + n^p$	$\langle a^{\widehat{\lambda}}, \mathscr{y}\rangle = 0$	$\widehat{\lambda}^{\perp} + \mathrm{i}\widehat{\lambda}^{\odot} = (p/T)\langle a^{\widehat{\lambda}}, b^{\widehat{\lambda}}\rangle$ $\theta^{\perp}_i + \mathrm{i}\theta^{\odot}_i = -\langle a^{\widehat{\lambda}}, b^{D_i}\rangle$
$(\Lambda + \mathrm{i}\Lambda')a^{\lambda} = b^{\lambda}$	$n^s + n^p$	—	$\lambda^{\perp} + \mathrm{i}\lambda^{\odot} = (p/T)\langle a^{\lambda}, b^{\lambda}\rangle$ $\chi^{\perp} + \mathrm{i}\chi^{\odot} = L^{00\lambda}a^{\lambda}$
$(\Lambda_{[\mathrm{e}]} + \mathrm{i}\Lambda'_{[\mathrm{e}]})a^{\lambda}_{[\mathrm{e}]} = b^{\lambda}_{[\mathrm{e}]}$	n^s	—	$\lambda^{\perp}_{[\mathrm{e}]} + \mathrm{i}\lambda^{\odot}_{[\mathrm{e}]} = (p/T)\langle \alpha^{\lambda}_{[\mathrm{e}]}, b^{\lambda}_{[\mathrm{e}]}\rangle$ $\chi^{\perp}_{[\mathrm{e}]} + \mathrm{i}\chi^{\odot}_{[\mathrm{e}]} = L^{00\lambda}_{[\mathrm{e}]}a^{\lambda}_{[\mathrm{e}]}$

Table 2: Typical Transport Linear Systems for nonisotrpic gases

The species diffusion velocities and the heat flux can also be rewritten in terms of the thermal diffusion ratios $\chi^{\parallel}_i$, $\chi^{\perp}_i$, and $\chi^{\odot}_i$, $i \in \mathcal{S}$, and the thermal conductivities $\lambda^{\parallel}$, $\lambda^{\perp}$, and $\lambda^{\odot}$ [30]

$$\begin{aligned}\mathbf{v}_i \,=\, &-\sum_{j\in\mathcal{S}} D^{\parallel}_{ij}\big(\boldsymbol{d}^{\parallel}_j + \chi^{\parallel}_j(\boldsymbol{\nabla}\log T)^{\parallel}\big) - \sum_{j\in\mathcal{S}} D^{\perp}_{ij}\big(\boldsymbol{d}^{\perp}_j + \chi^{\perp}_j(\boldsymbol{\nabla}\log T)^{\perp} + \chi^{\odot}_j(\boldsymbol{\nabla}\log T)^{\odot}\big)\\ &-\sum_{j\in\mathcal{S}} D^{\odot}_{ij}\big(\boldsymbol{d}^{\odot}_j + \chi^{\perp}_j(\boldsymbol{\nabla}\log T)^{\odot} - \chi^{\odot}_j(\boldsymbol{\nabla}\log T)^{\perp}\big),\end{aligned} \tag{3.4}$$

$$\boldsymbol{q} \,=\, -\big(\lambda^{\parallel}(\boldsymbol{\nabla}T)^{\parallel} + \lambda^{\perp}(\boldsymbol{\nabla}T)^{\perp} + \lambda^{\odot}(\boldsymbol{\nabla}T)^{\odot}\big) + p\sum_{i\in\mathcal{S}}(\chi^{\parallel}_i\mathbf{v}^{\parallel}_i + \chi^{\perp}_i\mathbf{v}^{\perp}_i + \chi^{\odot}_i\mathbf{v}^{\odot}_i) + \sum_{i\in\mathcal{S}}\rho_i\mathrm{Y}_i h_i\mathbf{v}_i. \tag{3.5}$$

3.2 Transport linear systems

The transport linear systems associated with transport coefficients parallel to the magnetic field are real and identical to that of isotropic mixtures already investigated in Section 2. These system are not further considered in this section. On the other hand, the tranport linear systems associated with anisotropic coefficients are complex, vector products with the magnetic field having been replaced by multiplications with imaginary numbers [23, 30]. The transport linear systems obtained from the kinetic theory take on either the regular form

$$(G + \mathrm{i}G')a = b, \tag{3.6}$$

or else the constrained singular form

$$\begin{cases}(G + \mathrm{i}G')a = b,\\ \langle a, \mathsf{g}\rangle = 0,\end{cases} \tag{3.7}$$

where $\mathrm{i}^2 = -1$, $G, G' \in \mathbb{R}^{n,n}$ denotes the system matrices, $b \in \mathbb{R}^n$ the right-hand side, $\mathsf{g} \in \mathbb{R}^n$ the constraint vector, and $\langle,\rangle$ the Hermitian scalar product. Both systems are typically associated with the evaluation of the transport coefficient $\mu^{\perp} + \mathrm{i}\mu^{\odot} = \langle a, b'\rangle$, where $b' \in \mathbb{R}^n$ is a given vector.

The transport linear systems corresponding to the first usual Sonine/Wang-Chang Uhlenbeck polynomial expansions are presented in Table 2. The successive approximations in the Chapman-Enskog expansion of transport coefficients are still known to converge more slowly in plasmas than in neutral mixtures [6, 8, 10]. Note that the variational framework for a direct evaluation of the thermal conductivity and the thermal diffusion ratios [16, 15] has been generalized to the anisotropic case [33].

3.3 Mathematical Structure

We introduce some notation associated with the complex transport linear systems. For $x, y \in \mathbb{C}^n$, $x = (x_1, \ldots, x_n)^t$, $y = (y_1, \ldots, y_n)^t$, the Hermitian scalar product $\langle x, y\rangle$ is given by $\langle x, y\rangle = \sum_{1\leq k\leq n} x_k \overline{y}_k$ and the nondegenerate nondefinite bilinear symmetric form (x, y) naturally associated with complex symmetric matrices is given is given by $(x, y) = \sum_{1\leq k\leq n} x_k y_k$. The real x and imaginary y parts $x, y \in \mathbb{R}$, of a complex number $z \in \mathbb{C}$, $z = x + \mathrm{i}y$, are written $x = \Re z$ and $y = \Im z$. When A is a real linear subspace $A \subset \mathbb{R}^n$, we denote by $A + \mathrm{i}A$ the corresponding complex linear space $\{z \in \mathbb{C}^n,\ z = x + \mathrm{i}y,\ x, y \in A\}$. If A is a real subspace, we denote by $A^\perp$ the orthogonal complement with respect to the Euclidean product whereas when B is a complex subspace, we denote by $B^\perp$ the orthogonal complement with respect to the nondegenerate bilinear form $(,)$. Note that if B has a basis of real vectors, the orthogonal complement is equivalently defined with the Hermitian scalar product. This is notably the case with the constraint $\langle a, \mathsf{g}\rangle = 0$ which can also be written $(a, \mathsf{g}) = 0$ since g is real. When $a, b \in \mathbb{C}^n$, the tensor product matrix $a{\otimes}b$ has components $a_k b_l$, $1 \leq k, l \leq n$ and for any $x \in \mathbb{C}^n$ we have $a{\otimes}b\ x = a(b, x)$.

The following results have been obtained from the properties of Boltzmann linearized operators under general assumptions on the variational approximation spaces [30, 32]. For the nonsingular systems, the matrix G satisfies (G_1) whereas the imaginary part is such that

(G_1') *The matrix G' is real diagonal.*

On the other hand, for the singular systems, the matrix G satisfies (G_2) wheras the imaginary part is such that

(G_2') *The matrix G' is real and given by $G' = Q\mathcal{D}'P$ where P and Q are the projector matrices $Q = P^t = I - \mathsf{g}{\otimes}\mathsf{z}/\langle \mathsf{z}, \mathsf{g}\rangle$ and $\mathcal{D}'$ is diagonal.*

Note that the matrix G' is symmetric and that $G'N(G) = 0$ in such a way that the nullspaces of G and G' are compatible [30, 32, 33]. The consequences of $(\mathsf{G}_1$-$\mathsf{G}_2)$ are investigated in Section 5. In particular, the transport linear systems are well posed, and the singular systems can also be cast into the nonsingular form $a = \big(G + \mathrm{i}G' + \alpha \mathsf{g}{\otimes}\mathsf{g}\big)^{-1} b$ where the matrix $G + \alpha \mathsf{g}{\otimes}\mathsf{g}$ is symmetric positive definite for any real number $\alpha > 0$ [15, 33].

4 Transport linear systems at thermodynamic nonequilibrium

We summarize in this section the transport fluxes and the transport linear systems in the situation of thermodynamic nonequilibrium. These results are obtained in a kinetic framework when both the Knudsen number and the electron mass simultaneously go to zero [35]. The species $\mathcal{S} = \mathcal{H} \cup \{\mathrm{e}\}$ must then be partitioned between the heavy species $\mathcal{H}$ and the electrons e and the proper convection velocity is the heavy species velocity $\boldsymbol{v}_h$ [35].

4.1 Heavy species transport fluxes

In the limit of zero electron mass, there is not anymore polarization effects for the heavy species and the corresponding transport fluxes can be written [35]

$$\boldsymbol{\Pi}_h = -\kappa(\boldsymbol{\nabla}{\cdot}\boldsymbol{v}_h)\boldsymbol{I} - \eta\big(\boldsymbol{\nabla}\boldsymbol{v}_h + (\boldsymbol{\nabla}\boldsymbol{v}_h)^t - \tfrac{2}{3}(\boldsymbol{\nabla}{\cdot}\boldsymbol{v}_h)\boldsymbol{I}\big), \tag{4.1}$$

$$\mathbf{v}_i = -\sum_{j\in\mathcal{H}} D_{ij}\widehat{\boldsymbol{d}}_j - \theta_i \boldsymbol{\nabla}\log T_h, \qquad i \in \mathcal{H}, \tag{4.2}$$

$$\boldsymbol{q}_h = -\widehat{\lambda}_h \boldsymbol{\nabla} T_h - p_h \sum_{i\in\mathcal{H}} \theta_{hi}\widehat{\boldsymbol{d}}_i + \sum_{i\in\mathcal{H}} \rho h_i \mathrm{Y}_i \mathbf{v}_i, \tag{4.3}$$

where $\boldsymbol{\Pi}_h$ is the heavy species viscous tensor, $\boldsymbol{I}$ the unit tensor in three dimensions, $\boldsymbol{v}_h$ the heavy species mass averaged flow velocity, $\mathbf{v}_i$, $i \in \mathcal{H}$, the heavy species diffusion velocities, $\widehat{\boldsymbol{d}}_i$, $i \in \mathcal{H}$, the heavy species effective diffusion driving forces, T_h the heavy species temperature, $\mathcal{H}$ the set of heavy species indices, $\boldsymbol{q}_h$ the heavy species heat flux, h_i, $i \in \mathcal{H}$, the heavy species enthalpy per unit mass,

and υ_i, $i \in \mathcal{H}$, the heavy species mass fractions. The vectors $\widehat{\boldsymbol{d}}_i$ incorporate the effects of various state variable gradients and external forces and are given by

$$\widehat{\boldsymbol{d}}_i = \frac{\boldsymbol{\nabla} p_i}{p_h} - \frac{n_i q_i}{p_h}(\boldsymbol{E} + \boldsymbol{v}_h \wedge \boldsymbol{B}) - \frac{n_i \boldsymbol{F}_{ie}}{p_h}, \qquad i \in \mathcal{H}, \tag{4.4}$$

where p_i, $i \in \mathcal{H}$, denotes the heavy species partial pressures, p_h the heavy species total pressure, q_i, $i \in \mathcal{H}$, the heavy species molar charges, and $\boldsymbol{F}_{ie}$, $i \in \mathcal{H}$, the average force of electrons acting on the ith heavy species. This force can be expanded in the form

$$\begin{aligned} \boldsymbol{F}_{ie} \,=\, & -p_{\mathrm{e}}\big(\alpha^{\parallel}_{ke}\boldsymbol{d}^{\parallel}_{\mathrm{e}} + \alpha^{\perp}_{ke}\boldsymbol{d}^{\perp}_{\mathrm{e}} + \alpha^{\odot}_{ke}\boldsymbol{d}^{\odot}_{\mathrm{e}} + \chi^{\parallel}_{ke}\boldsymbol{\nabla}\log T^{\parallel}_{\mathrm{e}} \\ & + \chi^{\perp}_{ke}\boldsymbol{\nabla}\log T^{\perp}_{\mathrm{e}} + \chi^{\odot}_{ke}\boldsymbol{\nabla}\log T^{\odot}_{\mathrm{e}}\big), \qquad i \in \mathcal{H}, \end{aligned} \tag{4.5}$$

where p_{e} is the electron partial pressure, and $\alpha^{\parallel}_{ie}$, $\alpha^{\perp}_{ie}$, $\alpha^{\odot}_{ie}$, $\chi^{\parallel}_{ie}$, $\chi^{\perp}_{ie}$ and $\chi^{\odot}_{ie}$ are second order coupling coefficients [35]. Alternatively, the heavy species diffusion velocities and heat flux may be written in terms of the heavy species thermal diffusion ratios χ_i, $i \in \mathcal{H}$, and the heavy species thermal conductivity λ_h as follows [35]

$$\mathbf{v}_i \,=\, -\sum_{j\in\mathcal{H}} D_{ij}(\widehat{\boldsymbol{d}}_j + \chi_j \boldsymbol{\nabla}\log T_h), \qquad i \in \mathcal{H}, \tag{4.6}$$

$$\boldsymbol{q}_h \,=\, -\lambda_h \boldsymbol{\nabla} T_h + p_h \sum_{i\in\mathcal{H}} \chi_i \mathbf{v}_i + \sum_{i\in\mathcal{H}} \rho h_i \upsilon_i \mathbf{v}_i. \tag{4.7}$$

4.2 Electron transport fluxes

The electron transport fluxes present polarization effects in the presence of strong magnetic fields. The second order electron diffusion velocities are found in the form [35]

$$\begin{aligned} \mathbf{v}_{\mathrm{e}} \,=\, & -D^{\parallel}_{\mathrm{ee}}\boldsymbol{d}^{\parallel}_{\mathrm{e}} - D^{\perp}_{\mathrm{ee}}\boldsymbol{d}^{\perp}_{\mathrm{e}} - D^{\odot}_{\mathrm{ee}}\boldsymbol{d}^{\odot}_{\mathrm{e}} - \theta^{\parallel}_{\mathrm{e}}(\boldsymbol{\nabla}\log T_{\mathrm{e}})^{\parallel} - \theta^{\perp}_{\mathrm{e}}(\boldsymbol{\nabla}\log T_{\mathrm{e}})^{\perp} \\ & -\theta^{\odot}_{\mathrm{e}}(\boldsymbol{\nabla}\log T_{\mathrm{e}})^{\odot} - \sum_{i\in\mathcal{H}}\big(\alpha^{\parallel}_{ie}\boldsymbol{d}^{2\parallel}_{i} + \alpha^{\perp}_{ie}\boldsymbol{d}^{2\perp}_{i} + \alpha^{\odot}_{ie}\boldsymbol{d}^{2\odot}_{i}\big), \end{aligned} \tag{4.8}$$

where $D^{\parallel}_{\mathrm{ee}}$, $D^{\perp}_{\mathrm{ee}}$ and $D^{\odot}_{\mathrm{ee}}$ are the electron diffusion coefficients parallel, perpendiclar and transverse to the magnetic field, and $\theta^{\parallel}_{\mathrm{e}}$, $\theta^{\perp}_{\mathrm{e}}$ and $\theta^{\odot}_{\mathrm{e}}$ the electron thermal diffusion coefficients parallel, perpendicular and transverse to the magnetic field. In these equation, the electron diffusion driving force $\boldsymbol{d}_{\mathrm{e}}$ and the second order diffusion driving forces $\boldsymbol{d}^2_i$, $i \in \mathcal{H}$, are given by

$$\widehat{d}_{\mathrm{e}} = \frac{\boldsymbol{\nabla} p_{\mathrm{e}}}{p_{\mathrm{e}}} - \frac{n_{\mathrm{e}} q_{\mathrm{e}}}{p_{\mathrm{e}}}(\boldsymbol{E} + \boldsymbol{v}_h \wedge \boldsymbol{B}), \qquad \boldsymbol{d}^2_i = -n_i \mathbf{v}_i, \quad i \in \mathcal{H}. \tag{4.9}$$

Similarly, the electron heat flux can be decomposed in the form

$$\begin{aligned} \boldsymbol{q}_{\mathrm{e}} \,=\, & -\widehat{\lambda}^{\parallel}_{\mathrm{e}}(\boldsymbol{\nabla} T_{\mathrm{e}})^{\parallel} - \widehat{\lambda}^{\perp}_{\mathrm{e}}(\boldsymbol{\nabla} T_{\mathrm{e}})^{\perp} - \widehat{\lambda}^{\odot}_{\mathrm{e}}(\boldsymbol{\nabla} T_{\mathrm{e}})^{\odot} - p_{\mathrm{e}}\big(\theta^{\parallel}_{\mathrm{e}}\boldsymbol{d}^{\parallel}_{\mathrm{e}} + \theta^{\perp}_{\mathrm{e}}\boldsymbol{d}^{\perp}_{\mathrm{e}} + \theta^{\odot}_{\mathrm{e}}\boldsymbol{d}^{\odot}_{\mathrm{e}}\big) \\ & -p_{\mathrm{e}}\sum_{i\in\mathcal{H}}\big(\chi^{\parallel}_{ie}\boldsymbol{d}^{2\parallel}_{\mathrm{e}} + \chi^{\perp}_{ie}\boldsymbol{d}^{2\perp}_{\mathrm{e}} + \chi^{\odot}_{ie}\boldsymbol{d}^{2\odot}_{\mathrm{e}}\big) + \rho_{\mathrm{e}} h_{\mathrm{e}} \mathbf{v}_{\mathrm{e}}, \end{aligned} \tag{4.10}$$

where $\widehat{\lambda}^{\parallel}_{\mathrm{e}}$, $\widehat{\lambda}^{\perp}_{\mathrm{e}}$ and $\widehat{\lambda}^{\odot}_{\mathrm{e}}$ are the electron partial thermal conductivities parallel, perpendicular and transverse to the magnetic field. Similar expressions can also be written in terms of the thermal diffusion ratios and the electron thermal conductivity but are omitted for the sake of brevity [35].

4.3 Transport linear systems

The kinetic theory investigations of Graille, Magin and Massot [35] have shown that the transport linear systems associated with the heavy species are similar to that of isotropic mixtures investigated in the Section 2 with the indexing set $\mathcal{S}$ replaced by $\mathcal{H}$. In particular, these systems share the same

mathematical structure as investigated in the Section 2 and there is not anymore anisotropy for the heavy species. On the other hand, the small transport linear systems associated with electrons are similar to that of the nonisotropic mixtures obtained in Section 3 without singularities [35].

Since we are interested in iterative solutions of the transport linear systems associated with a large number of species, only the mathematical structure of the transport linear systems associated with the heavy species and similar to that presented in Section 2 is therefore relevant in the nonequilibrium case. We do repeat the corresponding table of transport linear systems since they formally corresponds to changing the indexing set $\mathcal{S}$ into $\mathcal{H}$.

5 Generalized inverses and stationary iterative techniques

We first relate the solution of transport linear systems to generalized inverses with prescribed range and nullspace [28, 15, 19, 30, 33]. We next review projected stationary iterative techniques in order to solve constrained singular symmetric systems and to evaluate symmetric generalized inverses [28, 15, 19, 33]. These techniques are especially suited to the evaluation of diffusion matrices which may be expanded as convergent matrix series as investigated in Section 7. We next introduce an expansion of symmetric generalized inverses into dyadic products of conjugate direction and the corresponding more singular formulations of the transport linear systems. Both isotropic real systems and anisotropic complex systems are considered. The more singular formulations will then be used in conjunction with stationary projected iterative algorithms.

5.1 Generalized inverses and transport linear systems

In order to encompass the various structures of transport linear systems, either regular or singular as depending on transport coefficients and either real or complex as depending on magnetization, and also for future use, we introduce a common framework. We denote by $\mathbb{K}$ either $\mathbb{R}$ or $\mathbb{C}$, and for $A \in \mathbb{K}^{n,n}$ we denote by $R(A)$ and $N(A)$ the range and nullspace of the matrix A. For any complementary spaces $R \oplus S = \mathbb{K}^n$, $P_{R,S}$ denote the projector onto R parallel to S. We denote by $\langle x, y \rangle = \sum_{1 \leq k \leq n} x_k \overline{y}_k$ the Hermitian scalar product between $x, y \in \mathbb{C}^n$ or the Euclidean scalar product when $x, y \in \mathbb{R}^n$ and by $(x, y) = \sum_{1 \leq k \leq n} x_k y_k$ the nondegenerate nondefinite bilinear form between $x, y \in \mathbb{C}^n$ naturally associated with symmetric complex matrices. The tensor product matrix $a \otimes b$ has components $a_k b_l$, $1 \leq k, l \leq n$, so that $a \otimes b \, x = a(b, x)$ for $a, b, x \in \mathbb{C}^n$. The real x and imaginary y parts $x, y \in \mathbb{R}$, of a complex number $z \in \mathbb{C}$, $z = x + \mathrm{i}y$, are written $x = \Re z$ and $y = \Im z$. When A is a real linear subspace $A \subset \mathbb{R}^n$, we denote by $A + \mathrm{i}A$ the corresponding complexification $\{z \in \mathbb{C}^n,\ z = x + \mathrm{i}y,\ x, y \in A\}$. If A is a real subspace, we denote by $A^\perp$ the orthogonal complement with respect to the Euclidean product. When B is a complex subspace, we denote by $B^\perp$ the orthogonal complement with respect to the nondegenerate bilinear form $(,)$ and when B has a basis of real vectors, the orthogonal complement is equivalently defined with the Hermitian scalar product.

The transport linear systems associated with partially ionized gas mixtures can be written in the general form

$$\begin{cases} \mathcal{G} a = b, \\ a \in \mathcal{C}, \end{cases} \tag{5.1}$$

where $\mathcal{G} \in \mathbb{K}^{n,n}$, $\mathcal{C}$ is a linear subspace of $\mathbb{K}^n$, and $a, b \in \mathbb{K}^n$ are vectors. More specifically, in the isotropic case, we have $\mathbb{K} = \mathbb{R}$, $\mathcal{G} = G$, and either $\mathcal{C} = \mathbb{R}^n$ in the regular case or else $N(\mathcal{G}) = \mathbb{R}\mathsf{z}$ and $\mathcal{C} = \mathsf{g}^\perp$ in the singular case. In the nonisotropic case, we have $\mathbb{K} = \mathbb{C}$, $\mathcal{G} = G + \mathrm{i}G'$, and either $\mathcal{C} = \mathbb{C}^n$ in the regular case or else $N(\mathcal{G}) = \mathbb{C}\mathsf{z}$ and $\mathcal{C} = \mathsf{g}^\perp + \mathrm{i}\mathsf{g}^\perp$ in the singular case. All common properties between the real and complex cases will be written in terms of $\mathbb{K}$. When it is necessary to distinguish between these two situations, we will separately treat the real and complex cases. We will need the following result on generalized inverses with prescribed range and nullspace [2, 4, 29].

Proposition 5.1. *Let $\mathcal{G} \in \mathbb{K}^{n,n}$ be a matrix and let $\mathcal{C}$ and $\mathcal{S}$ be two subspaces of $\mathbb{K}^n$ such that $N(\mathcal{G}) \oplus \mathcal{C} = \mathbb{K}^n$ and $R(\mathcal{G}) \oplus \mathcal{S} = \mathbb{K}^n$. 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 $\mathcal{Z}\mathcal{G} = P_{\mathcal{C},N(\mathcal{G})}$.*

The well posedness of the transport linear systems (5.1) is obtained in the following proposition and its solution a is related to generalized inverses [28, 15, 19, 33]. First order multicomponent diffusion matrices will notably be expressed as generalized inverses of Stefan-Maxwell like matrices [28, 15, 30, 33]

Proposition 5.2. *Let $\mathcal{G} \in \mathbb{K}^{n,n}$ be a matrix and $\mathcal{C}$ be a subspace of $\mathbb{K}^n$. The constrained linear system (5.1) is well posed, i.e., admits a unique solution a for any $b \in R(\mathcal{G})$, if and only if*

$$N(\mathcal{G}) \oplus \mathcal{C} = \mathbb{K}^n. \tag{5.2}$$

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

In the real isotropic case the nullspace of the matrix $\mathcal{G} = G$ is obtained from ($\mathsf{G_1}$-$\mathsf{G_2}$) so that $N(\mathcal{G}) = \{0\}$ in the regular case whereas $N(\mathcal{G}) = \mathbb{R}\mathsf{z}$ in the singular case. In the complex case, the nullspace of the matrix $\mathcal{G} = G + \mathrm{i}G'$ is obtained in the following proposition where we use classical notation on complexifications [33].

Lemma 5.3. *Let $\mathcal{G} = G + \mathrm{i}G'$ where G, G' are real symmetric matrices, G is positive semi-definite and $G'N(G) = 0$. Then $N(\mathcal{G}) = N(G) + \mathrm{i}N(G)$ and $R(\mathcal{G}) = N(G)^\perp + \mathrm{i}N(G)^\perp$. Moreover, for any subspace $\mathcal{C} \subset \mathbb{R}^n$ complementary to $N(G)$, denoting $\mathcal{C} = \mathcal{C} + \mathrm{i}\mathcal{C}$ the complexification of $\mathcal{C}$, we have $N(\mathcal{G}) \oplus \mathcal{C} = \mathbb{C}^n$ and $P_{\mathcal{C},N(G)} = P_{\mathcal{C},N(\mathcal{G})}$.*

In the complex case, we thus have $N(\mathcal{G}) = \{0\}$ in the regular case and $N(\mathcal{G}) = \mathbb{C}\mathsf{z}$ in the singular case. The well posedness condition is then easily obtained in the real and complex cases since the constraint vector g is such that $\langle \mathsf{z}, \mathsf{g}\rangle \neq 0$ in such a way that $\mathbb{R}\mathsf{z} \cap \mathsf{g}^\perp = \{0\}$ in the isotropic case and $\mathbb{C}\mathsf{z} \cap (\mathsf{g}^\perp + \mathrm{i}\mathsf{g}^\perp) = \{0\}$ in the magnetized case. A further property is that the proper generalized inverses can be taken to be symmetric [19, 33]. We simultaneously investigate the real and complex case in the following proposition.

Proposition 5.4. *Let $\mathcal{G} = G + \mathrm{i}G'$ where G, G' are real symmetric matrices, G is positive semi-definite and $G'N(G) = 0$. Let $\mathcal{C} = \mathcal{C} + \mathrm{i}\mathcal{C}$ where $\mathcal{C} \subset \mathbb{R}^n$ is a subspace complementary to $N(G)$. Let $\mathcal{Z}$ be the generalized inverse of $\mathcal{G}$ with prescribed nullspace $N(\mathcal{Z}) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ and range $R(\mathcal{Z}) = \mathcal{C} + \mathrm{i}\mathcal{C}$. 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 $\mathcal{Z} = Z + \mathrm{i}Z'$, where $Z, Z' \in \mathbb{R}^{n,n}$, Z and Z' are symmetric matrices, Z is positive semi-definite, $Z'N(Z) = 0$ and $N(Z) = \mathcal{C}^\perp$. In the real case $\mathcal{G} = G$, we have $G' = Z' = 0$ and the generalized inverse $\mathcal{Z} = Z$ is real. The matrix Z is the unique symmetric generalized inverse of G with range $\mathcal{C}$. Furthermore, denoting by $\mathsf{z}_1, \ldots, \mathsf{z}_p$ a real basis of $N(G)$, where $p = \dim\big(N(G)\big) \geq 1$, there exist real vectors $\mathsf{g}_1, \ldots, \mathsf{g}_p$ spanning $\mathcal{C}^\perp$ such that $\langle \mathsf{g}_i, \mathsf{z}_j\rangle = \delta_{ij}$, $1 \leq i, j \leq p$. Then for any positive numbers α_i, β_i, $1 \leq i \leq p$, such that $\alpha_i\beta_i = 1$, $1 \leq i \leq p$, we have*

$$\mathcal{Z} = (\mathcal{G} + \sum_{1\leq i\leq p} \alpha_i\, \mathsf{g}_i{\otimes}\mathsf{g}_i)^{-1} - \sum_{1\leq i\leq p} \beta_i\, \mathsf{z}_i{\otimes}\mathsf{z}_i, \tag{5.3}$$

and the real part $G + \sum_{1\leq i\leq p} \alpha_i\, \mathsf{g}_i{\otimes}\mathsf{g}_i$ of the matrix $\mathcal{G} + \sum_{1\leq i\leq p} \alpha_i\, \mathsf{g}_i{\otimes}\mathsf{g}_i$ is symmetric positive definite. Therefore, for $b \in R(\mathcal{G})$, the solution a of (5.1) obtained from Proposition 5.2 also satisfies the regular system

$$(\mathcal{G} + \sum_{1\leq i\leq p} \alpha_i\, \mathsf{g}_i{\otimes}\mathsf{g}_i)a = b, \tag{5.4}$$

and we also have $P_{\mathcal{C},N(G)} = P_{\mathcal{C},N(\mathcal{G})} = \mathbb{I} - \sum_{1\leq i\leq p} \mathsf{z}_i{\otimes}\mathsf{g}_i$.

Considering then the transport linear systems in the real case (2.8) the proper generalized inverse Z of G is the one with range $\mathsf{g}^\perp$ and nullspace $\mathbb{R}\mathsf{g}$ and we then have $GZ = \mathbb{I} - \mathsf{g}{\otimes}\mathsf{z}/\langle \mathsf{g}, \mathsf{z}\rangle$ and $ZG = \mathbb{I} - \mathsf{z}{\otimes}\mathsf{g}/\langle \mathsf{g}, \mathsf{z}\rangle$. Considering the transport linear systems in the complex case (3.7) the proper generalized inverse $\mathcal{Z}$ of $\mathcal{G} = G + \mathrm{i}G'$ is the one with range $\mathsf{g}^\perp + \mathrm{i}\mathsf{g}^\perp$ and nullspace $\mathbb{C}\mathsf{g}$ and we have $\mathcal{G}\mathcal{Z} = \mathbb{I} - \mathsf{g}{\otimes}\mathsf{z}/\langle \mathsf{g}, \mathsf{z}\rangle$ and $\mathcal{Z}\mathcal{G} = \mathbb{I} - \mathsf{z}{\otimes}\mathsf{g}/\langle \mathsf{g}, \mathsf{z}\rangle$. This propostion also shows that there exist symmetric regular formulations of the transport linear systems. However, the singular formulations are more suited to iterative techniques [15].

5.2 Projected iterative algorithms

For a matrix $\mathcal{T} \in \mathbb{C}^{n,n}$, $\sigma(\mathcal{T})$ 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 $\lim_{i\to\infty} \mathcal{T}^i$ exists—not necessarily being zero [48]—and we have the following characterization [50, 44, 48, 4, 29].

Proposition 5.5. *A matrix $\mathcal{T} \in \mathbb{C}^{n,n}$ 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 $\mathcal{T}$ has only elementary divisors corresponding to the eigenvalue 1, that is, $N(I-\mathcal{T}) \cap R(I-\mathcal{T}) = \{0\}$.*

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

$$\mathcal{G} = \mathcal{M} - \mathcal{W}, \tag{5.5}$$

is a splitting if the matrix $\mathcal{M}$ is invertible. In order to solve the linear system $\mathcal{G}a = b$, where $b \in \mathbb{C}^n$, the splitting (5.5) induces the iterative scheme

$$z_{i+1} = \mathcal{T} z_i + \mathcal{M}^{-1} b, \qquad i \geq 0, \tag{5.6}$$

where $\mathcal{T} = \mathcal{M}^{-1}\mathcal{W}$. Assuming that $b \in R(\mathcal{G})$, we have $\mathcal{M}^{-1}b \in R(I-\mathcal{T})$, and the behavior of the sequence of iterates (5.6) is given in the next lemma [44, 4].

Lemma 5.6. *Let $\mathcal{T} \in \mathbb{K}^{n,n}$ and let $c \in \mathbb{K}^n$ such that $c \in R(I-\mathcal{T})$. Then the iterative scheme $z_{i+1} = \mathcal{T} z_i + c$, $i \geq 0$, converges for any $z_0 \in \mathbb{K}^n$ if and only if $\mathcal{T}$ is convergent. In this situation, the limit $\lim_{i\to\infty} z_i = z_\infty$ is given by $z_\infty = \bar{z}_\infty + P_{N(I-\mathcal{T}),R(I-\mathcal{T})} z_0$ where $\bar{z}_\infty$ is the unique solution of $(I-\mathcal{T})\bar{z}_\infty = c$ such that $\bar{z}_\infty \in R(I-\mathcal{T})$.*

We are now interested in solving the constrained singular system (5.1) by stationary iterative techniques. These techniques provide iterates which depend linearly on the right-hand side b, and this property may be important for some applications, as for instance for multicomponent diffusion matrices. For a given splitting $\mathcal{G} = \mathcal{M} - \mathcal{W}$ and for $b \in R(\mathcal{G})$, assuming that the iteration matrix $\mathcal{T} = \mathcal{M}^{-1}\mathcal{W}$ is convergent, the iterates (5.6) 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 use a projected iterative scheme [28, 19]

$$z'_{i+1} = \mathcal{P}\mathcal{T} z'_i + \mathcal{P}\mathcal{M}^{-1} b, \qquad i \geq 0, \tag{5.7}$$

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 $\{\, z'_i;\ i \geq 0 \,\}$ then satisfy the constraint $z'_i \in \mathcal{C}$. The spectral radius of the iteration matrix $\mathcal{P}\mathcal{T}$ associated with (5.7) can be estimated by using a theorem of Neumann and Plemmons [48] or the following result of Ern and Giovangigli [19, 33]. This theorem establishes that the spectral radius $\rho(\mathcal{P}\mathcal{T})$ of $\mathcal{P}\mathcal{T}$ is equal to $\gamma(\mathcal{T})$ when $\mathcal{T}$ is convergent.

Theorem 5.7. *Let $\mathcal{T} \in \mathbb{K}^{n,n}$ be a matrix 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 $N(I-\mathcal{T}) \oplus \mathcal{C} = \mathbb{K}^n$, and let also $\mathcal{P}$ be the oblique projector matrix onto the subspace $\mathcal{C}$ along $N(I-\mathcal{T})$. Then we have*

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

and the matrices $\mathcal{T}$ and $\mathcal{P}$ satisfy the relation $\mathcal{P}\mathcal{T} = \mathcal{P}\mathcal{T}\mathcal{P}$. In addition, if λ and $x \neq 0$ are such such that $\mathcal{T}x = \lambda x$, then $y = \mathcal{P}x$ is an eigenvector for the product $\mathcal{P}\mathcal{T}$ associated with the eigenvalue λ, that is, $\mathcal{P}\mathcal{T}y = \lambda y$.

In order to obtain convergent iteration matrices—and therefore convergent projected iterative scheme for the transport linear systems in the real case—we may use Keller's theorem [39].

Theorem 5.8. *Let $G \in \mathbb{R}^{n,n}$ be a symmetric matrix and let $G = M - W$ be a splitting such that M is symmetric and $M + W$ is positive definite. Then $T = M^{-1}W$ is convergent if and only if G is positive semi-definite.*

Combining then Keller's theorem, the spectral Theorem 5.7, and the mathematical structure resulting from the kinetic theory of gases, we may use in the real situation the splitting matrices

$$M = db(G) + \mathrm{diag}(\sigma_1, \ldots, \sigma_n), \tag{5.8}$$

where $db(G)$ is the sparse transport matrix and $\sigma_1, \ldots, \sigma_n$ are any nonnegative factors. Indeed, since $M+W = 2db(G) - G + 2\mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, we deduce that $M+W$ is positive definite from ($\mathsf{G_1}$-$\mathsf{G_2}$), and Keller's theorem can be used. The convergence of projected iterative algorithms and the asymptotic expansion of generalized inverses are then obtained as detailled in the following [19]. On the other hand, in the complex case, in order to obtain an iterative scheme with convergence properties valid for any matrix G', we may include the full imaginary part $\mathrm{i}G'$ of $\mathcal{G}$ in the splitting matrix $\mathcal{M}$

$$\mathcal{M} = db(G) + \mathrm{diag}(\sigma_1, \ldots, \sigma_n) + \mathrm{i}G', \tag{5.9}$$

so that $\mathcal{W} = \mathcal{G} - \mathcal{M}$ is real and if $\mathcal{M} = M + \mathrm{i}G'$ then $G = M - W$ is a splitting of the symmetric positive semi-definite matrix G. This can be done in practice since the resulting matrix $\mathcal{M} = M + \mathrm{i}G'$ is easily expressed in terms of the inverse of $M + \mathrm{i}\mathcal{D}'$ when G' is in the form $G' = Q\mathcal{D}'P$ [33]. Note that Keller's theorem cannot be applied directly as in the real case [19] since $\mathcal{G}$ is not Hermitian when G' is nonzero. The convergence and properties of the projected iterative algorithms (5.7) when applied to the real or complex symmetric constrained singular systems (5.1) are summarized in the following proposition [19, 33].

Theorem 5.9. *Let $\mathcal{G} = G + \mathrm{i}G'$ where G, G' are real symmetric matrices, G is positive semi-definite and $G'N(G) = 0$. Let $\mathcal{C} \subset \mathbb{R}^n$ be a subspace complementary to $N(G)$ and let $\mathcal{C}$ be the complexification of $\mathcal{C}$. Consider a splitting $G = M - W$, assume that M is symmetric and that $M+W$ is positive definite, so that M is also symmetric positive definite. Define $\mathcal{M} = M + \mathrm{i}G'$, $\mathcal{G} = \mathcal{M} - \mathcal{W}$, so that $\mathcal{W} = W$, and $\mathcal{T} = \mathcal{M}^{-1}\mathcal{W}$, $T = M^{-1}W$. Let $\mathcal{P} = P$ be the oblique projector matrix onto the subspace $\mathcal{C}$ along $N(G)$. Let also $b \in R(\mathcal{G})$, $z_0 \in \mathbb{C}^n$, $z'_0 = \mathcal{P}z_0$, and consider for $i \geq 0$ the iterates $z_{i+1} = \mathcal{T}z_i + M^{-1}b$ as in (5.6) and $z'_{i+1} = \mathcal{P}\mathcal{T}z'_i + \mathcal{P}M^{-1}b$ as in (5.7). Then $z'_i = \mathcal{P}z_i$ for all $i \geq 0$, the matrices $\mathcal{T}$, $\mathcal{P}\mathcal{T}$, T, and PT are convergent, $\rho(T) = \rho(\mathcal{T}) = 1$ when $\dim\big(N(G)\big) \geq 1$, $\rho(\mathcal{P}\mathcal{T}) = \gamma(\mathcal{T}) < 1$, $\rho(PT) = \gamma(T) < 1$, and*

$$\gamma(\mathcal{T}) \leq \gamma(T), \tag{5.10}$$

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

$$\lim_{i\to\infty} z'_i = \mathcal{P}(\lim_{i\to\infty} z_i) = a, \tag{5.11}$$

where a is the unique solution of (5.1). Each partial sum $\mathcal{Z}_i = \sum_{0\leq j\leq i-1}(\mathcal{P}\mathcal{T})^j\mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t$, $i \geq 1$, is symmetric and $\lim_{i\to\infty}\mathcal{Z}_i = \mathcal{Z}$ where

$$\mathcal{Z} = \sum_{0\leq j<\infty} (\mathcal{P}\mathcal{T})^j\mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t, \tag{5.12}$$

is the symmetric generalized inverse of $\mathcal{G}$ with prescribed nullspace $N(\mathcal{Z}) = \mathcal{C}^\perp + \mathrm{i}\mathcal{C}^\perp$ and range $R(\mathcal{Z}) = \mathcal{C} = \mathcal{C} + \mathrm{i}\mathcal{C}$. Similar properties hold in the real case where $G' = Z' = 0$ and $Z = \sum_{0\leq j<\infty}(PT)^jPM^{-1}P^t$ is real and is the generalized inverse of G with prescribed range $R(Z) = \mathcal{C}$ and nullspace $N(Z) = \mathcal{C}^\perp$, and each iterate $Z_i = \sum_{0\leq j<i-1}(PT)^jPM^{-1}P^t$ is positive semi-definite with $R(Z_i) = \mathcal{C}$.

The projected iterative algorithms applied to the transport linear systems have been successful for accurate evaluation of multicomponent diffusion matrices in nonionized gas mixtures [28, 15, 17, 19, 18]. When applied to partially ionized mixtures, these algorithms have been found efficient at law ionization levels [26, 33]. The convergence rates are also insensitive to the intensity of the magnetic when the whole complex part $\mathrm{i}G'$ is included in the splitting matrix $\mathcal{M} = M + \mathrm{i}G'$ as shown by the estimate (5.10).

However, as investigated by García Muñoz [26] for planetary atmosphere and reported by Giovangigli and Graille for high temperature air [33], the corresponding convergence rates deteriorate when ionization levels increase. The solution of this problem requires introducing new formulations of the transport linear systems investigated in the following section. The stationary projected iterative algorithms will then be performed with the new formulations.

5.3 Generalized inverses and conjugate directions

We consider in this section the transport linear system in the real singular case (2.8) under assumption (G_2). This situation is notably associated with isotropic multicomponent diffusion matrices. The complex case associated with nonisotropy will be investigated in the next section.

We expand in this section the matrix G and the symmetric generalized inverse Z with nullspace $\mathbb{R}\mathsf{g}$ and range $\mathsf{g}^\perp$ into dyadic products of conjugate directions. By truncating these expansions, we reformulate the transport linear systems and the corresponding generalized inverse problem in the real singular situation. The main idea is that a *more singular* formulation is required since by increasing the nullspace of the matrices G and Z we increase that of the projector matrix P and we may decrease the spectral radius of the corresponding product PT.

For the sake of notational simplicity, we will write $\mathsf{z}_1 = \mathsf{z}$ and $\mathsf{g}_1 = \mathsf{g}$ in this section. The matrix G is symmetric positive demi-definite, $N(G) = \mathbb{R}\mathsf{z}_1$, and defining Z as the generalized inverse of G with prescribed nullspace $N(Z) = \mathbb{R}\mathsf{g}_1$ and range $R(Z) = \mathsf{g}_1^\perp$, and letting $Q = P^t = \mathbb{I} - \mathsf{g}_1 \otimes \mathsf{z}_1 / \langle \mathsf{g}_1, \mathsf{z}_1 \rangle$, we have the relations

$$GZ = Q, \qquad ZG = P. \tag{5.13}$$

We know from Theorem 5.4 that Z is symmetric and positive semi-definite. We now select $\mathsf{z}_2^* \in \mathbb{R}^n$ such that $\mathsf{z}_2^* \notin \mathbb{R}\mathsf{z}_1$ and define

$$\mathsf{z}_2 = \mathsf{z}_2^* - \frac{\langle \mathsf{z}_2^*, \mathsf{g}_1 \rangle}{\langle \mathsf{z}_1, \mathsf{g}_1 \rangle} \mathsf{z}_1, \qquad \mathsf{g}_2 = G\mathsf{z}_2. \tag{5.14}$$

Note that $\langle \mathsf{z}_2, \mathsf{g}_2 \rangle > 0$ since $\langle \mathsf{z}_2, \mathsf{g}_2 \rangle = \langle \mathsf{z}_2, G\mathsf{z}_2 \rangle$ and $\mathsf{z}_2 \notin N(G) = \mathbb{R}\mathsf{z}_1$, and by construction we have $\langle \mathsf{z}_2, \mathsf{g}_1 \rangle = 0$ and $\langle \mathsf{z}_1, \mathsf{g}_2 \rangle = 0$, so that $\mathsf{g}_2 \notin \mathbb{R}\mathsf{g}_1$. We then introduce

$$G_2 = G - \frac{\mathsf{g}_2 \otimes \mathsf{g}_2}{\langle \mathsf{z}_2, \mathsf{g}_2 \rangle}, \qquad Z_2 = Z - \frac{\mathsf{z}_2 \otimes \mathsf{z}_2}{\langle \mathsf{z}_2, \mathsf{g}_2 \rangle}, \tag{5.15}$$

$$P_2 = \mathbb{I} - \frac{\mathsf{z}_1 \otimes \mathsf{g}_1}{\langle \mathsf{z}_1, \mathsf{g}_1 \rangle} - \frac{\mathsf{z}_2 \otimes \mathsf{g}_2}{\langle \mathsf{z}_2, \mathsf{g}_2 \rangle}, \qquad Q_2 = \mathbb{I} - \frac{\mathsf{g}_1 \otimes \mathsf{z}_1}{\langle \mathsf{z}_1, \mathsf{g}_1 \rangle} - \frac{\mathsf{g}_2 \otimes \mathsf{z}_2}{\langle \mathsf{z}_2, \mathsf{g}_2 \rangle}, \tag{5.16}$$

and by a direct calculation we obtain that

$$G_2 Z_2 = Q_2, \qquad Z_2 G_2 = P_2. \tag{5.17}$$

The expression

$$\langle G_2 x, x \rangle = \Big\langle G\big(x - \tfrac{\langle x, \mathsf{g}_2 \rangle}{\langle \mathsf{z}_2, \mathsf{g}_2 \rangle} \mathsf{z}_2\big), x - \tfrac{\langle x, \mathsf{g}_2 \rangle}{\langle \mathsf{z}_2, \mathsf{g}_2 \rangle} \mathsf{z}_2 \Big\rangle, \tag{5.18}$$

further yields that G_2 is positive semi-definite and $N(G_2) = \mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\}$. Indeed, if $G_2 x = 0$ we obtain that $x - \frac{\langle x, \mathsf{g}_2 \rangle}{\langle \mathsf{z}_2, \mathsf{g}_2 \rangle} \mathsf{z}_2 \in \mathbb{R}\mathsf{z}_1$ and $x \in \mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\}$ and conversely we have $\mathsf{z}_1, \mathsf{z}_2 \in N(G_2)$ by construction. Proceeding similarly for Z_2, we obtain that Z_2 is positive semi-definite and $N(Z_2) = \mathrm{span}\{\mathsf{g}_1, \mathsf{g}_2\}$. We thus deduce that Z_2 is the generalized inverse of G_2 with prescribed nullspace $N(Z_2) = \mathrm{span}\{\mathsf{g}_1, \mathsf{g}_2\}$ and range $R(Z_2) = \mathrm{span}\{\mathsf{g}_1, \mathsf{g}_2\}^\perp$, and G_2 is the generalized inverse of Z_2 with prescribed nullspace $N(G_2) = \mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\}$ and range $R(G_2) = \mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\}^\perp$. Letting $a_2 = Z_2 b$, $b_2 = Q_2 b$, we further obtain after some algebra the new transport linear system

$$\begin{cases} G_2 a_2 = b_2, \\ \langle a_2, \mathsf{g}_1 \rangle = \langle a_2, \mathsf{g}_1 \rangle = 0. \end{cases} \tag{5.19}$$

Thanks to $\langle \mathsf{z}_1, \mathsf{g}_2 \rangle = \langle \mathsf{z}_2, \mathsf{g}_1 \rangle = 0$, $\langle \mathsf{z}_1, \mathsf{g}_1 \rangle > 0$, and $\langle \mathsf{z}_2, \mathsf{g}_2 \rangle > 0$, it is easily checked that $N(G_2) \oplus \mathrm{span}\{\mathsf{g}_1, \mathsf{g}_2\}^\perp = \mathbb{R}^n$ and $b_2 \in R(G_2)$ by contruction so that we deduce from Proposition 5.2 that the system (5.19) is well posed. Therefore, its unique solution is given by $a_2 = Z_2 b$ and the solution of the original system a can be written

$$a = a_2 + \frac{\langle \mathsf{z}_2, b \rangle}{\langle \mathsf{z}_2, b \rangle} \mathsf{z}_2. \tag{5.20}$$

The main idea is that the projected iterative algorithm applied to the more singular system (5.19) will involve a matrix $P_2 T_2$ with a lower spectral radius than PT by properly tuning z_2. As a typical exemple, assume for instance that z_2 is an eigenvector for T associated with an eigenvalue nearby unity $1 - \epsilon$ where $\epsilon > 0$ so that $G\mathsf{z}_2 = \epsilon M \mathsf{z}_2$ with $\mathsf{z}_2 \neq 0$. From Theorem 5.7 we know that $1 - \epsilon$ is also an eigenvalue of the matrix PT with eigenvector $P\mathsf{z}_2$ and that all nonzero eigenvalue of PT are similarly nonunity eigenvalues of T. Then z_2 can be taken of order unity but $\mathsf{g}_2 = G\mathsf{z}_2 = \epsilon M \mathsf{z}_2$ is small, say

$\mathcal{O}(\epsilon)$. Then from (5.15) $G - G_2 = \mathcal{O}(\epsilon)$ and $Z - Z_2 = \mathcal{O}(1/\epsilon)$, and we may let for the sake of the argument $M_2 \simeq M_1 = M$, $W_2 \simeq W_1 = W$. Furthermore, it is established in [33] that

$$\gamma(T_i) = \sup\Big\{ \frac{|\langle W_i x, x\rangle|}{\langle M_i x, x\rangle};\ x \in \mathbb{R}^n,\ x \neq 0,\ \ \langle M_i \mathsf{z}_j, x\rangle = 0,\ 1 \leq j \leq i \Big\}, \tag{5.21}$$

where $i = 1, 2$. As a consequence, we see that the bad eigenvalue $1 - \epsilon$ of T associated with the vector z_2 is now eliminated when estimating $\gamma(T_2)$ since it has been made an exact singularity of G_2. More specifically, the relevant vectors to be considered for $\gamma(T_2)$ are now orthogonal to $M\mathsf{z}_2 = \mathsf{g}_2/\epsilon$ and this excludes z_2. In addition, from Theorem 5.7, all eigenvectors of P_2T_2 associated with nonzero eigenvalues are projections $P_2 w_2$ of eigenvectors w_2 of T_2 in such a way that all components of such eigenvectors of T_2 along $\mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\}$ are killed by P_2.

Remark 5.10. *The identity* (5.21) *is easily established by considering the new scalar product* $\langle\!\langle x, y\rangle\!\rangle = \langle Mx, y\rangle$, $x, y \in \mathbb{R}^n$. *With respect to this scalar product, the matrix* $T = M^{-1}W$ *is then symmetric since*

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

As a direct application of spectral properties of symmetric matrices, we know that T *has a complete set of real eigenvectors orthogonal with respect to* $\langle\!\langle\ ,\ \rangle\!\rangle$. *In addition, the eigenspace associated with the eigenvalue* 1 *is the eigenspace* $N(I - T) = N(G)$, $\langle\!\langle Tx, x\rangle\!\rangle = \langle Wx, x\rangle$, $\langle\!\langle x, x\rangle\!\rangle = \langle Mx, x\rangle$, *and* (5.21) *easily follows [33].*

Generalizing these ideas, we now expand the matrices G and Z into tensor products of conjugate directions and introduce the corresponding more singular formulations of the transport linear systems.

Theorem 5.11. *Assume that* G *is symmetric positive semi-definite,* $N(G) = \mathbb{R}\mathsf{z}$, $\langle \mathsf{z}, \mathsf{g}\rangle \neq 0$, *and let* Z *be the generalized inverse of* G *with nullspace* $\mathbb{R}\mathsf{g}$ *and range* $\mathsf{g}^\perp$. *Let* z_i^*, $1 \leq i \leq n$, *be a basis of* $\mathbb{R}^n$ *with* $\mathsf{z}_1^* = \mathsf{z}$, *and define for convenience* $\mathsf{z}_1 = \mathsf{z}_1^* = \mathsf{z}$, $\mathsf{g}_1 = \mathsf{g}$, $G_1 = G$, $Z_1 = Z$, $P_1 = P$, $Q_1 = Q$, $G_0 = G_1 + \mathsf{g}_1 \otimes \mathsf{g}_1/\langle \mathsf{z}_1, \mathsf{g}_1\rangle$, *and* $Z_0 = Z_1 + \mathsf{z}_1 \otimes \mathsf{z}_1/\langle \mathsf{z}_1, \mathsf{g}_1\rangle$. *Define then inductively for* $k \geq 1$ *the vectors*

$$\mathsf{z}_k = \mathsf{z}_k^* - \sum_{1 \leq j \leq k-1} \frac{\langle \mathsf{z}_k^*, \mathsf{g}_j\rangle}{\langle \mathsf{z}_j, \mathsf{g}_j\rangle} \mathsf{z}_j, \qquad \mathsf{g}_k = G_{k-1}\mathsf{z}_k, \tag{5.22}$$

the linear operators

$$G_k = G_{k-1} - \frac{\mathsf{g}_k \otimes \mathsf{g}_k}{\langle \mathsf{z}_k, \mathsf{g}_k\rangle}, \qquad Z_k = Z_{k-1} - \frac{\mathsf{z}_k \otimes \mathsf{z}_k}{\langle \mathsf{z}_k, \mathsf{g}_k\rangle}, \tag{5.23}$$

and the projectors

$$Q_k = \mathbb{I} - \sum_{1 \leq i \leq k} \frac{\mathsf{g}_i \otimes \mathsf{z}_i}{\langle \mathsf{z}_i, \mathsf{g}_i\rangle}, \qquad P_k = \mathbb{I} - \sum_{1 \leq i \leq k} \frac{\mathsf{z}_i \otimes \mathsf{g}_i}{\langle \mathsf{z}_i, \mathsf{g}_i\rangle}. \tag{5.24}$$

Then the vectors z_i, g_i, $1 \leq i \leq n$, *is such that* $\langle \mathsf{z}_i, \mathsf{g}_i\rangle > 0$, $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_i\} = \mathrm{span}\{\mathsf{z}_1^*, \ldots, \mathsf{z}_i^*\}$, $\mathsf{g}_i = G_{i-1}\mathsf{z}_i$, $\mathsf{z}_i = Z_{i-1}\mathsf{g}_i$, $1 \leq i \leq n$, $\langle \mathsf{z}_i, \mathsf{g}_j\rangle = 0$ *if* $i \neq j$, $1 \leq i, j \leq n$. *Moreover, for any* $0 \leq k \leq n$ *we have the relations*

$$G_k Z_k = Q_k, \qquad Z_k G_k = P_k, \tag{5.25}$$

where P_k *is the projector onto* $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}^\perp$ *parallel to* $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}$, Q_k *is the projector onto* $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}^\perp$ *parallel to* $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}$, *and* $P_0 = Q_0 = \mathbb{I}$, $G_0 Z_0 = Z_0 G_0 = \mathbb{I}$, $G_n = Z_n = P_n = Q_n = 0$. *In addition, for any* $0 \leq k \leq n$, G_k *and* Z_k *are symmetric positive semi-definite,* $N(G_k) = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}$, $R(G_k) = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}^\perp$, Z_k *is the generalized inverse of* G_k *with prescribed nullspace* $N(Z_k) = \mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}$ *and range* $R(Z_k) = \mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}^\perp$, *and* G_k *is the generalized inverse of* Z_k *with nullspace* $N(G_k) = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}$ *and range* $R(G_k) = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}^\perp$. *Finally, we have* $\mathsf{g}_i = G\mathsf{z}_i$, $\mathsf{z}_i = Z\mathsf{g}_i$, $2 \leq i \leq n$, $\mathsf{g}^\perp = \mathrm{span}\{\mathsf{z}_2, \ldots, \mathsf{z}_n\}$, *the directions* z_i, $2 \leq i \leq n$, *are conjugate for* G, *the directions* g_i, $2 \leq i \leq n$ *are conjugate for* Z, *and we have the decompositions*

$$G = \sum_{2 \leq j \leq n} \frac{\mathsf{g}_i \otimes \mathsf{g}_i}{\langle \mathsf{z}_i, \mathsf{g}_i\rangle}, \qquad Z = \sum_{2 \leq j \leq n} \frac{\mathsf{z}_i \otimes \mathsf{z}_i}{\langle \mathsf{z}_i, \mathsf{g}_i\rangle}, \tag{5.26}$$

$$\mathbb{I} = \sum_{1 \leq j \leq n} \frac{\mathsf{g}_i \otimes \mathsf{z}_i}{\langle \mathsf{z}_i, \mathsf{g}_i\rangle} = \sum_{1 \leq j \leq n} \frac{\mathsf{z}_i \otimes \mathsf{g}_i}{\langle \mathsf{z}_i, \mathsf{g}_i\rangle}. \tag{5.27}$$

Proof. The proof is established by induction and we have already established the properties of z_2, g_2, G_2, Z_2, P_2 and Q_2. Assume now that k steps of the procedure have been taken and that $2 \leq k < n$ and consider the vector z_{k+1} defined from (5.22). From this definition we obtain that $\langle \mathsf{z}_{k+1}, \mathsf{g}_l \rangle = 0$ for $1 \leq l \leq k$ and it is easily checked that $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\} = \mathrm{span}\{\mathsf{z}_1^*, \ldots, \mathsf{z}_{k+1}^*\}$. Defining $\mathsf{g}_{k+1} = G_k \mathsf{z}_{k+1}$ we obtain that $\langle \mathsf{g}_{k+1}, \mathsf{z}_l \rangle = 0$ for $1 \leq l \leq k$, since $R(G_k) = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}^\perp$, and similarly that $\mathsf{z}_{k+1} = Z_k \mathsf{g}_{k+1}$ since $\mathsf{z}_{k+1} \in \mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}^\perp$ and $Z_k G_k = \mathbb{I} - \sum_{1 \leq i \leq k} \mathsf{z}_k \otimes \mathsf{g}_k / \langle \mathsf{z}_k, \mathsf{g}_k \rangle$ from the induction hypothesis. Moreover, $\langle \mathsf{z}_{k+1}, \mathsf{g}_{k+1} \rangle > 0$ since z_{k+1}^* and thus z_{k+1} does not belong to $N(G_k) = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}$ and this also show that $\mathsf{g}_{k+1} \notin \mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}$. Upon defining G_{k+1} and Z_{k+1} from (5.23) these matrices G_{k+1} and Z_{k+1} are symmetric and from

$$\langle G_{k+1} x, x \rangle = \Big\langle G_k \big(x - \tfrac{\langle x, \mathsf{g}_{k+1} \rangle}{\langle \mathsf{z}_{k+1}, \mathsf{g}_{k+1} \rangle} \mathsf{z}_{k+1}\big), \big(x - \tfrac{\langle x, \mathsf{g}_{k+1} \rangle}{\langle \mathsf{z}_{k+1}, \mathsf{g}_{k+1} \rangle} \mathsf{z}_{k+1}\big) \Big\rangle, \tag{5.28}$$

we deduce that G_{k+1} is positive semi-definite since G_k is positive semi-definite. Moreover we easily deduce that $N(G_{k+1}) = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\}$ since $N(G_k) = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}$. Similarly, Z_{k+1} is positive semi-definite with $N(Z_{k+1}) = \mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_{k+1}\}$. A direct calculation also yields $G_{k+1} Z_{k+1} = Q_{k+1}$ and $Z_{k+1} G_{k+1} = P_{k+1}$ and it is straightforward to check that and P_{k+1} is the projector onto $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_{k+1}\}^\perp$ parallel to $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\}$, and Q_{k+1} is the projector onto $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\}^\perp$ parallel to $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_{k+1}\}$. As a consequence, Z_{k+1} is the generalized inverse of G_{k+1} with prescribed nullspace $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_{k+1}\}$ and range $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_{k+1}\}^\perp$ and G_{k+1} is the generalized inverse of Z_{k+1} with prescribed nullspace $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\}$ and range $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\}^\perp$. The relation $G_0 Z_0 = \mathbb{I}$ is also established directly from the definitions of G_0, Z_0, and $GZ = \mathbb{I} - \mathsf{g}_1 \otimes \mathsf{z}_1 / \langle \mathsf{g}_1, \mathsf{z}_1 \rangle$.

The induction is therefore established and since $N(G_n) = N(Z_n) = \mathbb{R}^n$ we deduce that $G_n = Z_n = P_n = Q_n = 0$. Thanks to the relations (5.23) and $G_n = 0$ we next obtain that $G = \sum_{2 \leq j \leq n} \mathsf{g}_k \otimes \mathsf{g}_k / \langle \mathsf{z}_k, \mathsf{g}_k \rangle$ and similarly that $Z = \sum_{2 \leq j \leq n} \mathsf{z}_k \otimes \mathsf{z}_k / \langle \mathsf{z}_k, \mathsf{g}_k \rangle$. These relation also implies (5.27) from $G_0 Z_0 = \mathbb{I}$.

In addition, since $\dim\big(\mathrm{span}\{\mathsf{z}_2, \ldots, \mathsf{z}_n\}\big) = n - 1$ and $\langle \mathsf{g}, \mathsf{z}_l \rangle = 0$, $2 \leq l \leq n$, we deduce that $\mathsf{g}^\perp = \mathrm{span}\{\mathsf{z}_2, \ldots, \mathsf{z}_n\}$. Moreover, we have $\langle \mathsf{g}_k, \mathsf{z}_l \rangle = 0$ for $2 \leq k < l \leq n$, and $\mathsf{g}_k = G_{k-1} \mathsf{z}_k$. However, $G_{k-1} \mathsf{z}_k = G \mathsf{z}_k$ thanks to the relations (5.23) in such a way that $\langle G \mathsf{z}_k, \mathsf{z}_l \rangle = 0$ for $2 \leq k < l \leq n$ and thus for $2 \leq k, l \leq n$ and $k \neq l$, and the directions z_k, $2 \leq k \leq n$ are conjugate for G. The proof for Z and the directions g_k, $2 \leq k \leq n$ is similar and the proof is complete. □

In the following corollary we obtain the proper generalization of the transport linear systems (2.8) and (5.19) corresponding respectively to $k = 1$ and $k = 2$.

Corollary 5.12. *Keeping the notation of the preceding theorem, and letting $b_k = Q_k b$, the linear system*

$$\begin{cases} G_k a_k = b_k, \\ \langle a_k, \mathsf{g}_l \rangle = 0, \quad 1 \leq l \leq k, \end{cases} \tag{5.29}$$

is well posed, its solution is $a_k = Z_k b$, and we have the expansion

$$a = a_k + \sum_{1 \leq l \leq k} \frac{\langle \mathsf{z}_k, b \rangle}{\langle \mathsf{z}_k, \mathsf{g}_k \rangle} \mathsf{z}_k, \tag{5.30}$$

where $a = a_1$ is the unique solution of $Ga = b$ such that $\langle a, \mathsf{g} \rangle = 0$.

Proof. From Theorem 5.11 we know that $N(G_k) = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}$ and the constraint space associated with (5.29) is $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}^\perp$. These spaces are respectively of dimension k and $n - k$ and their intersection is zero

$$\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\} \cap \mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}^\perp = \{0\}.$$

Indeed, if $z = \alpha_1 \mathsf{z}_1 + \cdots + \alpha_k \mathsf{z}_k$ and $\langle z, \mathsf{g}_l \rangle = 0$, $1 \leq l \leq k$, we directly obtain that $\alpha_l = 0$, $1 \leq l \leq k$ since $\langle \mathsf{z}_i, \mathsf{g}_l \rangle = 0$ if $i \neq l$ and $\langle \mathsf{z}_i, \mathsf{g}_i \rangle > 0$ for $1 \leq i \leq k$. This shows that $N(G_k) \oplus \mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}^\perp = \mathbb{R}^n$ and (5.29) is well posed. From the relation $G_k Z_k = Q_k$ and $b_k = Q_k b$ we directly obtain that $a_k = Z_k b$ and from the relations between the generalized inverses Z_k, $k \geq 1$, we obtain (5.30). □

5.4 Conjugate directions in the anisotropic situation

We consider in this section the transport linear system in the complex singular case (3.7) under assumptions $(\mathsf{G}_2)(\mathsf{G}_2')$. In this situation, the matrix $\mathcal{G}$ is in the form $\mathcal{G} = G + \mathrm{i}G'$, where G, G' are symmetric, G positive demi-definite, $N(G) = \mathbb{R}\mathsf{z}$, $G'\mathsf{z} = 0$, and we define $\mathcal{Z}$ as the generalized inverse of $G + \mathrm{i}G'$ with prescribed nullspace $N(\mathcal{Z}) = \mathbb{C}\mathsf{g}$ and range $R(\mathcal{Z}) = \mathsf{g}^\perp + \mathrm{i}\mathsf{g}^\perp$. We then have the relations

$$\mathcal{G}\mathcal{Z} = Q, \qquad \mathcal{Z}\mathcal{G} = P, \tag{5.31}$$

where $Q = P^t = \mathbb{I} - \mathsf{g}\otimes\mathsf{z}/\langle \mathsf{g}, \mathsf{z}\rangle$, and we know from Theorem 5.4 that $\mathcal{Z}$ is symmetric. However, the conjugate direction expansion cannot be performed as easily as in the real case. Indeed, the nondegenerate bilinear form $(z, z') = \sum_{1\le i\le n} z_i z_i'$ naturally associated with complex symmetric matrices is not definite in $\mathbb{C}^n$. As a consequence, we may encounter breakdowns arising from zero scalar product in the decomposition into conjugate directions. In order to avoid such problems we will use the special structure of the matrices $\mathcal{G}$ and restrict the vectors z_i^*, $1 \le i \le n$, to be *real* vectors.

Theorem 5.13. *Assume that G is symmetric positive semi-definite, G' is symmetric, $\mathsf{z}, \mathsf{g} \in \mathbb{R}^n$, $N(G) = \mathbb{R}\mathsf{z}$, $G'\mathsf{z} = 0$, $\mathcal{G} = G + \mathrm{i}G'$, $\langle \mathsf{z}, \mathsf{g}\rangle \ne 0$, and let $\mathcal{Z}$ be the generalized inverse of $\mathcal{G}$ with nullscace $\mathbb{C}\mathsf{g}$ and range $\mathsf{g}^\perp + \mathrm{i}\mathsf{g}^\perp$. Let z_i^*, $1 \le i \le n$, be a basis of $\mathbb{R}^n$ with $\mathsf{z}_1^* = \mathsf{z}$, and define for convenience $\mathsf{z}_1 = \mathsf{z}_1^* = \mathsf{z}$, $\mathsf{g}_1 = \mathsf{g}$, $\mathcal{G}_1 = \mathcal{G}$, $\mathcal{Z}_1 = \mathcal{Z}$, $\mathcal{Q}_1 = Q$, $\mathcal{P}_1 = P$, $\mathcal{G}_0 = \mathcal{G}_1 + \mathsf{g}_1\otimes\mathsf{g}_1/(\mathsf{z}_1, \mathsf{g}_1)$, and $\mathcal{Z}_0 = \mathcal{Z}_1 + \mathsf{z}_1\otimes\mathsf{z}_1/(\mathsf{z}_1, \mathsf{g}_1)$. Define then inductively for $k \ge 1$ the vectors*

$$\mathsf{z}_k = \mathsf{z}_k^* - \sum_{1\le j\le k-1} \frac{(\mathsf{z}_k^*, \mathsf{g}_j)}{(\mathsf{z}_j, \mathsf{g}_j)}\mathsf{z}_j, \qquad \mathsf{g}_k = \mathcal{G}_{k-1}\mathsf{z}_k, \tag{5.32}$$

the linear operators

$$\mathcal{G}_k = \mathcal{G}_{k-1} - \frac{\mathsf{g}_k\otimes\mathsf{g}_k}{(\mathsf{z}_k, \mathsf{g}_k)}, \qquad \mathcal{Z}_k = \mathcal{Z}_{k-1} - \frac{\mathsf{z}_k\otimes\mathsf{z}_k}{(\mathsf{z}_k, \mathsf{g}_k)}, \tag{5.33}$$

and the projectors

$$\mathcal{Q}_k = \mathbb{I} - \sum_{1\le i\le k} \frac{\mathsf{g}_i\otimes\mathsf{z}_i}{(\mathsf{z}_i, \mathsf{g}_i)}, \qquad \mathcal{P}_k = \mathbb{I} - \sum_{1\le i\le k} \frac{\mathsf{z}_i\otimes\mathsf{g}_i}{(\mathsf{z}_i, \mathsf{g}_i)}. \tag{5.34}$$

Then the sequence of vectors z_i, g_i, $1 \le i \le n$, is such that $\Re(\mathsf{z}_i, \mathsf{g}_i) > 0$, $\mathrm{span}\{\mathsf{z}_1, \dots, \mathsf{z}_i\} = \mathrm{span}\{\mathsf{z}_1^*, \dots, \mathsf{z}_i^*\}$, $\mathsf{g}_i = \mathcal{G}_{i-1}\mathsf{z}_i$, $\mathsf{z}_i = \mathcal{Z}_{i-1}\mathsf{g}_i$, $1 \le i \le n$, $(\mathsf{z}_i, \mathsf{g}_j) = 0$ if $i \ne j$, $1 \le i, j \le n$. Moreover, for any $0 \le k \le n$ we have the relations

$$\mathcal{G}_k\mathcal{Z}_k = \mathcal{Q}_k, \qquad \mathcal{Z}_k\mathcal{G}_k = \mathcal{P}_k, \tag{5.35}$$

where $\mathcal{P}_k$ is the projector onto $\mathrm{span}\{\mathsf{g}_1, \dots, \mathsf{g}_k\}^\perp$ parallel to $\mathrm{span}\{\mathsf{z}_1, \dots, \mathsf{z}_k\}$, $\mathcal{Q}_k$ is the projector onto $\mathrm{span}\{\mathsf{z}_1, \dots, \mathsf{z}_k\}^\perp$ parallel to $\mathrm{span}\{\mathsf{g}_1, \dots, \mathsf{g}_k\}$, and $\mathcal{P}_0 = \mathcal{Q}_0 = \mathbb{I}$, $\mathcal{G}_0\mathcal{Z}_0 = \mathcal{Z}_0\mathcal{G}_0 = \mathbb{I}$, $\mathcal{G}_n = \mathcal{Z}_n = \mathcal{P}_n = \mathcal{Q}_n = 0$. In addition, for any $0 \le k \le n$, $\mathcal{G}_k$ and $\mathcal{Z}_k$ are symmetric, $N(\mathcal{G}_k) = \mathrm{span}\{\mathsf{z}_1, \dots, \mathsf{z}_k\}$, $R(\mathcal{G}_k) = \mathrm{span}\{\mathsf{z}_1, \dots, \mathsf{z}_k\}^\perp$, the matrix $\Re(\mathcal{G}_k)$ is positive semi-definite and $N\big(\Re(\mathcal{G}_k)\big) = \mathrm{span}\{\mathsf{z}_1, \dots, \mathsf{z}_k\}$, and $N\big(\Re(\mathcal{G}_k)\big) \subset N\big(\Im(\mathcal{G}_k)\big)$. Moreover, $\mathcal{Z}_k$ is the generalized inverse of $\mathcal{G}_k$ with prescribed nullspace $N(\mathcal{Z}_k) = \mathrm{span}\{\mathsf{g}_1, \dots, \mathsf{g}_k\}$, and range $R(\mathcal{Z}_k) = \mathrm{span}\{\mathsf{g}_1, \dots, \mathsf{g}_k\}^\perp$. Conversely, $\mathcal{G}_k$ is the generalized inverse of $\mathcal{Z}_k$ with prescribed nullspace $N(\mathcal{G}_k) = \mathrm{span}\{\mathsf{z}_1, \dots, \mathsf{z}_k\}$, and range $R(\mathcal{G}_k) = \mathrm{span}\{\mathsf{z}_1, \dots, \mathsf{z}_k\}^\perp$. Finally, we have $\mathsf{g}_i = \mathcal{G}\mathsf{z}_i$, $\mathsf{z}_i = \mathcal{Z}\mathsf{g}_i$, $2 \le i \le n$, $\mathsf{g}^\perp = \mathrm{span}\{\mathsf{z}_2, \dots, \mathsf{z}_n\}$, the directions z_i, $2 \le i \le n$, are conjugate for $\mathcal{G}$ whereas the directions g_i, $2 \le i \le n$, are conjugate for $\mathcal{Z}$, and we have the decompositions

$$\mathcal{G} = \sum_{2\le j\le n} \frac{\mathsf{g}_i\otimes\mathsf{g}_i}{(\mathsf{z}_i, \mathsf{g}_i)}, \qquad \mathcal{Z} = \sum_{2\le j\le n} \frac{\mathsf{z}_i\otimes\mathsf{z}_i}{(\mathsf{z}_i, \mathsf{g}_i)}, \tag{5.36}$$

$$\mathbb{I} = \sum_{1\le j\le n} \frac{\mathsf{g}_i\otimes\mathsf{z}_i}{(\mathsf{z}_i, \mathsf{g}_i)} = \sum_{1\le j\le n} \frac{\mathsf{z}_i\otimes\mathsf{g}_i}{(\mathsf{z}_i, \mathsf{g}_i)}. \tag{5.37}$$

Proof. The proof is established by induction on k as in the real case and the main idea in order to avoid breakdowns is to use the fact that any subspace $F \subset \mathbb{C}^n$ spanned by real vectors is such that $F = \overline{F}$ as in the proof of the positivity of the real part of diagonal coefficients in a complex Choleski method [33].

We have already defined $\mathsf{z}_1 = \mathsf{z}_1^* = \mathsf{z}$ and z_2 and g_2 are easily constructed as in the real case by letting

$$\mathsf{z}_2 = \mathsf{z}_2^* - \frac{(\mathsf{z}_2^*, \mathsf{g}_1)}{(\mathsf{z}_1, \mathsf{g}_1)}\mathsf{z}_1, \qquad \mathsf{g}_2 = \mathcal{G}\mathsf{z}_2. \tag{5.38}$$

Then we have $\mathsf{z}_2 \in \mathbb{R}^n$, $\mathsf{g}_2 \in \mathbb{C}^n$, $(\mathsf{z}_2, \mathsf{g}_1) = 0$, $(\mathsf{g}_2, \mathsf{z}_1) = (\mathcal{G}\mathsf{z}_2, \mathsf{z}_1) = (\mathsf{z}_2, \mathcal{G}\mathsf{z}_1) = 0$, $\Re(\mathsf{z}_2, \mathsf{g}_2) = \langle G\mathsf{z}_2, \mathsf{z}_2\rangle \neq 0$ since $\mathsf{z}_2 \notin N(G) = \mathbb{R}\mathsf{z}_1$. Moreover $\mathcal{Z}\mathsf{g}_2 = \mathcal{Z}\mathcal{G}\mathsf{z}_2 = \mathsf{z}_2$ since $(\mathsf{z}_2, \mathsf{g}_1) = 0$ and obviously $\mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\} = \mathrm{span}\{\mathsf{z}_1^*, \mathsf{z}_2^*\}$. Defining then $\mathcal{G}_2$, $\mathcal{Z}_2$, $\mathcal{P}_2$, and $\mathcal{Q}_2$, from (5.33)(5.34) with $k = 2$ a direct calculation yields the relations $\mathcal{G}_2\mathcal{Z}_2 = \mathcal{Q}_2$, $\mathcal{Z}_2\mathcal{G}_2 = \mathcal{P}_2$, and it is straighforward to check that $\mathcal{P}_2$ is the projector onto $\mathrm{span}\{\mathsf{g}_1, \mathsf{g}_2\}^\perp$ parallel to $\mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\}$, and $\mathcal{Q}_2$ is the projector onto $\mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\}^\perp$ parallel to $\mathrm{span}\{\mathsf{g}_1, \mathsf{g}_2\}$. Moreover, since $N(\mathcal{G}) = \mathbb{C}\mathsf{z}_1$ and by construction

$$\mathcal{G}_2 x = \mathcal{G}\Big(x - \tfrac{(\mathcal{G}\mathsf{z}_2, x)}{(\mathsf{z}_2, \mathcal{G}\mathsf{z}_2)}\mathsf{z}_2\Big),$$

we deduce that $\mathcal{G}_2 x = 0$ implies $x \in \mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\}$ and conversely $\mathcal{G}_2\mathsf{z}_1 = \mathcal{G}_2\mathsf{z}_2 = 0$ so that $N(\mathcal{G}_2) = \mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\}$. This now implies that $R(\mathcal{G}_2) = \mathrm{span}\{\mathsf{z}_1, \mathsf{z}_2\}^\perp$ and proceeding similarly we obtain that $N(\mathcal{Z}_2) = \mathrm{span}\{\mathsf{g}_1, \mathsf{g}_2\}$ and $R(\mathcal{Z}_2) = \mathrm{span}\{\mathsf{g}_1, \mathsf{g}_2\}^\perp$.

Assume then that k steps of the procedure have been taken where $2 \leq k < n$ and consider the vector z_{k+1} defined from (5.32). From this definition we obtain that $(\mathsf{z}_{k+1}, \mathsf{g}_l) = 0$ for $1 \leq l \leq k$, and it is easily established that $\mathrm{span}\{\mathsf{z}_1^*, \ldots, \mathsf{z}_{k+1}^*\} = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\}$. Defining $\mathsf{g}_{k+1} = \mathcal{G}_k\mathsf{z}_{k+1}$ we obtain that $(\mathsf{g}_{k+1}, \mathsf{z}_l) = 0$ for $1 \leq l \leq k$, since $R(\mathcal{G}_k) = \mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}^\perp$, and similarly that $\mathsf{z}_{k+1} = \mathcal{Z}_k\mathsf{g}_{k+1}$ since $\mathsf{z}_{k+1} \in \mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}^\perp$ and $\mathcal{Z}_k\mathcal{G}_k = \mathbb{I} - \sum_{1\leq i\leq k} \mathsf{z}_k{\otimes}\mathsf{g}_k/(\mathsf{z}_k, \mathsf{g}_k)$ from the induction hypothesis. We now establish that $\Re(\mathsf{z}_{k+1}, \mathsf{g}_{k+1}) > 0$ and this will also prove that $\mathsf{g}_{k+1} \notin \mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\}$. Indeed, we have $(\mathsf{g}_{k+1}, \mathsf{z}_{k+1}) = (\mathcal{G}_k\mathsf{z}_{k+1}, \mathsf{z}_{k+1})$ so that $(\mathsf{g}_{k+1}, \mathsf{z}_{k+1}) = (\mathcal{G}_k\mathsf{z}_{k+1}, \mathsf{z}_{k+1}^*)$ since $(\mathsf{g}_{k+1}, \mathsf{z}_l) = 0$, $1 \leq l \leq k$, and similarly $(\mathsf{g}_{k+1}, \mathsf{z}_{k+1}) = (\mathcal{G}_k\mathsf{z}_{k+1}, \overline{\mathsf{z}}_{k+1})$ since $\mathsf{z}_{k+1} - \mathsf{z}_{k+1}^* \in \mathrm{span}\{\mathsf{z}_1^*, \ldots, \mathsf{z}_k^*\}$ and thus $\overline{\mathsf{z}}_{k+1} - \mathsf{z}_{k+1}^* \in \mathrm{span}\{\mathsf{z}_1^*, \ldots, \mathsf{z}_k^*\}$ since $\mathsf{z}_1^*, \ldots, \mathsf{z}_k^*$ are real vectors. We have thus established that $(\mathsf{g}_{k+1}, \mathsf{z}_{k+1}) = (\mathcal{G}_k\mathsf{z}_{k+1}, \overline{\mathsf{z}}_{k+1}) = \langle \mathcal{G}_k\mathsf{z}_{k+1}, \mathsf{z}_{k+1}\rangle$ and we may now use $\mathcal{G}_k\mathsf{z}_{k+1} = \mathcal{G}\mathsf{z}_{k+1}$ which is a consequence of (5.33) and $(\mathsf{z}_{k+1}, \mathsf{g}_l) = 0$, $1 \leq l \leq k$, to obtain that $(\mathsf{g}_{k+1}, \mathsf{z}_{k+1}) = \langle \mathcal{G}\mathsf{z}_{k+1}, \mathsf{z}_{k+1}\rangle$. We may now use the identity $\Re\langle \mathcal{G}z, z\rangle = \langle Gx, x\rangle + \langle Gy, y\rangle$ valid for $z \in \mathbb{C}^n$, $x, y \in \mathbb{R}^n$, $z = x + \mathrm{i}y$ to conclude that $\Re(\mathsf{g}_{k+1}, \mathsf{z}_{k+1}) > 0$ since $\mathsf{z}_{k+1} \notin \mathbb{C}\mathsf{z}_1$ for $k \geq 1$.

Upon defining $\mathcal{G}_{k+1}$ and $\mathcal{Z}_{k+1}$ from (5.33), $\mathcal{G}_{k+1}$ and $\mathcal{Z}_{k+1}$ are symmetric and the nullspace of $\mathcal{G}_{k+1}$ is easily deduced from that of $\mathcal{G}_k$ as in the special case $k = 1$. We thus deduce the range of $\mathcal{G}_{k+1}$ and we can proceed similarly for $\mathcal{Z}_{k+1}$. A direct calculation also yields $\mathcal{G}_{k+1}\mathcal{Z}_{k+1} = \mathcal{Q}_{k+1}$ and $\mathcal{Z}_{k+1}\mathcal{G}_{k+1} = \mathcal{P}_{k+1}$ and it is straightforward to check that and $\mathcal{P}_{k+1}$ is the projector onto $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_{k+1}\}^\perp$ parallel to $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\}$, and $\mathcal{Q}_{k+1}$ is the projector onto $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\}^\perp$ parallel to $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_{k+1}\}$. As a consequence, $\mathcal{Z}_{k+1}$ is the generalized inverse of $\mathcal{G}_{k+1}$ with prescribed nullspace $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_{k+1}\}$ and range $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_{k+1}\}^\perp$ and $\mathcal{G}_{k+1}$ is the generalized inverse of $\mathcal{Z}_{k+1}$ with prescribed nullspace $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\}$ and range $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_{k+1}\}^\perp$. The relation $\mathcal{G}_0\mathcal{Z}_0 = \mathbb{I}$ is also established directly from the definitions of $\mathcal{G}_0$, $\mathcal{Z}_0$, and $\mathcal{G}\mathcal{Z} = \mathbb{I} - \mathsf{g}_1{\otimes}\mathsf{z}_1/(\mathsf{g}_1, \mathsf{z}_1)$.

The induction is therefore established, aside from the positivity properties of $\Re(\mathcal{G}_k)$, and since $N(\mathcal{G}_n) = N(\mathcal{Z}_n) = \mathbb{C}^n$ we deduce that $\mathcal{G}_n = \mathcal{Z}_n = \mathcal{P}_n = \mathcal{Q}_n = 0$. From $\mathcal{G}_n = 0$ and (5.33) we deduce that $\mathcal{G} = \sum_{2\leq j\leq n} \mathsf{g}_k{\otimes}\mathsf{g}_k/(\mathsf{z}_k, \mathsf{g}_k)$ and similarly that $\mathcal{Z} = \sum_{2\leq j\leq n} \mathsf{z}_k{\otimes}\mathsf{z}_k/(\mathsf{z}_k, \mathsf{g}_k)$. These relations finally implies the expansions (5.37) from $\mathcal{G}_0\mathcal{Z}_0 = \mathbb{I}$.

We now show that $\Re(\mathcal{G}_k)$ is positive definite with nullspace $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}$. To establish this property, we will prove that $\big(\Re(\mathcal{G}_k)z, z\big) \geq 0$ when $z \in \mathbb{R}^n$ and that $\big(\Re(\mathcal{G}_k)z, z\big) = 0$ if and only if $z \in \mathrm{span}\{\mathsf{z}_1^*, \ldots, \mathsf{z}_k^*\}$. An easy induction first establishes that $\mathrm{span}\{\mathsf{g}_1, \ldots, \mathsf{g}_k\} = \mathrm{span}\big\{\mathcal{G}_0(\mathsf{z}_1^*), \ldots, \mathcal{G}_0(\mathsf{z}_k^*)\big\}$, thanks to $\mathsf{g}_k = \mathcal{G}_{k-1}\mathsf{z}_k = \mathcal{G}_0\mathsf{z}_k$ and $\mathsf{z}_k - \mathsf{z}_k^* \in \mathrm{span}\{\mathsf{z}_1^*, \ldots, \mathsf{z}_{k-1}^*\}$. As a consequence,

$$\mathrm{span}\{\mathsf{z}_1^*, \ldots, \mathsf{z}_k^*\} \oplus \mathrm{span}\big\{\mathcal{G}_0(\mathsf{z}_1^*), \ldots, \mathcal{G}_0(\mathsf{z}_k^*)\big\}^\perp = \mathbb{C}^n,$$

and for any $z \in \mathbb{C}^n$ we may write $z = \sum_{1\leq i\leq k} \alpha_i\mathsf{z}_i^* + w$ where $(w, \mathsf{g}_l) = 0$, $1 \leq l \leq k$, and $\big(w, \mathcal{G}_0(\mathsf{z}_l^*)\big) = 0$, $1 \leq l \leq k$. After some algebra, upon denoting γ the inverse of the matrix $\big((\mathsf{z}_i^*, \mathcal{G}(\mathsf{z}_j^*)\big)_{1\leq i,j\leq k}$, we obtain that $w = \big(\mathbb{I} - \sum_{1\leq i,j\leq k} \gamma_{ij}\mathsf{z}_i^*{\otimes}\mathcal{G}_0(\mathsf{z}_j^*)\big)z$. We now have the properties that $\mathcal{G}_k z = \mathcal{G}_k w$ and that $\mathcal{G}_k w = \mathcal{G}_0 w$ in such a way that $\mathcal{G}_k z = \mathcal{G}_0 w$ and $\mathcal{G}_k = \mathcal{G}_0 - \sum_{1\leq i,j\leq k} \gamma_{ij}\mathcal{G}_0(\mathsf{z}_i^*){\otimes}\mathcal{G}_0(\mathsf{z}_j^*)$. In addition $(\mathcal{G}_k z, z) = (\mathcal{G}_0 w, z)$ but since $w - z \in \mathrm{span}\{\mathsf{z}_1^*, \ldots, \mathsf{z}_k^*\}$ we also have $\overline{w} - z \in \mathrm{span}\{\mathsf{z}_1^*, \ldots, \mathsf{z}_k^*\}$ when $z \in \mathbb{R}^n$ and thus $(\mathcal{G}_k z, z) = (\mathcal{G}_0 w, \overline{w}) = \langle \mathcal{G}_0 w, w\rangle$ when $z \in \mathbb{R}^n$. Now if $w = a + \mathrm{i}b$ we have $\Re\langle \mathcal{G}_0 w, w\rangle = \langle G_0 a, a\rangle + \langle G_0 b, b\rangle$ where $G_0 = G + \mathsf{g}_1{\otimes}\mathsf{g}_1/\langle \mathsf{z}_1, \mathsf{g}_1\rangle$ is positive definite so that $\Re(\mathcal{G}_k z, z) \geq 0$ when $z \in \mathbb{R}^n$ and it is zero if and only if $w = 0$. Finally, the properties $\mathsf{g}_i = \mathcal{G}\mathsf{z}_i$, $\mathsf{z}_i = \mathcal{Z}\mathsf{g}_i$, $2 \leq i \leq n$, $\mathsf{g}^\perp = \mathrm{span}\{\mathsf{z}_2, \ldots, \mathsf{z}_n\}$, and the fact that the directions z_i, $2 \leq i \leq n$, are conjugate for $\mathcal{G}$ and the directions g_i, $2 \leq i \leq n$, are conjugate for $\mathcal{Z}$, are established as in the real case and the proof is complete. □

Corollary 5.14. *Keeping the notation of the preceding theorem, and letting $b_k = \mathcal{Q}_k b$, the linear system*

$$\begin{cases} \mathcal{G}_k a_k = b_k, \\ (a_k, \mathsf{g}_l) = 0, \quad 1 \leq l \leq k, \end{cases} \tag{5.39}$$

is well posed, its solution is $a_k = \mathcal{Z}_k b$, *and we have the expansion*

$$a = a_k + \sum_{1 \le l \le k} \frac{(\mathsf{z}_k, b)}{(\mathsf{z}_k, \mathsf{g}_k)} \mathsf{z}_k, \tag{5.40}$$

where $a = a_1$ *is the unique solution of* $\mathcal{G}a = b$ *such that* $\langle a, \mathsf{g} \rangle = 0$.

Proof. The proof is similar to that of the real case. □

As a special important case we have

$$\mathcal{G}_2 = \mathcal{G} - \mathsf{g}_2 \otimes \mathsf{g}_2 / (\mathsf{z}_2, \mathsf{g}_2), \qquad \mathcal{Z}_2 = \mathcal{Z} - \mathsf{z}_2 \otimes \mathsf{z}_2 / (\mathsf{z}_2, \mathsf{g}_2), \tag{5.41}$$

and

$$\mathcal{G}_2 \mathcal{Z}_2 = \mathcal{Q}_2, \qquad \mathcal{Z}_2 \mathcal{G}_2 = \mathcal{P}_2. \tag{5.42}$$

Moreover, $\mathcal{Z}_2$ is the generalized inverse of $\mathcal{G}_2$ with prescribed nullspace $N(\mathcal{Z}_2) = \text{span}\{\mathsf{g}_1, \mathsf{g}_2\}$ and range $R(\mathcal{Z}_2) = \text{span}\{\mathsf{g}_1, \mathsf{g}_2\}^\perp$, and $\mathcal{G}_2$ is the generalized inverse of $\mathcal{Z}_2$ with prescribed nullspace $N(\mathcal{G}_2) = \text{span}\{\mathsf{z}_1, \mathsf{z}_2\}$ and range $R(\mathcal{G}_2) = \text{span}\{\mathsf{z}_1, \mathsf{z}_2\}^\perp$. Letting $a_2 = \mathcal{Z}_2 b$, $b_2 = \mathcal{Q}_2 b$, we obtain the new transport linear system

$$\begin{cases} \mathcal{G}_2 a_2 = b_2, \\ (a_2, \mathsf{g}_1) = (a_2, \mathsf{g}_1) = 0. \end{cases} \tag{5.43}$$

This system is well posed and its unique solution is given by $a_2 = \mathcal{Z}_2 b$ and the solution of the original system a can be written

$$a = a_2 + \frac{(\mathsf{z}_2, b)}{(\mathsf{z}_2, b)} \mathsf{z}_2. \tag{5.44}$$

We now investigate more closely the structure of the matrices $\Re(\mathcal{G}_2)$ and $\Im(\mathcal{G}_2)$. We evaluate the matrix $\Re(\mathcal{G}_2)$ and establish that $\Im(\mathcal{G}_2)$ shares a similar form with $\Im(\mathcal{G}_1) = G'$ when the later matrix reads $G' = Q\mathcal{D}'P$. After some lengthy algebra, thanks to $\mathsf{z}_2 \in \mathbb{R}^n$, one can indeed establish that

$$\begin{aligned} \Re(\mathcal{G}_2) &= G - \frac{G\mathsf{z}_2 \otimes G\mathsf{z}_2}{\langle G\mathsf{z}_2, \mathsf{z}_2 \rangle} + \frac{r_2 \otimes r_2}{\langle G\mathsf{z}_2, \mathsf{z}_2 \rangle m^2}, \\ \Im(\mathcal{G}_2) &= \big(\mathbb{I} - \mathsf{s}_1 \otimes \mathsf{z}_1 - \mathsf{s}_2 \otimes \mathsf{z}_2\big) \mathcal{D}' \big(\mathbb{I} - \mathsf{z}_1 \otimes \mathsf{s}_1 - \mathsf{z}_2 \otimes \mathsf{s}_2\big), \end{aligned}$$

where $\mathcal{D}'$ is the diagonal matrix such that $G' = Q\mathcal{D}'P$, $m^2 = (G\mathsf{z}_2, \mathsf{z}_2)^2 + (G'\mathsf{z}_2, \mathsf{z}_2)^2$, and where

$$r_2 = (G'\mathsf{z}_2, \mathsf{z}_2) G\mathsf{z}_2 - (G\mathsf{z}_2, \mathsf{z}_2) G'\mathsf{z}_2,$$

$$\mathsf{s}_1 = \frac{\mathsf{g}_1}{\langle \mathsf{z}_1, \mathsf{g}_1 \rangle} \qquad \mathsf{s}_2 = \frac{mG\mathsf{z}_2 + (G\mathsf{z}_2, \mathsf{z}_2) G\mathsf{z}_2 + (G'\mathsf{z}_2, \mathsf{z}_2) G'\mathsf{z}_2}{m\big(m + (G\mathsf{z}_2, \mathsf{z}_2)\big)}.$$

These expressions greatly simplify when $(G'\mathsf{z}_2, \mathsf{z}_2) = 0$ and then $m = (G\mathsf{z}_2, \mathsf{z}_2)$ which is often the case in practice as discussed in Section 7. Thanks to the special structure of $\Im(\mathcal{G}_2)$, the inverse of a matrix in the form $M + \mathrm{i}\Im(\mathcal{G}_2)$, where $M \in \mathbb{R}^{n,n}$ is symmetric positive definite, is easily expressed in terms of the inverse of $M + \mathrm{i}\mathcal{D}'$ as described in [33].

6 Orthogonal residual algorithms

Conjugate gradients-type methods—used with preconditioning—are among the most effective iterative procedures for solving Hermitian systems [37, 41, 34]. Projected conjugate gradients methods have been introduced in particular to solve real symmetric constrained singular semi-definite systems arising from multicomponent transport [28, 15, 19]. For general linear systems, however, one cannot obtain short recurrence algorithms which globally minimize some error norm over the corresponding Krylov subspaces unless the matrix has certain rather special spectral properties [21]. Complex symmetric systems have been investigated motivated by electromagnetic applications [22, 24, 25, 3, 32, 33]. In particular, projected orthogonal residuals have been investigated in order to solve the complex symmetric constrained singular systems arising from magnetized multicomponent transport [22, 32, 33].

These algorithms reduce to projected conjugate gradients methods in the absence of magnetization, that is, when the imaginary part of the system matrix vanishes.

We investigate in this section the links between orthogonal residuals techniques and the expansions into conjugate directions obtained in the previous section. We establish that projected orthogonal residuals algorithms applied to the more singular formulations of the transport linear systems are equivalent to constraining the first search directions.

6.1 Projected orthogonal directions

We present in this section a projected orthogonal residuals method for constrained singular linear systems arising from multicomponent transport [33]. We consider again a matrix in the form $\mathcal{G} = G + \mathrm{i}G'$ where G, G' are real symmetric matrices, G is positive semi-definite and $G'N(G) = 0$, a vector $b \in R(\mathcal{G})$, a subspace $\mathcal{C} \subset \mathbb{R}^n$ complementary to $N(G)$ and $\mathcal{C}$ the complexification of $\mathcal{C}$. This algorithms is associated 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 [22]. Note that the projector onto $\mathcal{C}$ parallel to $N(G) + \mathrm{i}N(G) = N(G + \mathrm{i}G')$ coincide with the projector onto $\mathcal{C}$ parallel to $N(G)$ and is denoted by $\mathcal{P}$.

Assuming that $M \in \mathbb{R}^{n,n}$ is hermitian positive definite, the projected preconditioned orthogonal residuals algorithm can be described as follows. Let $z_0 \in \mathbb{C}^n$, be an initial guess, $z'_0 = \mathcal{P}z_0$, $r'_0 = b - \mathcal{G}z'_0$, $p'_0 = \mathcal{P}M^{-1}r'_0$. 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 $\prod_{0\leq i\leq k-1}\langle \mathcal{G}p'_i, p'_i\rangle \neq 0$, $r'_i = b - \mathcal{G}z'_i$, $0 \leq i \leq k$, and

$$\langle M^{-1}r'_i, r'_j\rangle = 0, \qquad 0 \leq j < i \leq k, \tag{6.1}$$

$$\langle \mathcal{G}p'_i, p'_j\rangle = 0, \qquad 0 \leq j < i \leq k, \tag{6.2}$$

$$\langle r'_i, p'_j\rangle = 0, \qquad 0 \leq j < i \leq k, \tag{6.3}$$

$$\begin{aligned} &\mathcal{K}_i = \mathrm{span}(r'_0, \ldots, r'_i), = \mathrm{span}(r'_0, \ldots, (\mathcal{G}M^{-1})^i r'_0), \qquad 0 \leq i \leq k, \\ &\mathcal{K}'_i = \mathrm{span}(p'_0, \ldots, p'_i) = \mathcal{P}M^{-1}\mathcal{K}_i, \qquad \mathcal{K}_i = \mathcal{H}\mathcal{K}'_i, \qquad 0 \leq i \leq k, \end{aligned} \tag{6.4}$$

where $\dim(\mathcal{K}_i) = i + 1$ for $0 \leq i \leq k - 1$ and where $\mathcal{H} = \mathbb{I} - \sum_{1\leq i,j\leq p} \gamma_{ij}\mathsf{z}_i \otimes M\mathsf{z}_j$ and $(\gamma_{ij})_{1\leq i,j\leq p}$ is the inverse of the matrix $\big(\langle M\mathsf{z}_i, \mathsf{z}_j\rangle\big)_{1\leq i,j\leq p}$ and $\dim(\mathcal{K}_i) = \dim(\mathcal{K}'_i) = i + 1$ 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. On the other hand if $\langle \mathcal{G}p'_k, p'_k\rangle \neq 0$ we introduce the solution $\nu'_{k0}, \ldots, \nu'_{kk}$ of the linear systems

$$\begin{pmatrix} \langle \mathcal{G}p'_0, p'_0\rangle & & & \\ \langle \mathcal{G}p'_0, p'_1\rangle & \langle \mathcal{G}p'_1, p'_1\rangle & & \\ \vdots & \vdots & \ddots & \\ \langle \mathcal{G}p'_0, p'_k\rangle & \langle \mathcal{G}p'_1, p'_k\rangle & \ldots & \langle \mathcal{G}p'_k, p'_k\rangle \end{pmatrix} \begin{pmatrix} \nu'_{k0} \\ \nu'_{k1} \\ \vdots \\ \nu'_{kk} \end{pmatrix} = \begin{pmatrix} \langle \mathcal{G}M^{-1}\mathcal{G}p'_k, p'_0\rangle \\ \langle \mathcal{G}M^{-1}\mathcal{G}p'_k, p'_1\rangle \\ \vdots \\ \langle \mathcal{G}M^{-1}\mathcal{G}p'_k, p'_k\rangle \end{pmatrix}, \tag{6.5}$$

$\sigma'_k = \langle r'_k, p'_k\rangle / \langle \mathcal{G}p'_k, p'_k\rangle$ and we set

$$p'_{k+1} = \mathcal{P}M^{-1}\mathcal{G}p'_k - \sum_{0\leq j\leq k} \nu'_{kj}p'_j, \qquad z'_{k+1} = z'_k + \sigma'_k p'_k, \qquad r'_{k+1} = r'_k - \sigma'_k \mathcal{G}p'_k. \tag{6.6}$$

Theorem 6.1. *The projected preconditioned orthogonal residuals algorithm is well defined and converges in at most* $\mathrm{rank}(\mathcal{G})$ *steps towards the unique solution a of $\mathcal{G}a = b$ and $a \in \mathcal{C}$. Moreover, the iterates z'_k, $k \geq 1$, are the projections of the iterates z_k, $k \geq 1$, of the corresponding unprojected algorithm [33].*

When the magnetic part G' vanishes and $\mathcal{G} = G$ is positive semi-definite we recover the projected version of the conjugate gradient algorithm [22, 19].

Remark 6.2. *The preceding algorithm correspond to the unpreconditioned version applied to a the system rewritten in the form*

$$\begin{cases} \mathcal{B}^{-1}\mathcal{G}\mathcal{B}^{-*}(\mathcal{B}^* a) = \mathcal{B}^{-1}b, \\ \mathcal{B}^* a \in \mathcal{B}^*\mathcal{C}, \end{cases} \tag{6.7}$$

where $\mathcal{B}$ is an invertible matrix, $\mathcal{B}^*$ its adjoint and $\mathcal{B}^{-*}$ the inverse of the adjoint. The resulting algorithm is then rewritten with the help of the hermitian matrix $M = \mathcal{B}\mathcal{B}^*$. In order to precondition the orthogonal residuals algorithm one may also consider the following reformulation of (5.1)

$$\begin{cases} \mathcal{B}^{-1}\mathcal{G}\mathcal{B}^{-1}(\mathcal{B}a) = \mathcal{B}^{-1}b, \\ \mathcal{B}a \in \mathcal{B}\mathcal{C}, \end{cases} \tag{6.8}$$

where $\mathcal{B}$ is an invertible matrix. The corresponding iterative scheme is more complex than the algorithm associated with (6.7) *and is not guarantee to converge.*

6.2 Conjugate directions versus conjugate gradients

When applied to a symmetric positive semi-definite matrix G the projected orthogonal residuals algorithm yield the projected conjugate gradient algorithm for singular systems [22, 33]. Starting form $x_0 = 0$, the approximate solution is then obtained in the form

$$p'_0 \frac{\langle p'_0, r'_0\rangle}{\langle Gp'_0, p'_0\rangle} + \cdots + p'_l \frac{\langle p'_l, r'_l\rangle}{\langle Gp'_l, p'_l\rangle},$$

where $l+1$ is the dimension of the subspace spanned by the vectors $G^k b$, $k \geq 0$. Thanks to the symmetry of G we then have the classical relations $\langle p'_l, r'_l\rangle = \langle p'_l, r'_0\rangle = \langle p'_l, b\rangle$ in such a way that the generalized inverse Z is approximated in the form

$$\frac{p'_0 \otimes p'_0}{\langle Gp'_0, p'_0\rangle} + \cdots + \frac{p'_l \otimes p'_l}{\langle Gp'_l, p'_l\rangle},$$

over the Krylov subspace $\mathrm{span}\{b, \ldots, G^l b\}$. An important difference with the expansion into conjugate directions (5.26) obtained in Theorem 5.11 in therefore that the fixed subspaces $\mathrm{span}\{\mathsf{z}_1, \ldots, \mathsf{z}_k\}$, $k \geq 1$, which are independent of b, are now replaced by the Krylov subspaces $\mathrm{span}\{b, \ldots, G^i b\}$, $i \geq 0$. Moreover, the algorithm associated with the expansion (5.26) is linear whereas orthogonal residuals algorithms are non linear. Finally, we further obtain with the orthogonal residuals algorithm the important relations $\langle M^{-1} r'_i, r'_j\rangle = 0$, $0 \leq i, j \leq l$. Since the expansion associated with the more singular formulation is associated with a decomposition of Z in the form

$$Z = \frac{\mathsf{z}_2 \otimes \mathsf{z}_2}{\langle G\mathsf{z}_2, \mathsf{z}_2\rangle} + Z_2,$$

we conclude that using the more singular formulation with projected conjugate gradients would constrain the first projected search direction p'_0 to be the vector z_2 and the subsequent directions would then chosen in the Krylov subspaces associated with G_2.

Similarly, in the complex magnetized case, starting from $z_0 = 0$, the approximate solution is then obtained in the form

$$p'_0 \frac{\langle p'_0, r'_0\rangle}{\langle \mathcal{G}p'_0, p'_0\rangle} + \cdots + p'_l \frac{\langle p'_l, r'_l\rangle}{\langle \mathcal{G}p'_l, p'_l\rangle}, \tag{6.9}$$

where $l+1$ is the dimension of the subspace spanned by the vectors $\mathcal{G}^k b$, $k \geq 0$. When $\mathcal{G}$ is not Hermitian, we do not have a simple relation between $\langle p'_i, r'_i\rangle$ and $\langle p'_i, r'_0\rangle$, $i \geq 1$, where $r'_0 = \mathcal{P}b = b$. However, when z_2 is a real vector, we have $(\mathcal{G}\mathsf{z}_2, \mathsf{z}_2) = \langle \mathcal{G}\mathsf{z}_2, \mathsf{z}_2\rangle$ and we may still interpret the first term of the expansion

$$\mathcal{Z} = \frac{\mathsf{z}_2 \otimes \mathsf{z}_2}{(\mathcal{G}\mathsf{z}_2, \mathsf{z}_2)} + \mathcal{Z}_2,$$

as the first term of an expansion contraining the first projected search direction p'_0 to be the real direction z_2.

After some algebra, one can further establish, by induction on i, expressions in the form

$$\langle r'_i, p'_i\rangle = \langle r'_0, p'_i\rangle - \sum_{0 \leq j \leq i-1} \alpha_{ij} \langle r'_0, p'_j\rangle,$$

where the complex coefficients α_{ij}, $1 \leq i \leq l$, $0 \leq j \leq i-1$, involve the quantities $\langle \mathcal{G}p'_k, p'_l\rangle$, $0 \leq k \leq l \leq i-1$. This yields expansions of the generalized inverse $\mathcal{Z}$ of $\mathcal{G}$ in the form

$$\sum_{1 \leq i \leq l} \Big(\frac{p_i \otimes \overline{p}_i}{\langle \mathcal{G}p'_i, p'_i\rangle} - \sum_{0 \leq j \leq i-1} \alpha_{ij} \frac{p_i \otimes \overline{p}_j}{\langle \mathcal{G}p'_i, p'_i\rangle} \Big), \tag{6.10}$$

over the Krylov subspace span$\{b, \ldots, \mathcal{G}^l b\}$. In other words, since the orthogonal residuals algorithm needs to use a positive definite scalar product, the Hermitian scalar product has been used. The price to pay in then that only half of the conjugacy relations are generally satisfied, since $\mathcal{G}$ is symmetric but not Hermitian, and the resulting expansion of $\mathcal{Z}$ is more complex than the expansions obtained in a symmetric framework in Theorem 5.13. However, the orthogonal residuals algorithm is guarantee to converge at variance with the symmetric expansion (5.36) which has been restricted to directions spanned by real vectors. In addition, only the expansion (6.9) is used in practice, not the resulting matrix expression (6.10).

Remark 6.3. *The orthogonality relations between residuals do not necessarily hold when the search directions are in prescribed subspaces as in Theorems 5.11 and 5.13. Letting for instance*

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix} \qquad p_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad b = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

we obtain for $x_0 = 0$ *that* $r_0 = b$ *and* $\sigma_0 = \langle r_0, p_0 \rangle / \langle A p_0, p_0 \rangle = 0$ *so that* $r_1 = r_0$ *and* $\langle r_1, r_0 \rangle > 0$.

7 Application to diffusion matrices

Numerical simulation of reactive flows with complex chemistry and detailed transport requires to evaluate diffusion fluxes. When only the species diffusion velocities are to be evaluated—and not the diffusion matrices—Stefan-Maxwell type equations can be solved by using either a projected conjugate gradient method or—in the complex case—a projected orthogonal residuals algorithm as investigated in Section 8. Only the diffusion velocities are required when an explicit time marching technique is use 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 time step' is taken to be explicit. On the other hand, when an implicit time marching method is used, the diffusion coefficients are then to be evaluated. We thus investigate in this section the use of stationary iterative techniques in order to evaluate multicomponent diffusion matrices.

We first discuss the expansions of diffusion matrices obtained by using the theory of projected iterative algorithms for constrained singular systems and the natural formulation of the transport linear systems. We then discuss the new expansions associated with the more singular formulations of the transport linear systems. We consider the first order diffusion in the isotropic case and then in the nonisotropic magnetized case. We subsequently consider the higher order diffusion matrices which are important in plasma modeling especially in order to evaluate the electrical conductivities.

In order to asses the accuracy of the resulting algorithms, numerical experiments are performed with high temperature air. The correponding mixture is constituted by the $n^s = 11$ species N_2, O_2, NO, N, O, N_2^+, O_2^+, NO^+, N^+, O^+, and e. The Thermodynamic properties have been estimated from Gupta, Yos, Thomson and Lee [36] and the collision integrals from Wright, Bose, Palmer, and Levin [55]. We have considered typical mixtures in the form

$$\mathrm{x}_{\mathrm{N}_2} = \mathrm{x}_{\mathrm{O}_2} = \mathrm{x}_{\mathrm{NO}} = \mathrm{x}_{\mathrm{N}} = \mathrm{x}_{\mathrm{O}} = 0.2(1 - 10x)$$

$$\mathrm{x}_{\mathrm{N}_2^+} = \mathrm{x}_{\mathrm{O}_2^+} = \mathrm{x}_{\mathrm{NO}^+} = \mathrm{x}_{\mathrm{N}^+} = \mathrm{x}_{\mathrm{O}^+} = x, \qquad \mathrm{x}_{\mathrm{e}} = 5x,$$

where x_{A} is the mole fraction of species A, the ionization parameter x is such that $0 \leq x \leq 0.1$, and the ionization level or degree is $\mathrm{x}_{\mathrm{e}} = 5x$. The accuracy of the asymptotic expansions is investigated as depending on the ionization parameter x and on the intensity of the magnetic field B. The corresponding mass fractions are denoted by $\mathrm{Y}_1, \ldots, \mathrm{Y}_{n^s}$ and are such that $\mathrm{Y}_k > 0$, $k \in \mathcal{S}$, and $\sum_{k \in \mathcal{S}} \mathrm{Y}_k = 1$. In all the numerical experiments, the pressure is taken to be $p = 0.1$ atm and the temperature $T = T_h = 10000$ K. Using other pressures or temperature would not significantly modify the accuracy of the asymptotic expansions.

7.1 The real first order matrix

We investigate in this section the evaluation of the first order diffusion matrix $D_{[00]}$. The corresponding n^s systems presented in Table 1 are of size $n = n^s$ and written in the form

$$\begin{cases} \Delta a_{[00]}^{D_k} = b_{[00]}^{D_k} \\ \langle a_{[00]}^{D_k}, \mathsf{y} \rangle = 0, \end{cases} \qquad k \in \mathcal{S}, \tag{7.1}$$

and the first order diffusion coefficients are then evaluated from

$$D_{[00]kl} = \langle a_{[00]}^{D_k}, b_{[00]}^{D_l} \rangle, \qquad k, l \in \mathcal{S}. \tag{7.2}$$

The Stefan-Maxwell matrix Δ can be written in the form [11, 23, 28, 29]

$$\Delta_{kk} = \sum_{\substack{l \in \mathcal{S} \\ l \neq k}} \frac{\mathrm{x}_k \mathrm{x}_l}{\mathcal{D}_{kl}}, \qquad \Delta_{kl} = -\frac{\mathrm{x}_k \mathrm{x}_l}{\mathcal{D}_{kl}}, \qquad k, l \in \mathcal{S}, \quad k \neq l,$$

where $\mathrm{x}_1, \ldots, \mathrm{x}_{n^s}$ are the species mole fractions and $\mathcal{D}_{kl}$, $k, l \in \mathcal{S}$, are the species binary diffusion coefficients. This matrix Δ is symmetric positive definite with nullspace $N(\Delta) = \mathbb{R}\mathsf{u}$, $R(\Delta) = \mathsf{u}^\perp$, where $\mathsf{u} \in \mathbb{R}^{n^s}$ is given by $\mathsf{u} = (1, \ldots, 1)^t$, $2\mathrm{diag}(\Delta) - \Delta$ is positive definite and Δ is a singular M-matrix [49, 28]. The right hand sides $b_{[00]}^{D_k}$ are given by

$$b_{[00]}^{D_k} = \mathsf{e}^k - \mathsf{y}, \qquad k \in \mathcal{S},$$

where e^k, $k \in \mathcal{S}$, are the standard basis vectors of $\mathbb{R}^{n^s}$ and y is the mass fractions vector $\mathsf{y} = (\mathrm{Y}_1, \ldots, \mathrm{Y}_{n^s})^t$ in such a way that $b_{[00]i}^{D_k} = \delta_{ki} - \mathrm{Y}_i$, $i, k \in \mathcal{S}$. Since $b_{[00]}^{D_k} \in R(\Delta)$, $k \in \mathcal{S}$, and $\langle \mathsf{u}, \mathsf{y} \rangle = 1$, the transport linear systems (7.1) are well posed and from $D_{[00]kl} = \langle \Delta b_{[00]}^{D_k}, b_{[00]}^{D_l} \rangle$ and the symmetry of Δ, we deduce the symmetry of $D_{[00]}$. We also have $D_{[00]kl} = \langle a_{[00]}^{D_k}, b_{[00]}^{D_l} \rangle = \langle a_{[00]}^{D_k}, \mathsf{e}^l \rangle$ since $\langle a_{[00]}^{D_k}, \mathsf{y} \rangle = 0$ in such a way that $D_{[00]kl} = a_{[00]l}^{D_k} = a_{[00]k}^{D_l}$. Thanks these relations and to linearity, the transport linear systems (7.1) imply the matrix relations $\Delta D_{[00]} = Q$, and $D_{[00]}\mathsf{y} = 0$ where $Q = \mathbb{I} - \mathsf{y} \otimes \mathsf{u} = [b_{[00]}^{D_1}, \ldots, b_{[00]}^{D_{n^s}}]$. Since $D_{[00]}\mathsf{y} = 0$ and $D_{[00]}$ is symmetric we next obtain that $R(D_{[00]}) \subset \mathsf{y}^\perp$. In addition, since $D_{[00]}$ and Δ are symmetric, we deduce from $\Delta D_{[00]} = Q$ upon transposing that $D_{[00]}\Delta = P$ so that $R(P) = \mathsf{y}^\perp \subset R(D_{[00]})$ and thus $R(D_{[00]}) = \mathsf{y}^\perp$ and $N(D_{[00]}) = \mathbb{R}\mathsf{y}$. Multiplying on the right $\Delta D_{[00]} = Q$ by Δ and on the left by $D_{[00]}$ we finally obtain that $\Delta D_{[00]}\Delta = \Delta$ and $D_{[00]}\Delta D_{[00]} = D_{[00]}$ since $\Delta\mathsf{u} = 0$, $\Delta = \Delta^t$, and $D_{[00]}\mathsf{y} = 0$. Therefore, $D_{[00]}$ is the generalized inverse of Δ with prescribed nullspace $\mathbb{R}\mathsf{y}$ and range $\mathsf{y}^\perp$ [27, 28, 19]. In particular, for any $a > 0$ we have $D_{[00]} = (\Delta + a\mathsf{y}\otimes\mathsf{y})^{-1} - (1/a)\mathsf{u}\otimes\mathsf{u}$.

As a direct application of Section 5, from the convergence of the projected iterative algorithm applied to (7.1), or equivalently from the expansion of generalized inverses (5.12), we deduce that upon using the splitting $\Delta = M - W$, with $M = \mathcal{D}$ where

$$\mathcal{D} = \mathrm{diag}\Big(\frac{\Delta_{11}}{1 - \mathrm{Y}_1}, \ldots, \frac{\Delta_{n^s,n^s}}{1 - \mathrm{Y}_{n^s}}\Big), \tag{7.3}$$

and letting $T = M^{-1}W$ and $P = Q^t = \mathbb{I} - \mathsf{u}\otimes\mathsf{y}$, we have the convergent asymptotic expansion

$$D_{[00]} = \sum_{0 \leq j < \infty} (PT)^j P M^{-1} P^t. \tag{7.4}$$

In the first term $PM^{-1}P^t$ the matrix M^{-1} corresponds to the Hischfelder-Curtiss approximation and the projector operation P to the addition of a species independent mass conservation corrector [51, 28]. In other words, if $\boldsymbol{d} = (\boldsymbol{d}_1, \ldots, \boldsymbol{d}_{n^s})^t$ is a constrained diffusion driving force vector whose components sum up to zero, we have $\boldsymbol{d} = P^t\boldsymbol{d}$, so that $\mathbf{v} = (\mathbf{v}_1, \ldots, \mathbf{v}_{n^s})^t$ is given by $\mathbf{v} = -M^{-1}\boldsymbol{d} + \mathsf{u}\langle \mathsf{y}, \boldsymbol{d} \rangle$ where $-M^{-1}\boldsymbol{d}$ is the Hirschfelder-Curtiss approximation and $\mathsf{u}\langle \mathsf{y}, \boldsymbol{d} \rangle$ a species independent mass conservation corrector [51]. However, the next approximation of $D_{[00]}$ with two terms is more interesting since it is much more accurate and still yields $(n^s)^2$ coefficients within $\mathcal{O}\big((n^s)^2\big)$ operations [28, 20].

The rescaled errors of the various iterates associated with the classical expansion (7.4) are presented in Figure 1 for the ionization parameters $x = 10^{-4}$, $x = 10^{-3}$, and $x = 10^{-2}$. These errors are calculated with the Frobenius matrix norm $\|A\|^2 = \sum_{1 \leq i,j \leq n} a_{ij}^2$ and rescaled by the initial error. We can see that the convergence rates deteriorate as the ionization parameter x increases as first investigated by Garcia Muñoz [26]. In particular, the convergence rate for $x = 10^{-2}$, one of the worse case encountered, is not satisfactory.

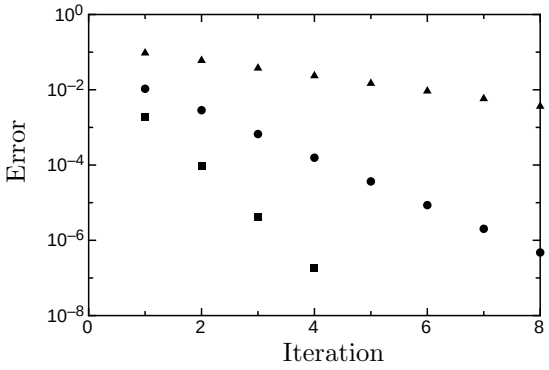

Figure 1: Reduced errors of first order diffusion matrix classical approximations for various ionized mixures; ■ $x = 10^{-4}$, ● $x = 10^{-3}$, and ▲ $x = 10^{-2}$

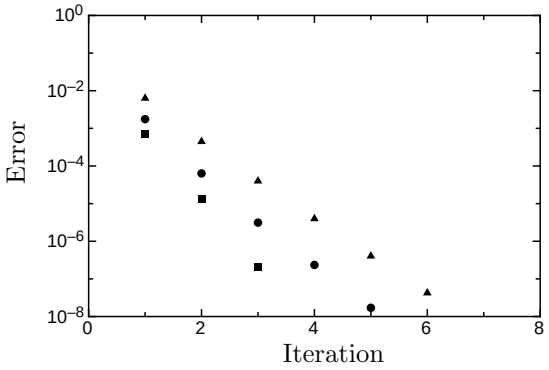

Figure 2: Reduced errors of first order diffusion matrix new approximations for various ionized mixures; ■ $x = 10^{-4}$, ● $x = 10^{-3}$, and ▲ $x = 10^{-2}$

We also investigated a splitting matrix M taking into account the line and column corresponding to the electron in Δ. This matrix M is defined by $M_{ij} = \mathcal{D}_{ij}$ if $i \neq n^s$ and $j \neq n^s$, and $M_{ij} = \Delta_{ij}$ otherwise. However, it only *marginally* improved the bad convergence rates observed with increasing ionization levels, suggesting that the small coefficients in Δ and the large coefficient in $D_{[00]}$ associated with electron [31] is not at the origin of the problem. This has been confirmed by investigating the heavy species first order diffusion matrix associated with non equilibrium models—where the electron species is suppressed—which yielded similar results as those presented in Figure 1.

In order to improve the convergence rates for increasing ionization levels, we have used the *more singular* formulation (5.17) with the vector u_2^* defined by $(\mathsf{u}_2)_k^* = 1$ if $k \in \mathcal{I}$ and $(\mathsf{u}_2)_k^* = 0$ otherwise, where $\mathcal{I}$ denotes the set of ionized species. Letting $\mathrm{Y}_c = \sum_{k\in\mathcal{I}} \mathrm{Y}_k$ the resulting vector u_2 is such that $(\mathsf{u}_2)_k = 1 - \mathrm{Y}_c$ if $k \in \mathcal{I}$ and $(\mathsf{u}_2)_k = -\mathrm{Y}_c$ otherwise. We then define $\mathsf{u}_1 = \mathsf{u}$, $\mathsf{y}_1 = \mathsf{y}$, $\mathsf{y}_2 = \Delta\mathsf{u}_2$, $\Delta_2 = \Delta - \mathsf{y}_2\otimes\mathsf{y}_2/\langle\mathsf{u}_2,\mathsf{y}_2\rangle$ $(D_{[00]})_2 = D_{[00]} - \mathsf{u}_2\otimes\mathsf{u}_2/\langle\mathsf{u}_2,\mathsf{y}_2\rangle$, and we have $\Delta_2(D_{[00]})_2 = Q_2$, $N\big((D_{[00]})_2\big) = \mathrm{span}\{\mathsf{y}_1,\mathsf{y}_2\}$, $Q_2 = Q - \mathsf{u}_2\otimes\mathsf{y}_2/\langle\mathsf{u}_2,\mathsf{y}_2\rangle$. The more singular formulation associated with (7.1) can then be written

$$\begin{cases} \Delta_2(a_{[00]}^{D_k})_2 = (b_{[00]}^{D_k})_2, \\ \big\langle(a_{[00]}^{D_k})_2,\mathsf{y}_1\big\rangle = \big\langle(a_{[00]}^{D_k})_2,\mathsf{y}_2\big\rangle = 0, \end{cases} \qquad k \in \mathcal{S}, \tag{7.5}$$

where $(b_{[00]}^{D_k})_2 = Q_2 b_{[00]}^{D_k}$ and $(D_{[00]})_2$ can equivalently be defined by

$$(D_{[00]})_{2kl} = \big\langle(a_{[00]}^{D_k})_2,(b_{[00]}^{D_l})_2\big\rangle = 0, \qquad k,l \in \mathcal{S}.$$

We now set $\Delta_2 = M_2 - W_2$ with $M_2 = \mathcal{D}_2$ where

$$\mathcal{D}_2 = \mathrm{diag}\Big(\frac{(\Delta_2)_{11}}{1-(\mathsf{y}_1)_1-(\mathsf{y}_2)_1},\ldots,\frac{(\Delta_2)_{n^s,n^s}}{1-(\mathsf{y}_1)_{n^s}-(\mathsf{y}_2)_{n^s}}\Big), \tag{7.6}$$

and when all mass fractions are positive the coefficients $(\Delta_2)_{kk}$ and $(Q_2)_{kk} = 1-(\mathsf{y}_1)_k-(\mathsf{y}_2)_k$ are always positive, provided there are at least two neutral and two ionized species. Upon letting $T_2 = M_2^{-1}W_2$

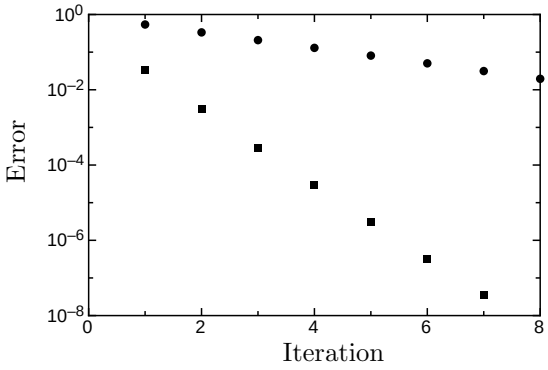

Figure 3: Reduced errors of heavy species first order diffusion matrix approximations for $x = 10^{-2}$; • classical expansion, ■ new expansion with Δ_2

and $P_2 = Q_2^t = \mathbb{I} - \mathsf{u}_1 \otimes \mathsf{y}_1 / \langle \mathsf{u}_1, \mathsf{y}_1 \rangle - \mathsf{u}_2 \otimes \mathsf{y}_2 / \langle \mathsf{u}_2, \mathsf{y}_2 \rangle$, and thanks to Theorem 5.9 and (5.12) we have the expansion

$$D_{[00]} = \frac{\mathsf{u}_2 \otimes \mathsf{u}_2}{\langle \mathsf{u}_2, \mathsf{y}_2 \rangle} + \sum_{1 \le j < \infty} (P_2 T_2)^j P_2 M_2^{-1} P_2^t. \tag{7.7}$$

The resulting errors of the successive approximations are presented in Figure 2 for the ionization parameters $x = 10^{-4}$, $x = 10^{-3}$, and $x = 10^{-2}$. These results show the much better convergence behavior of the modified iterates (7.7). Using a more singular formulation with the matrices Δ_3 and $(D_{[00]})_3$ and a nullspace of dimension 3 did not significantly improved the convergence rates since after elimination of the worse eigenvalue of T there remains a group of several 'quasi largest' similar eigenvalues in T_2 which cannot be taken into account with one single extra nullspace vector.

An eigenvalue analysis reveals that there is indeed one relatively isolated bad eigenvalue of the matrix T associated with (7.4). The corresponding eigenvector further suggests the use of the vector u_2^* defined by $(\mathsf{u}_2)_k^* = 1$ if $k \in \mathcal{I}$ and $(\mathsf{u}_2)_k^* = 0$ otherwise. This eigenvalue may be associated with the small values of the binary diffusion coefficients between positively charged ions. This explains why bad convergence rates are still observed for the heavy species diffusion matrices. Finally, in Figure 3 are presented the errors associated with the classical and new expansions of the heavy species first order diffusion matrices for $x = 10^{-2}$. This figure shows that the modified iterates also improve the convergence rates for the heavy species first order diffusion matrices. Similar results have also been found for other choices of the mixture mole fractions.

Remark 7.1. *The modified diffusion matrix $D_{[00]} + \alpha \mathsf{u} \otimes \mathsf{u}$ can be used instead of $D_{[00]}$ to improve the structure of Jacobian matrices of discretized systems of equations when all the mass fractions are considred as independent unknowns and to suppress artificial singularities [27, 29].*

7.2 The complex first order matrix

We investigate in this section the evaluation of the first order magnetized diffusion matrix $D_{[00]}^{\perp} + \mathrm{i} D_{[00]}^{\odot}$. The first order diffusion matrix parallel to the magnetic field $D_{[00]}^{\parallel}$ can be evaluated as in the previous section and is not further discussed. The corresponding n^s systems presented in Table 2 are of size $n = n^s$ and written in the form

$$\begin{cases} (\Delta + \mathrm{i}\Delta') a_{[00]}^{D_k} = b_{[00]}^{D_k} \\ \langle a_{[00]}^{D_k}, \mathsf{y} \rangle = 0, \end{cases} \qquad k \in \mathcal{S}, \tag{7.8}$$

where where $\mathrm{i}^2 = -1$ and Δ' is the magnetized part of the complex Stefan-Maxwell matrix. This matrix is in the form $\Delta' = (\mathbb{I} - \mathsf{y} \otimes \mathsf{u})\, \mathcal{D}' (\mathbb{I} - \mathsf{u} \otimes \mathsf{y})$ and $\mathcal{D}'$ is the diagonal matrix such that $\mathcal{D}'_{kk} = n_k q_k B / p$ where B denotes the intensity of the magnetic field, n_k, $k \in \mathcal{S}$, the species mole per unit volume, q_k, $k \in \mathcal{S}$, the species molar charges, and by p the pressure [32]. The first order diffusion coefficients are then evaluated from

$$D_{[00]kl}^{\perp} + \mathrm{i} D_{[00]kl}^{\odot} = \langle a_{[00]}^{D_k}, b_{[00]}^{D_l} \rangle, \qquad k, l \in \mathcal{S}. \tag{7.9}$$

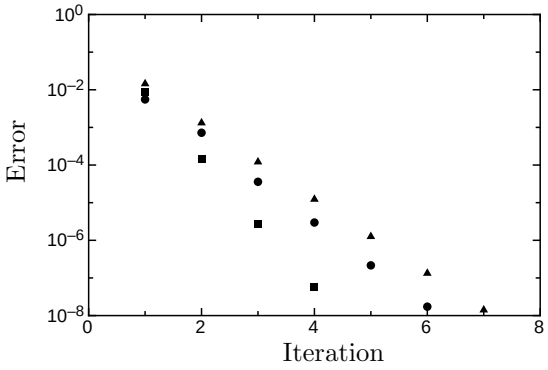

Figure 4: Reduced errors of first order magnetized diffusion matrix new approximations for various ionized mixures and $B = 10^3$; ■ $x = 10^{-4}$, • $x = 10^{-3}$, and ▲ $x = 10^{-2}$

The symmetry properties of $D^{\perp}_{[00]}$ and $D^{\odot}_{[00]}$ as well as the nullspace and range of $D^{\perp}_{[00]kl} + \mathrm{i}D^{\odot}_{[00]kl}$ are derived as in the real case and the details are omitted. Furthermore, as in the isotropic case, the transport linear systems imply the matrix relations $(\Delta+\mathrm{i}\Delta')(D^{\perp}_{[00]}+\mathrm{i}D^{\odot}_{[00]}) = Q$ and $(D^{\perp}_{[00]}+\mathrm{i}D^{\odot}_{[00]})\mathsf{y} = 0$.

The matrix $\Delta+\mathrm{i}\Delta'$ is such that $N(\Delta+\mathrm{i}\Delta') = \mathbb{C}\mathsf{u}$, $R(\Delta+\mathrm{i}\Delta') = \mathsf{u}^{\perp}+\mathrm{i}\mathsf{u}^{\perp}$ and it is easily established that $D^{\perp}_{[00]} + \mathrm{i}D^{\odot}_{[00]}$ is the generalized inverse of $\Delta + \mathrm{i}\Delta'$ with prescribed nullspace $\mathbb{C}\mathsf{y}$ and range $\mathsf{y}^{\perp}$. In addition, for any $\alpha > 0$, we have $D^{\perp}_{[00]} + \mathrm{i}D^{\odot}_{[00]} = (\Delta + \mathrm{i}\Delta' + \alpha\mathsf{y}\otimes\mathsf{y})^{-1} - (1/\alpha)\mathsf{u}\otimes\mathsf{u}$.

As a direct application of the stationary iterative algorithms introduced in Section 5, we deduce that, upon using the splitting $\Delta+\mathrm{i}\Delta' = \mathcal{M} - \mathcal{W}$ where $\mathcal{M} = \mathcal{D}+\mathrm{i}\Delta'$ and $\mathcal{D}$ is the diagonal matrix (7.3) such that $\mathcal{D}_{kk} = \Delta_{kk}/(1-\mathrm{Y}_k)$, and letting $\mathcal{T} = \mathcal{M}^{-1}\mathcal{W}$ and $\mathcal{P} = P = \mathbb{I} - \mathsf{u}\otimes\mathsf{y}$, we have the convergent asymptotic expansion

$$D^{\perp}_{[00]} + \mathrm{i}D^{\odot}_{[00]} = \sum_{0\le j\le\infty} (\mathcal{P}\mathcal{T})^j\mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t.$$

Furthermore, since $\Delta' = (\mathbb{I} - \mathsf{y}\otimes\mathsf{u})\,\mathcal{D}'(\mathbb{I} - \mathsf{u}\otimes\mathsf{y})$, where $\mathcal{D}'$ is diagonal, the inverse of $\mathcal{M} = \mathcal{D} + \mathrm{i}\Delta'$ can easily be expressed in terms of the inverse of the diagonal matrix $\mathcal{D} + \mathrm{i}\mathcal{D}'$ in such a way that the iterates are easily evaluated [32, 33]. Various approximations can then be obtained by truncating this convergent series. The first approximation $\mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t$ generalizes the Hirschfelder-Curtiss approximation with a mass corrector to the magnetized case [32]. The errors associated with the classical expansion are similar to that of Figure 1 and are omitted.

In order to improve the convergence rates for increasing ionization levels, we have used the *more singular* formulation (5.42) with the vector $(\mathsf{u}_2)_k = 1-\mathrm{Y}_c$ if $k \in \mathcal{I}$ and $(\mathsf{u}_2)_k = -\mathrm{Y}_c$ otherwise. Defining $\mathsf{u}_1 = \mathsf{u}$, $\mathsf{y}_1 = \mathsf{y}$, $\mathsf{y}_2 = (\Delta+\mathrm{i}\Delta')\mathsf{u}_2$, $(\Delta+\mathrm{i}\Delta')_2 = (\Delta+\mathrm{i}\Delta') - \mathsf{y}_2\otimes\mathsf{y}_2/(\mathsf{u}_2,\mathsf{y}_2)$, and $(D^{\perp}_{[00]}+\mathrm{i}D^{\odot}_{[00]})_2 = (D^{\perp}_{[00]}+\mathrm{i}D^{\odot}_{[00]}) - \mathsf{u}_2\otimes\mathsf{u}_2/\langle\mathsf{u}_2,\mathsf{y}_2\rangle$, we have $(\Delta + \mathrm{i}\Delta')_2(D^{\perp}_{[00]} + \mathrm{i}D^{\odot}_{[00]})_2 = \mathcal{Q}_2$, $N\big((D^{\perp}_{[00]} + \mathrm{i}D^{\odot}_{[00]})_2\big) = \mathrm{span}\{\mathsf{y}_1,\mathsf{y}_2\}$, where $\mathcal{Q}_2 = \mathcal{Q} - \mathsf{u}_2\otimes\mathsf{y}_2/\langle\mathsf{u}_2,\mathsf{y}_2\rangle$. The more singular formulation can then be written in the form

$$\begin{cases} (\Delta + \mathrm{i}\Delta')_2(a^{D_k}_{[00]})_2 = (b^{D_k}_{[00]})_2, \\ \big\langle(a^{D_k}_{[00]})_2, \mathsf{y}_1\big\rangle = \big\langle(a^{D_k}_{[00]})_2, \mathsf{y}_2\big\rangle = 0, \end{cases} \qquad k \in \mathcal{S}, \tag{7.10}$$

and $(D^{\perp}_{[00]} + \mathrm{i}D^{\odot}_{[00]})_2$ can equivalently be defined by

$$(D^{\perp}_{[00]} + \mathrm{i}D^{\odot}_{[00]})_{2kl} = \big\langle(a^{D_k}_{[00]})_2, (b^{D_l}_{[00]})_2\big\rangle = 0, \qquad k,l \in \mathcal{S}.$$

Upon letting $(\Delta + \mathrm{i}\Delta')_2 = \mathcal{M}_2 - \mathcal{W}_2$ and $\mathcal{M}_2 = \mathcal{D}_2 + \mathrm{i}\Delta'$ where $\mathcal{D}_2$ is the diagonal matrix (7.6), and $\mathcal{T}_2 = \mathcal{M}_2^{-1}\mathcal{W}_2$, $\mathcal{P}_2 = \mathcal{Q}_2^t = \mathbb{I} - \mathsf{u}_1\otimes\mathsf{y}_1/\langle\mathsf{u}_1,\mathsf{y}_1\rangle - \mathsf{u}_2\otimes\mathsf{y}_2/\langle\mathsf{u}_2,\mathsf{y}_2\rangle$, we have the expansion

$$D^{\perp}_{[00]} + \mathrm{i}D^{\odot}_{[00]} = \frac{\mathsf{u}_2\otimes\mathsf{u}_2}{(\mathsf{u}_2,\mathsf{y}_2)} + \sum_{1\le j<\infty} (\mathcal{P}_2\mathcal{T}_2)^j\mathcal{P}_2\mathcal{M}_2^{-1}\mathcal{P}_2^t. \tag{7.11}$$

The errors corresponding to the new expansion are presented in Figure 4. The errors are calculated with the complex Frobenius matrix norm $\|A\|^2 = \sum_{1\le i,j\le n}|a_{ij}|^2$ and are rescaled by the initial error. These results show the much better convergence behavior of the modified iterates (7.7). Finally, similar results have been found for other choices of the mixture mole fractions.

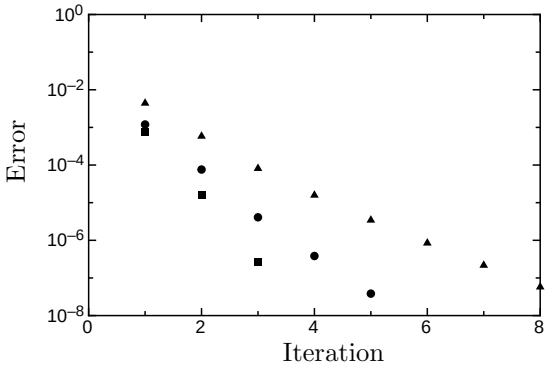

Figure 5: Reduced errors of higher order diffusion matrix new approximations for various ionized mixures; ■ $x = 10^{-4}$, ● $x = 10^{-3}$, and ▲ $x = 10^{-2}$

7.3 Higher order diffusion matrices

We investigate in this section the evaluation of higher order approximations of diffusion matrices, also accounting for the energy of the molecules. The corresponding n^s linear systems presented in Table 1 are of size $n = 2n^s + n^p$, where n^p denotes the number of polyatomic species of the mixture, and can be written in the form

$$\begin{cases} La^{D_k} = b^{D_k} \\ \langle a^{D_k}, \mathcal{Y} \rangle = 0, \end{cases} \qquad k \in \mathcal{S}. \tag{7.12}$$

The diffusion coefficients are then given by

$$D_{kl} = \langle a^{D_k}, b^{D_l} \rangle, \qquad k, l \in \mathcal{S}. \tag{7.13}$$

The coefficents of the matrix L are intricate expressions involving collision integrals and internal energy relaxation times that are detailed in references [15, 32]. The matrix L is symmetric positive definite, $N(L) = \mathbb{R}\mathcal{U}$, $R(L) = \mathcal{U}^\perp$, and $2db(L) - L$ is positive definite when $n^s \geq 3$. Upon partitionning $\mathbb{R}^{2n^s+n^p}$ into $\mathbb{R}^{n^s} \times \mathbb{R}^{n^s+n^p}$, the nullspace vector $\mathcal{U}$, the contraint vector $\mathcal{Y}$, and the right hand sides b^{D_k}, $k \in \mathcal{S}$, are given by

$$\mathcal{U} = \begin{pmatrix} \mathsf{u} \\ 0 \end{pmatrix}, \qquad \mathcal{Y} = \begin{pmatrix} \mathsf{y} \\ 0 \end{pmatrix}, \qquad b^{D_k} = \begin{pmatrix} b^{D_k}_{[00]} \\ 0 \end{pmatrix}, \quad k \in \mathcal{S}, \tag{7.14}$$

where 0 denote the vector with zero components in $\mathbb{R}^{n^s+n^p}$, and u, y, $b^{D_k}_{[00]}$, $k \in \mathcal{S}$, have been defined in the previous section in connection with the first order diffusion matrix. The right hand sides b^{D_k}, $k \in \mathcal{S}$, can also be written

$$b^{D_k} = \mathsf{e}^k - \mathcal{Y}, \qquad k \in \mathcal{S}.$$

where e^k, $k \in \mathcal{S}$, are the standard basis vectors of $\mathbb{R}^n = \mathbb{R}^{2n^s+n^p}$. Since $b^{D_k} \in R(L)$, $k \in \mathcal{S}$, and $\langle \mathcal{U}, \mathcal{Y} \rangle = 1$, the transport linear systems (7.12) are well posed and from $D_{kl} = \langle Lb^{D_k}, b^{D_l} \rangle$ and the symmetry of L, we deduce the symmetry of D. We also have $D_{kl} = \langle a^{D_k}, b^{D_l} \rangle = \langle a^{D_k}, \mathsf{e}^l \rangle$ since $\langle a^{D_k}, \mathcal{Y} \rangle = 0$ in such a way that $D_{kl} = a^{D_k}_l = a^{D_l}_k$, $1 \leq k, l \leq n^s$.

Upon defining the blocks $a^D = [a^{D_1}, \ldots, a^{D_{n^s}}]$ and $b^D = [b^{D_1}, \ldots, b^{D_{n^s}}]$ the linear systems imply the matrix relations $L\, a^D = b^D$, and $\mathcal{Y}^t a^D = 0$. We introduce the projectors $\mathcal{Q} = \mathcal{P}^t = \mathbb{I}_n - \mathcal{Y} \otimes \mathcal{U}$, the rectangular matrix Π, and we have the block decompositions

$$a^D = \begin{pmatrix} D \\ X \end{pmatrix}, \quad b^D = \begin{pmatrix} Q \\ \mathcal{O} \end{pmatrix}, \quad \Pi = \begin{pmatrix} \mathbb{I}_{n^s} \\ \mathcal{O} \end{pmatrix}, \quad \mathcal{Q} = \begin{pmatrix} Q & \mathcal{O}^t \\ \mathcal{O} & \mathbb{I}_{n^s+n^p} \end{pmatrix}, \tag{7.15}$$

where $\mathcal{O}$ denotes the zero matrix in $\mathbb{R}^{n^s+n^p,n^s}$, X a nonzero matrix in $\mathbb{R}^{n^s+n^p,n^s}$, and $\mathbb{I}_s$ the unit matrix of size s.

We next introduce the generalized inverse $\mathcal{Z}$ of L with nullspace $\mathcal{Y}$ and range $\mathcal{Y}^\perp$ which satisfies $L\,\mathcal{Z} = \mathcal{Q}$, $\mathcal{Z}\,L = \mathcal{P}$, $N(\mathcal{Z}) = \mathbb{R}\mathcal{Y}$, and $R(\mathcal{Z}) = \mathcal{Y}^\perp$, and we also know that $a^{D_k} = \mathcal{Z}b^{D_k}$, $k \in \mathcal{S}$. As a consequence, we have the relations

$$b^D = \mathcal{Q}\Pi, \qquad a^D = \mathcal{Z}\Pi, \tag{7.16}$$

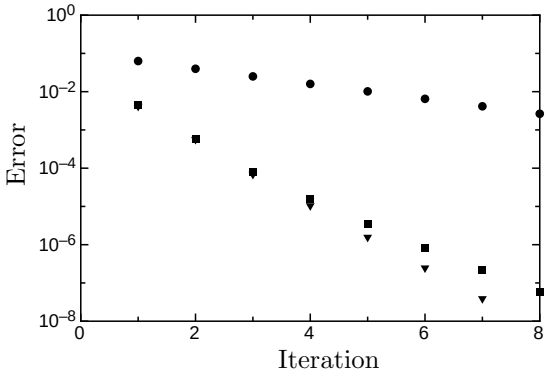

Figure 6: Reduced errors of higher order diffusion matrix classical • L, new ■ L_2, and ▼ L_3 expansions for $x = 10^{-2}$

since $a^D = \mathcal{Z}b^D = \mathcal{Z}\mathcal{Q}\Pi = \mathcal{Z}\Pi$, and the higher order coefficients are given by $D = \Pi^t a^D = \Pi^t \mathcal{Z}\Pi$.

Projected stationary iterative algorithms can be used for solutions of (7.12) by using splittings in the form $L = \mathcal{M} - \mathcal{W}$ with $\mathcal{M} = db(L) + \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$ [15]. We then have the convergent asymptotic expansion

$$a^D = \sum_{0 \le j \le \infty} (\mathcal{P}\mathcal{T})^j \mathcal{P}\mathcal{M}^{-1} b^D, \tag{7.17}$$

and the higher order matrix D is then evaluated from $D = \Pi^t a^D$. The iterates $(a^D)^j$, $j \ge 0$, satisfy $(a^D)^{j+1} = \mathcal{P}\mathcal{T}(a^D)^j + \mathcal{P}\mathcal{M}^{-1}b^D$ and only involve the product of the matrix $\mathcal{P}\mathcal{T} \in \mathbb{R}^{2n^s+n^p, 2n^s+n^p}$ by $(a^D)^j \in \mathbb{R}^{2n^s+n^p, n^s}$. The iterates can also be deduced from the expansion (5.12) of generalized inverse $\mathcal{Z}$ since $a^D = \mathcal{Z}b^D$ and $b^D = \mathcal{Q}b^D$. Since $b^D = \mathcal{Q}\Pi$, these relations also imply the identity

$$D = \Pi^t \Big(\sum_{0 \le j \le \infty} (\mathcal{P}\mathcal{T})^j \mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t \Big) \Pi,$$

but the iterates must be taken on the block a^D prior to evaluate D.

In order to improve the convergence rates for increasing ionization levels, we have used the *more singular* formulation (5.17) with the vector $\mathcal{u}_2$ defined by

$$\mathcal{u}_2 = \begin{pmatrix} \mathsf{u}_2 \\ 0 \end{pmatrix} \tag{7.18}$$

where $\mathsf{u}_2 \in \mathbb{R}^{n^s}$ has been defined for the first order matrices $(\mathsf{u}_2)_k = 1 - \mathrm{Y}_c$ if $k \in \mathcal{I}$ and $(\mathsf{u}_2)_k = -\mathrm{Y}_c$ otherwise where $\mathrm{Y}_c = \sum_{k \in \mathcal{I}} \mathrm{Y}_k$. Upon letting $\mathcal{u}_1 = \mathcal{u}$, $\mathcal{y}_1 = \mathcal{y}$, $\mathcal{y}_2 = L\mathcal{u}_2$, $L_2 = L - \mathcal{y}_2 \otimes \mathcal{y}_2 / \langle \mathcal{u}_2, \mathcal{y}_2 \rangle$, $\mathcal{Z}_2 = \mathcal{Z} - \mathcal{u}_2 \otimes \mathcal{u}_2 / \langle \mathcal{u}_2, \mathcal{y}_2 \rangle$, and $a_2^D = a^D - \mathcal{u}_2 \otimes \mathsf{u}_2 / \langle \mathcal{u}_2, \mathcal{y}_2 \rangle$, we have $L_2\mathcal{Z}_2 = \mathcal{Q}_2$, $a_2^D = \mathcal{Z}_2 b^D$, $b_2^D = \mathcal{Q}_2 b^D$, $N(\mathcal{Z}_2) = \mathrm{span}\{\mathcal{y}_1, \mathcal{y}_2\}$, $\mathcal{Q}_2 = \mathcal{Q} - \mathcal{y}_2 \otimes \mathcal{u}_2 / \langle \mathcal{u}_2, \mathcal{y}_2 \rangle$, and the more singular formulation can be written

$$\begin{cases} L_2 a_2^{D_k} = b_2^{D_k}, \\ \langle a_2^{D_k}, \mathcal{y}_1 \rangle = \langle a_2^{D_k}, \mathcal{y}_2 \rangle = 0, \end{cases} \qquad k \in \mathcal{S}. \tag{7.19}$$

Letting $L_2 = \mathcal{M}_2 - \mathcal{W}_2$, $\mathcal{M}_2 = db(L_2) + \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, where σ_i, $1 \le i \le n$, are nonnegative weights, $\mathcal{T}_2 = \mathcal{M}_2^{-1}\mathcal{W}_2$ and $\mathcal{P}_2 = \mathcal{Q}_2^t = \mathbb{I} - \mathcal{u}_1 \otimes \mathcal{y}_1 / \langle \mathcal{u}_1, \mathcal{y}_1 \rangle - \mathcal{u}_2 \otimes \mathcal{y}_2 / \langle \mathcal{u}_2, \mathcal{y}_2 \rangle$, we have the expansion

$$a_2^D = \sum_{0 \le j \le \infty} (\mathcal{P}_2\mathcal{T}_2)^j \mathcal{P}_2 \mathcal{M}_2^{-1} b_2^D, \tag{7.20}$$

and finally $D = \mathsf{u}_2 \otimes \mathsf{u}_2 / \langle \mathcal{u}_2, \mathcal{y}_2 \rangle + \Pi^t a_2^D$ or equivalently

$$D = \frac{\mathsf{u}_2 \otimes \mathsf{u}_2}{\langle \mathcal{u}_2, \mathcal{y}_2 \rangle} + \Pi^t \sum_{1 \le j < \infty} (\mathcal{P}_2\mathcal{T}_2)^j \mathcal{P}_2 \mathcal{M}_2^{-1} \mathcal{P}_2^t \, \Pi. \tag{7.21}$$

Only these modified formulations yield satisfactory results for all ionization levels. The resulting errors of the successive approximations of D are presented in Figure 5 for the ionization parameters $x = 10^{-4}$, $x = 10^{-3}$, and $x = 10^{-2}$. These results show that the good convergence rates observed

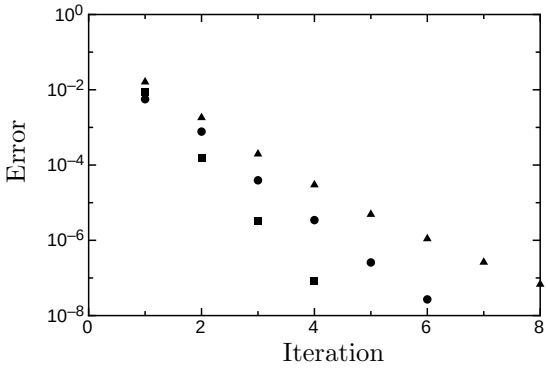

Figure 7: Reduced errors of higher order magnetized diffusion matrix new approximations for various ionized mixures and $B = 10^3$; ■ $x = 10^{-4}$, • $x = 10^{-3}$, and ▲ $x = 10^{-2}$

for first order matrices also hold for higher order matrices. The improvement of the convergence rates is exhibited in Figure 6 where the convergence history of the expansions obtained from L and L_2 are presented. We have also experimented an even more singular formulation with the matrix L_3 and various vectors $\mathcal{U}_3$ but no significant improvements have been obtained. The errors presented on Figure 6 corresponds to the vector $\mathcal{U}_3 = (0_{n^s}, \mathsf{u}_2, 0_{n^p})^t$.

In the magnetized case, we have to solve the n^s complex systems

$$\begin{cases} (L + \mathrm{i}L')\, a^{D_k} = b^{D_k}, \\ (a^{D_k}, \mathcal{Y}) = 0, \end{cases} \qquad k \in \mathcal{S}, \tag{7.22}$$

where $L' = (\mathbb{I} - \mathcal{Y} \otimes \mathcal{U})\, \mathsf{L}' (\mathbb{I} - \mathcal{U} \otimes \mathcal{Y})$, and L' is a diagonal matrix such that $\mathsf{L}'_{kk} = n_k q_k B/p$, for $k \in \mathcal{S}$, $\mathsf{L}'_{n^s+k,n^s+k} = \frac{5}{2} n_k q_k B/p$, for $k \in \mathcal{S}$, and $\mathsf{L}'_{2n^s+k,2n^s+k} = c_k^{\mathrm{int}} m_k n_k q_k B/Rp$, for $k \in \mathcal{P}$, where R is the gas constant, m_k the molar mass of the kth species, and c_k^{int} the internal specific heat per unit mass of the kth species. The matrix $\mathcal{L} = L + \mathrm{i}L'$ is complex symmetric, $N(L + \mathrm{i}L') = \mathbb{C}\mathcal{U}$, and $R(L + \mathrm{i}L') = \mathcal{U}^{\perp} + \mathrm{i}\mathcal{U}^{\perp}$. Introducing the generalized inverse $\mathcal{Z}$ of $L + \mathrm{i}L'$ with nullspace $\mathbb{C}\mathcal{Y}$ and nullspace $\mathcal{Y}^{\perp}$ we have as in the real case the relations $b^D = \mathcal{Q}\Pi$, $a^D = \mathcal{Z}\Pi$. Upon using splittings in the form $L + \mathrm{i}L' = \mathcal{M} - \mathcal{W}$ with $\mathcal{M} = db(L) + \mathrm{i}L' + \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, we obtain from the general results of Section 5 similar expansions

$$D^{\perp} + \mathrm{i}D^{\odot} = \Pi \Big(\sum_{0 \le j \le \infty} (\mathcal{P}\mathcal{T})^j \mathcal{P}\mathcal{M}^{-1}\mathcal{P}^t \Big) \Pi^t,$$

but the convergence rates of these expansions decrease as ionization levels increase. As in the real case, we have to use a more singular formulation in order to obtain a better convergence behavior for higher ionization levels. These expansions are similar to real case and the details are omitted. The resulting errors of the successive approximations of $D^{\perp} + \mathrm{i}D^{\odot}$ are presented in Figure 7 for $B = 10^3$ and $x = 10^{-4}$, $x = 10^{-3}$, and $x = 10^{-2}$. These results show that the good convergence rates observed for isotropic higher order matrices also hold for magnetized higher order matrices.

The higher order effects usually have a minor impact on the diffusion matrix of neutral species mixtures [15]. They have a more important impact, however, on ionized mixtures. Our numerical test for high temperature air have shown that the relative error in matrix norms $\|D^{\parallel} - D^{\parallel}_{[00]}\|/\|D^{\parallel}\|$, $\|D^{\perp} - D^{\perp}_{[00]}\|/\|D^{\perp}\|$, and $\|D^{\odot} - D^{\odot}_{[00]}\|/\|D^{\parallel}\|$, can be large for ionization levels above 10^{-3}. In addition, higher order effects due to the energy of the molecules are always important, even for weakly ionized mixtures, in order to evaluate the electrical conductivities [23, 6, 8, 9, 10].

8 Application to thermal conductivity and Stefan-Maxwell equations

We investigate in this section iterative techniques in order to evaluate the thermal conductivity coefficients and the species diffusion velocities. Both problems can be solved by using generalized conjugate

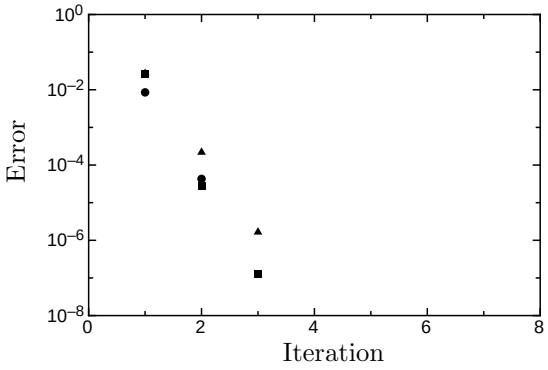

Figure 8: Reduced errors for conjugate gradient approximate thermal conductivities λ and various ionized mixtures; ■ $x = 10^{-4}$, ● $x = 10^{-3}$, and ▲ $x = 10^{-2}$

gradient techniques. We consider both the isotropic case as well as the nonisotropic magnetized case. In order to asses the accuracy of the resulting algorithms, numerical experiments are again performed with high temperature air. In contrast with stationary techniques, it is found that generalized conjugate gradient techniques are efficient for all ionization levels and magnetic field intensities. Using the more singular formulations only introduce a shift in the convergence history.

8.1 Transport linear systems associated with λ and χ

The linear system associated with the thermal conductivity presented in Table 1 is of size $n = n^s + n^p$ and written in the form

$$\Lambda a^\lambda = b^\lambda, \tag{8.1}$$

where the coefficients of the matrix Λ are intricate expressions that are detailed in reference [15]. This system can directly be obtained from a variational formulation in the isotropic as well as in the magnetized case [16, 32]. The matrix Λ is symmetric positive definite [15] and the thermal conductivities and the thermal diffusion ratios are evaluated from the following products

$$\lambda = \frac{p}{T}\langle a^\lambda, b^\lambda\rangle, \qquad \chi = L^{00\lambda} a^\lambda, \tag{8.2}$$

where $L^{00\lambda}$ is the upper right block of L of size $n^s \times (n^s + n^p)$ in such a way that L has the bloc decomposition

$$L = \begin{pmatrix} \Delta & L^{00\lambda} \\ L^{\lambda 00} & \Lambda \end{pmatrix}. \tag{8.3}$$

The coefficients of the matrices $L^{00\lambda}$ and $L^{00\lambda} = (L^{00\lambda})^t$ are given in [15] and the rescaled thermal diffusion ratios $\widetilde{\chi}$ are also obtained from the rescaled version $\widetilde{L}^{00\lambda}$ of the block $L^{00\lambda}$ [20]. More specifically, if $\widetilde{L}^{00\lambda}$ is the matrix such that $\mathrm{diag}(\mathrm{x}_1, \ldots, \mathrm{x}_{n^s})\widetilde{L}^{00\lambda} = L^{00\lambda}$ then we have $\mathrm{x}_i\widetilde{\chi}_i = \chi_i$, $i \in \mathcal{S}$, where $\widetilde{\chi}$ is evaluated from $\widetilde{\chi} = \widetilde{L}^{00\lambda} a^\lambda$.

In the nonisotropic case, the linear system associated with the thermal conductivities presented in Table 2 is written in the form

$$(\Lambda + \mathrm{i}\Lambda')a^\lambda = b^\lambda, \tag{8.4}$$

where Λ' is the diagonal matrix given by $(\Lambda')_{kk} = \frac{5}{2} n_k q_k B/p$, for $k \in \mathcal{S}$, and $(\Lambda')_{n^s+k, n^s+k} = c_k^{\mathrm{int}} m_k n_k q_k B/Rp$, for $k \in \mathcal{P}$, where R is the gas constant, m_k the molar mass of the kth species, and c_k^{int} the internal specific heat per unit mass of the kth species. The thermal conductivities and the thermal diffusion ratios are given by the following products

$$\lambda^\perp + \mathrm{i}\lambda^\odot = \frac{p}{T}\langle a^\lambda, b^\lambda\rangle, \qquad \chi^\perp + \mathrm{i}\chi^\odot = L^{00\lambda} a^\lambda, \tag{8.5}$$

and the rescaled thermal diffusion ratios are similarly obtained from the rescaled block $\widetilde{L}^{00\lambda}$ [20].

In the numerical experiments, the matrices Λ, Λ' and $L^{00\lambda}$ have been evaluated following the approximations presented in [20]. The rotational relaxation times for internal energy of the polyatomic ionized molecules have been approximated as the relaxation time of the corresponding neutral molecules [1]. The isotropic systems (8.1) have been solved with a projected conjugate gradients technique and

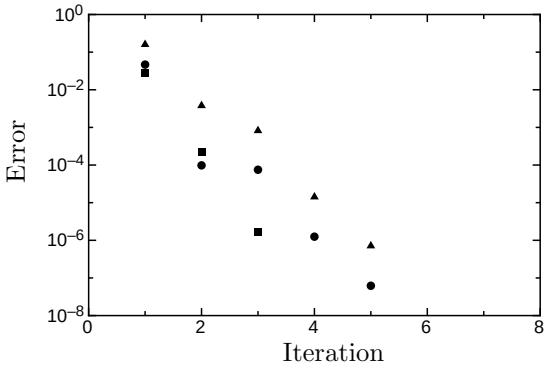

Figure 9: Reduced errors for orthogonal residuals approximate thermal conductivities $\lambda^{\parallel}$, $\lambda^{\perp}$, and $\lambda^{\odot}$ and $x = 10^{-2}$

the magnetized systems (8.4) by using a projected orthogonal residuals technique. In both situations, a diagonal preconditionning matrix has been used. In Figure 8 are presented the convergence history for various values of the ionization parameter $x = 10^{-4}$, $x = 10^{-3}$, and $x = 10^{-2}$ and without magnetization. The errors are defined by $|\lambda - \lambda^k|/\lambda$ where λ is the thermal conductivity and λ^k the kth iterate. In Figure 9 are presented the convergence history for $x = 10^{-2}$ and $B = 10^3$ for $\lambda = \lambda^{\parallel}$, $\lambda^{\perp}$, and $\lambda^{\odot}$. The errors are defined similarly by $|\lambda^{\parallel} - \lambda^{\parallel k}|/\lambda^{\parallel}$, $|\lambda^{\perp} - \lambda^{\perp k}|/\lambda^{\perp}$, and $|\lambda^{\odot} - \lambda^{\odot k}|/|\lambda^{\odot}|$. These figures shows the good behavior of the generalized conjugate gradient techniques independently of the ionization level and of the magnetic field intensity.

These numerical simulations with partially ionized air have also shown that three iterations are generally required in order to evaluate the thermal diffusion ratios with a good accuracy, whereas two iterates are generally sufficient for the thermal conductivities.

8.2 Stefan-Maxwell equations

When only the species diffusion velocities are required—and not the diffusion coefficients—some type of Stefan-Maxwell equations can be solved by using orthogonal residuals algorithms. The particular form of the Stefan-Maxwell equations depends on the order of accuracy of the diffusion velocities and on magnetization. As a general rule, the Stefan-Maxwell equations are easily derived from the tranport linear systems upon multiplying on the right by the proper diffusion driving force vectors.

In the real isotropic case, multiplying on the right the system (7.1) by the species diffusion driving forces vector $\boldsymbol{d}_k$, and summing over k, letting $\mathbf{v}_{[00]} = (\mathbf{v}_{[00]1}, \ldots, \mathbf{v}_{[00]n^s})^t$, $\boldsymbol{d} = (\boldsymbol{d}_1, \ldots, \boldsymbol{d}_{n^s})^t$, and using $\mathbf{v}_{[00]i} = -\sum_{j\in\mathcal{S}} D_{[00]ij}\boldsymbol{d}_j$, we obtain the classical Stefan-Maxwell relations

$$\begin{cases} -\Delta\mathbf{v}_{[00]} = \boldsymbol{d} - \mathsf{y}\sum_{l\in\mathcal{S}} \boldsymbol{d}_l, \\ \langle \mathbf{v}_{[00]}, \mathsf{y}\rangle = 0. \end{cases} \tag{8.6}$$

One may equivalently multiply the matrix form $\Delta D_{[00]}$ by $\boldsymbol{d} = (\boldsymbol{d}_1, \ldots, \boldsymbol{d}_{n^s})^t$. The right hand side $Q\boldsymbol{d} = \boldsymbol{d} - \mathsf{y}\sum_{l\in\mathcal{S}} \boldsymbol{d}_l$ is the constrained diffusion driving forces vector whose components $\boldsymbol{d}_i - \mathrm{Y}_i\langle \boldsymbol{d}, \mathsf{u}\rangle$, $i \in \mathcal{S}$, sum up to zero. The corresponding equations with Soret effect are obtained in a similar way by using the modified the diffusion driving forces vector $\boldsymbol{d} + \chi\boldsymbol{\nabla}\log T$ where $\chi = (\chi_1, \ldots, \chi_{n^s})^t$ is the thermal diffusion ratio vector. The Stefan-Maxwell equation can then be solved by a projected conjugate gradient method in each spatial direction [15].

In the nonisotropic case, a complex form of the Stefan-Maxwell equations is similarly obtained [32] by multiplying the system (7.8) on the right by the complex vector $\boldsymbol{d}_k^{\perp} - \mathrm{i}\boldsymbol{d}_k^{\odot}$ and summing over $k \in \mathcal{S}$. Letting $\mathbf{v}_{[00]}^{\perp} = (\mathbf{v}_{[00]1}^{\perp}, \ldots, \mathbf{v}_{[00]n^s}^{\perp})^t$, and $\mathbf{v}_{[00]}^{\odot} = (\mathbf{v}_{[00]1}^{\odot}, \ldots, \mathbf{v}_{[00]n^s}^{\odot})^t$, the complex form of the Stefan-Maxwell equations is found in the form

$$\begin{cases} -(\Delta + \mathrm{i}\Delta')(\mathbf{v}_{[00]}^{\perp} - \mathrm{i}\mathbf{v}_{[00]}^{\odot}) = \boldsymbol{d}^{\perp} - \mathrm{i}\boldsymbol{d}^{\odot} - \mathsf{y}\sum_{l\in\mathcal{S}}(\boldsymbol{d}_l^{\perp} - \mathrm{i}\boldsymbol{d}_l^{\odot}), \\ \langle \mathbf{v}_{[00]}^{\perp} - \mathrm{i}\mathbf{v}_{[00]}^{\odot}, \mathsf{y}\rangle = 0. \end{cases} \tag{8.7}$$

The proper modifications of the complex Stefan-Maxwell equations in the presence of Soret effect correspond to including the temperature gradient terms in the diffusion driving forces as discussed

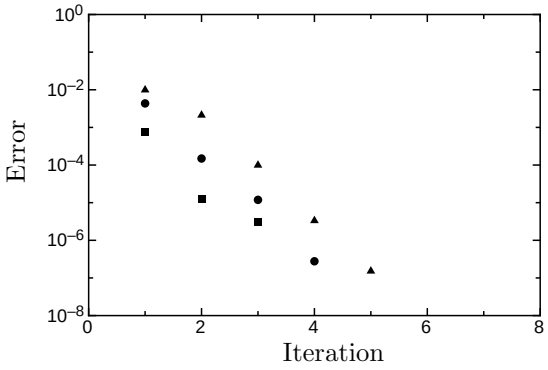

Figure 10: Reduced errors for conjugate gradient approximate diffusion velocities $\mathbf{v}$ and various ionized mixtures; ■ $x = 10^{-4}$, ● $x = 10^{-3}$, and ▲ $x = 10^{-2}$

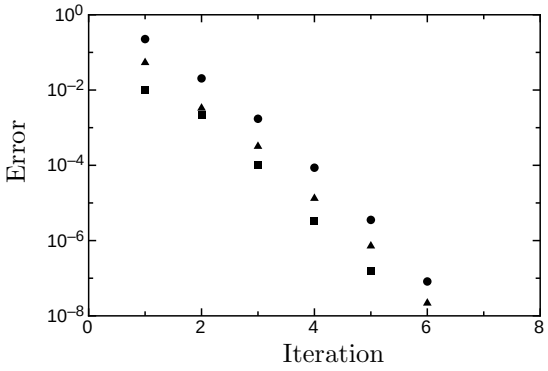

Figure 11: Reduced errors for conjugate gradient approximate nonisotropic diffusion velocities with $x = 10^{-2}$; ■ $\mathbf{v}^{\parallel}$, ● $\mathbf{v}^{\perp}$, and ▲ $\mathbf{v}^{\odot}$

in [33]. The nonisotropic magnetized Stefan-Maxwell equation can then be solved by an orthogonal residuals method in each spatial direction [33].

Indeed, the Stefan-Maxwell relations between the velocity vectors $\mathbf{v}_{[00]1}, \ldots, \mathbf{v}_{[00]n^s}$ and the diffusion driving force vectors $\boldsymbol{d}_1, \ldots, \boldsymbol{d}_{n^s}$ which are vectors of $\mathbb{R}^3$, only involve scalar coefficients, they may be decomposed on the canonical basis of $\mathbb{R}^3$, and it is then sufficient to consider the case of scalar diffusion velocities $\mathrm{v}_{[00]1}, \ldots, \mathrm{v}_{[00]n^s}$ and scalar diffusion driving forces $d_1, \ldots, d_n$, real for isotropic systems, and complex for magnetized systems.

In the numerical tests, we have arbitrary selected a scalar diffusion driving force proportional to the charge per unit volume $(\mathrm{x}_1 q_1, \ldots, \mathrm{x}_{n^s} q_{n^s})^t$. Other arbitrary selected diffusion driving forces have yield similar convergence behavior. In Figure 10 are presented the convergence history without magnetization $B = 0$ for the various ionization parameters $x = 10^{-4}$, $x = 10^{-3}$, and $x = 10^{-2}$. The errors are defined by $\|\mathrm{v}_{[00]} - \mathrm{v}^k_{[00]}\|/\|\mathrm{v}_{[00]}\|$ where $\mathrm{v}_{[00]} = (\mathrm{v}_{[00]1}, \ldots, \mathrm{v}_{[00]n^s})^t$ is the scalar diffusion velocity $\mathrm{v}^k_{[00]} = (\mathrm{v}^k_{[00]1}, \ldots, \mathrm{v}^k_{[00]n^s})^t$ the kth iterate, and $\|a\|$ denotes the Euclidean norm of $a \in \mathbb{R}^n$. Similarly, in Figure 11 are presented the convergence history for $x = 10^{-2}$ and $B = 10^3$ for $\mathrm{v}_{[00]} = \mathrm{v}^{\parallel}_{[00]}$, $\mathrm{v}^{\perp}_{[00]}$, and $\mathrm{v}^{\odot}_{[00]}$. The errors are defined similarly by $\|\mathrm{v}^{\parallel}_{[00]} - \mathrm{v}^{k\parallel}_{[00]}\|/\|\mathrm{v}^{\parallel}_{[00]}\|$, $\|\mathrm{v}^{\perp}_{[00]} - \mathrm{v}^{k\perp}_{[00]}\|/\|\mathrm{v}^{\perp}_{[00]}\|$, and $\|\mathrm{v}^{\odot}_{[00]} - \mathrm{v}^{k\odot}_{[00]}\|/\|\mathrm{v}^{\odot}_{[00]}\|$. These figures show the good behavior of the generalized conjugate gradient techniques independently of the ionization rate and of the intensity of the magnetic field.

Finally in Figure 12 are presented the convergence history of the conjugate gradient method without magnetization $B = 0$ for $x = 10^{-2}$ with the classical are the more singular formulation. The more singular formulation is easily obtained from (7.5) upon multiplying on the right by the diffusion driving forces $\boldsymbol{d}_k$ and summing over $k \in \mathcal{S}$. Upon defining $(\mathbf{v}_{[00]})_2 = -(D_{[00]})_2 \boldsymbol{d}$, it is easily obtained that

$$\begin{cases} -\Delta_2 (\mathbf{v}_{[00]})_2 = Q_2 \boldsymbol{d}, \\ \big\langle (\mathbf{v}_{[00]})_2, \mathrm{y}_1 \big\rangle = \big\langle (\mathbf{v}_{[00]})_2, \mathrm{y}_2 \big\rangle = 0. \end{cases} \tag{8.8}$$

We see that the conjugate gradient method is able to solve the linear system in its original form and

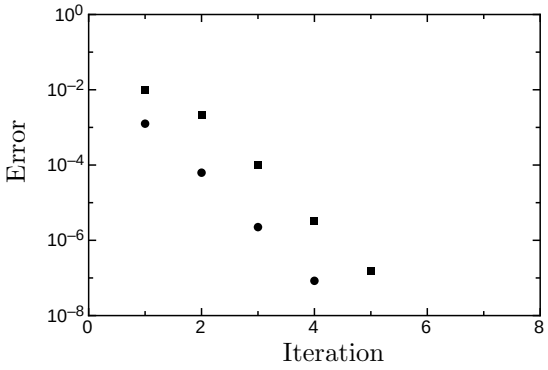

Figure 12: Reduced errors for conjugate gradient approximate diffusion velocities $\mathbf{v}$ for $x = 10^{-2}$ with the classical ■ and the new • formulations of the transport linear systems

that there is simply a shift of one iterate in the error estimates in agreement with the fact that with the more singular formulation there is one additional already prescribed search direction.

Higher order Stefan-Maxwell equations are easily derived from the transport linear systems but can also be rewritten in terms of Schur complements. In the isotropic case, the higher order Stefan-Maxwell equations are obtained by either multiplying the linear system (7.12) on the right by $\boldsymbol{d}_k$ and then summing over $k \in \mathcal{S}$, or equivalently by multiplying the matrix form $La^D = b^D$ on the right by $\boldsymbol{d} = (\boldsymbol{d}_1, \dots, \boldsymbol{d}_{n^s})^t$. Upon defining $\mathfrak{v} = -a^D\boldsymbol{d}$, in such a way that $\mathfrak{v}_l = -a^D_l\boldsymbol{d}$, $1 \leq l \leq 2n^s + n^p$, we have $\mathfrak{v} \in (\mathbb{R}^3)^n$ and the higher order Stefan-Maxwell equations are found in the form

$$\begin{cases} -L\mathfrak{v} = b^D\boldsymbol{d}, \\ \langle \mathfrak{v}, \mathcal{Y} \rangle = 0. \end{cases} \tag{8.9}$$

Upon partitionning $(\mathbb{R}^3)^{2n^s+n^p}$ into $(\mathbb{R}^3)^{n^s} \times (\mathbb{R}^3)^{n^s+n^p}$ and similarly $\mathbb{R}^{2n^s+n^p}$ into $\mathbb{R}^{n^s} \times (\mathbb{R}^3)^{n^s+n^p}$ we have the block decompositions

$$\mathfrak{v} = \begin{pmatrix} \mathbf{v} \\ \mathbf{r} \end{pmatrix}, \qquad b^D\boldsymbol{d} = \begin{pmatrix} Q\boldsymbol{d} \\ 0 \end{pmatrix}, \qquad \mathcal{Y} = \begin{pmatrix} \mathsf{y} \\ 0 \end{pmatrix}, \tag{8.10}$$

so that $\mathbf{v} = \Pi^t\mathfrak{v}$ and $\langle \mathfrak{v}, \mathcal{Y} \rangle = \langle \mathbf{v}, \mathsf{y} \rangle = 0$ where $\mathbf{v} = (\mathbf{v}_1, \dots, \mathbf{v}_{n^s})^t$ and the diffusion velocities are defined as $\mathbf{v}_i = -\sum_{j\in\mathcal{S}} D_{ij}\boldsymbol{d}_j$. Moreover, using the block decomposition (8.3) of the matrix L, and that of $\mathfrak{v}$, we obtain that $\Delta\mathbf{v} + L^{00\lambda}\mathbf{r} = Q\boldsymbol{d}$ and $L^{\lambda 00}\mathbf{v} + \Lambda\mathbf{r} = 0$. We may then write $\mathbf{r} = -\Lambda^{-1}L^{\lambda 00}\mathbf{v}$ and finally eliminate $\mathbf{r}$ to obtain the alternative form involving only the velocity vector $\mathbf{v}$

$$-\big(\Delta - L^{00\lambda}\Lambda^{-1}L^{\lambda 00}\big)\mathbf{v} = Q\boldsymbol{d}. \tag{8.11}$$

These equations show that, in comparison with the first order velocities $\mathbf{v}_{[00]}$, the higher order diffusion velocities $\mathbf{v}$ require to modify the matrix Δ by the corrective terms $L^{00\lambda}\Lambda^{-1}L^{\lambda 00}$. Schur complements have also been investigated by Muckenfusss and Curtiss [46] and Monchick, Munn, and Mason [45]. However, from a numerical point of view, evaluating the product of the matrix $\Delta - L^{00\lambda}\Lambda^{-1}L^{\lambda 00}$ by a vector is costly since it requires solving a linear system with the matrix Λ. Therefore, iterative methods are more conveniently designed with the matrix L than with the Schur complement $\Delta - L^{00\lambda}\Lambda^{-1}L^{\lambda 00}$. In other words, since Λ is a full matrix, the formulation (8.9) with the enlarged velocity vector $\mathfrak{v}$ is more interesting for iterative techniques than the alternative formulation (8.11) only involving $\mathbf{v}$.

The corresponding modifications required in order to take into account Soret effects simply coreponds to adding the temperature gradients terms in the diffusion driving forces [32]. These higher order Stefan-Maxwell equations have been generalized to the complex nonisotropic case including Soret effects but the details are omitted [32]. The convergence rates observed for the higher order Sefan-Maxwell equations has been found similar to that of first order Stefan-Maxwell equations.

Finally note that higher order Stefan-Maxwell equations for mixtures of monatomic gases have also been investigated by Kolesnikov and Tirsky by using vectorial perturbed distribution functions [40]. More specifically, instead of deriving the usual transport linear systems that are next multiplied by the proper diffusion driving forces, it is also possible to consider vectorial species perturbed distribution functions and next to derive the transport linear systems for the diffusion velocities as elegantly done

by Kolesnikov and Tirsky. The resulting higher order Stefan-Maxwell linear equation derived from both methods are easily shown to be equivalent after some matrix manipulations.

9 Conclusion

We have investigated iterative algorithms for solving transport linear systems in partially ionized multicomponent flows. Stationary algorithms as well as generalized conjugate gradient techniques have been considered. New stationary iterative algorithms have been introduced by considering sequences of generalized inverses with nullspaces of increasing dimensions. The resulting algorithms yield low cost accurate approximations of the transport coefficients and are relevant to multicomponent multidimensional numerical simulations. The accuracy of the resulting algorithms have been assesed by comprehensive numerical tests with high temperature air.

A Bloc structure of the transport linear systems

The transport linear systems are derived from a variational procedure used to solve constrained systems of linearized Boltzmann integral equations. The finite dimensional functional space used in the variational procedure can generally be written $\mathcal{A} = \text{span}\{\ \xi^{rk},\ (r,k) \in \mathcal{B}\ \}$, where ξ^{rk}, $(r,k) \in \mathcal{B}$, are basis functions. Here $\mathcal{B}$ denotes the set of basis function indices which has n elements. In the notation (r,k) the index k refers to the species and the index r to the function type that is considered. The basis functions ξ^{rk} are generally expressed in terms of the Laguerre-Sonine polynomials and the Wang Chang and Uhlenbeck polynomials in the internal energy, thus accounting for the polyatomic nature of the molecules [15].

The set $\mathcal{B}$ can be used as a natural indexing set and the components of any vector $x \in \mathbb{R}^n$ are then denoted by $x = (x_k^r)_{(r,k)\in\mathcal{B}}$. We can correspondingly write $G = (G_{kl}^{rs})_{(r,k),(s,l)\in\mathcal{B}}$ the coefficients of the matrix G. For any function type r, we consider the subset $\mathcal{S}_r \subset \mathcal{S}$ given by $\mathcal{S}_r = \{\ k \in \mathcal{S},\ (r,k) \in \mathcal{B}\ \}$ and we denote by n_r the number of elements of $\mathcal{S}_r$. Note that $\mathcal{S}_r$ may differ from $\mathcal{S}$ since some types of functions do not appear for certain species. For instance, functions in the internal energy must not be considered for the monatomic species. The transport linear system matrix $G = (G_{kl}^{rs})_{(r,k),(s,l)\in\mathcal{B}}$ in $\mathbb{R}^{n,n}$ can then be partitioned into the blocks $G^{rs} = (G_{kl}^{rs})_{k\in\mathcal{S}_r,\, l\in\mathcal{S}_s}$ of size $n_r * n_s$. For instance, for the thermal conductivity, the indexing set is given by $\mathcal{B}^\lambda = \{10\}\times\mathcal{S} \ \cup\ \{01\}\times\mathcal{P}$, where $\mathcal{P}$ is the set of polyatomic species indices, and $\mathcal{B}^\lambda$ has $n = n^s + n^p$ elements. Thus, the system matrix $\Lambda \in \mathbb{R}^{n^s+n^p,n^s+n^p}$ admits the block-decomposition

$$\Lambda = \begin{pmatrix} \Lambda^{1010} & \Lambda^{1001} \\ \Lambda^{0110} & \Lambda^{0101} \end{pmatrix},$$

with $\Lambda^{1010} \in \mathbb{R}^{n^s,n^s}$, $\Lambda^{1001} \in \mathbb{R}^{n^s,n^p}$, $\Lambda^{0110} \in \mathbb{R}^{n^p,n^s}$, and $\Lambda^{0101} \in \mathbb{R}^{n^p,n^p}$. The matrix $\big(\text{diag}(G^{rs})\big)_{kl} = G_{kl}^{rs}\delta_{kl}$, $(r,k),(s,l) \in \mathcal{B}$, is defined as the diagonal of the rectangular block G^{rs}.

The sparse transport matrix is then formed by the diagonals of all the rectangular blocks G^{rs} of G. This matrix is denoted by $db(G) \in \mathbb{R}^{n,n}$ and can be written

$$db(G)_{kl}^{rs} = G_{kl}^{rs}\delta_{kl}, \qquad (r,k),(s,l) \in \mathcal{B}, \tag{A.1}$$

where δ_{kl} is the Kronecker symbol. With respect to the matrix Λ for instance, we have the block decomposition

$$db(\Lambda) = \begin{pmatrix} \text{diag}(\Lambda^{1010}) & \text{diag}(\Lambda^{1001}) \\ \text{diag}(\Lambda^{0110}) & \text{diag}(\Lambda^{0101}) \end{pmatrix}.$$

The matrices G and $db(G)$ have a general mathematical structure inherited from the properties of the Boltzmann linearized collision operator and the properties of the variational approximation spaces associated with the transport linear systems [15].

B Zero mass fractions

Zero mass fractions lead to artificial singularities in the transport linear systems which are eliminated by considering rescaled versions of the original systems [15]. Provided the diffusion matrix is replaced by the flux diffusion matrix $\widetilde{D}_{kl} = \mathrm{Y}_k D_{kl}$, $k, l \in \mathcal{S}$, it is proven in [15] that all the transport coefficients are smooth rational functions of the mass fractions and admit finite limits when some mass fractions become arbitrarily small. Moreover, the iterative algorithms obtained for positive mass fractions can be rewritten in terms of a rescaled system matrix that is still defined for nonnegative mass fractions and yield the same sequence of iterates [15]. This result establishes rigorously the validity of a common practice in numerical calculations, which consists in evaluating transport properties of a given gas mixture by first adding to all the species mass fractions a very small number, typically lower than the machine precision.

Even though the singularities disapear by using the flux diffusion matrix $C = \mathrm{diag}(\mathrm{Y}_1, \ldots, \mathrm{Y}_{n^s})D$ we have still evaluated the numerical errors with the Frobenius norm of the original symmetric diffusion matrices D. However, similar convergence behavior have been observed with the errors measured trough the matrix C.

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