On the Schur complement form of the Dirichlet-to-Neumann operator

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Abstract

The Dirichlet-to-Neumann operator relates the values of the normal derivative of a scalar field to the values of the field itself on the boundary of a simply connected domain. Although it is easy to prove analytically that the Dirichlet-to-Neumann operator is self-adjoint, the discretization of the pertinent Green’s integral equation by means of the usual Galerkin approach generally results in a non-symmetric matrix representation of that operator. In this paper we remedy this by means of a Hamiltonian Schur complement method and compare it with other symmetrization approaches. It is also shown that the problem of E-wave scattering by a lossy dielectric cylinder can be nicely simplified by means of the Dirichlet-to-Neumann operator. A numerical Galerkin implementation demonstrates the strength and versatility of the present approach.

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1. Introduction

The Dirichlet-to-Neumann [1] or Poincaré–Steklov [2] operator \( \mathcal{Y} \) relates the values of the normal derivative \( E_n \) of a scalar electric field \( E \) to the values of the field itself on the boundary \( c \) of a simply connected domain \( D \). In other words we have \( E_n = \mathcal{Y} E \). Inside the domain \( D \) we suppose that the field \( E \) satisfies the Helmholtz equation for a homogeneous, non-magnetic material, i.e.,

\[
\nabla^2 E + k^2 E = 0
\]

with \( k = \sqrt{-j\omega \mu_0 (\sigma + j\omega \epsilon)} \). Hence \( \mathcal{Y} \) is dependent on the wavenumber \( k \). For any two fields \( u, v \) satisfying (1), we readily find by Green’s theorem that

\[
0 = \int_c (vu_n - uv_n) \, ds = \int_c (v\mathcal{Y}u - u\mathcal{Y}v) \, ds
\]
which implies that the operator \( \mathcal{Y} \) is self-adjoint. More precisely, we have that \( \mathcal{Y} \) is a self-adjoint pseudo-differential operator of order 1 [1], with domain the space \( H_{1/2}(\epsilon) \) and range the dual space \( H_{-1/2}(\epsilon) \) [3,4]. One of the striking facts concerning the Dirichlet-to-Neumann operator is the observation [5] that the wavenumber in the domain \( D \) may be replaced with the wavenumber \( k_0 \) of the surrounding region, provided we introduce an equivalent surface current density \( j_s \), related to the value of the electric field \( E \) on the boundary \( \epsilon \) by means of a differential surface admittance operator \( Y \) defined by:

\[
j_s = \mathcal{Y}E \overset{\text{def}}{=} \frac{1}{j_0k_0} [Y_k - Y_{k_0}]E
\]

(3)

Note that in the sequel we will generally adopt the notation \( \mathcal{Y} = \mathcal{Y}_k \) and \( \mathcal{Y}_0 = \mathcal{Y}_{k_0} \). It is shown in [5] that the introduction of this equivalent surface current density greatly simplifies skin effect calculations of good (but not perfect) conductors in the presence of external fields. A possible description of the Dirichlet-to-Neumann operator is given by the well-known boundary integral equation

\[
\frac{1}{2}E(r) = \int_\epsilon \left[ \left( \frac{\partial}{\partial n} g(r - r') \right) E(r') - g(r - r') E_n(r') \right] ds' \tag{4}
\]

where the Green's function is \( g(r - r') = \frac{i}{2} H_0^{(2)}(k|r - r'|) \). This can be compactly written in an easily understood operator format:

\[
\frac{1}{2}E = g_s E - g E_n \tag{5}
\]

Hence, formally, from Eq. (5) we find

\[
\mathcal{Y} = g^{-1}(g_s - I/2) \tag{6}
\]

where \( I \) is the identity operator. It is seen that the self-adjoint character of \( \mathcal{Y} \) is not apparent in Eq. (6) at first glance. Nevertheless, from the single layer potential representation

\[
E(r) = \int_\epsilon g(r - r') \xi(r') ds' \tag{7}
\]

with normal derivative [6]:

\[
E_n(r) = -\frac{1}{2} \xi(r) + \int_\epsilon \left( \frac{\partial}{\partial n} g(r - r') \right) \xi(r') ds' \tag{8}
\]

which can be formally written as \( E = g \xi \) and \( E_n = -\xi/2 + g_n \xi \), we obtain:

\[
\mathcal{Y} = (g_n - I/2)g^{-1} = \mathcal{Y}' \tag{9}
\]

thereby proving the self-adjointness of \( \mathcal{Y} \). Here we have utilized the fact that \( (g_n)' = g_n' \) and \( g' = g \).

However, discretizing and solving the integral equation (4) by means of a Galerkin approach generally results in a non-symmetric matrix representation of the operator \( \mathcal{Y} \), and hence the reciprocity relation (2) at first sight does not seem to have a discrete equivalent. This is of course counter-intuitive and un-physical. In Section 2 we remedy this formally (in an involutive algebra setting ¹, see [7]) by means of a Hamiltonian Schur complement approach. In Section 3 we successfully apply this to the problem of E-wave or transverse magnetic (TM) scattering by a lossy dielectric cylinder: it is shown that the single integral equation treatment of [8] can be nicely simplified by means of the Dirichlet-to-Neumann operator. In Sections 4 and 5 pertinent Galerkin schemes are proposed, documented and implemented in order to find the Schur and other explicitly symmetric discretized matrix formulations of the Dirichlet-to-Neumann operator. Finally, typical low fre-

¹ An involutive algebra is an operator algebra together with an involution ¹ such that \( (a')' = a, (a + b)' = a' + b', (ab)' = b'a' \). The operator \( a' \) is called the adjoint operator of \( a \). When \( a' = a \) the operator \( a \) is called self-adjoint. In a matrix context \( a' \) can stand for the transpose \( a^\top \) (real involution) or the Hermitian transpose \( a^H \) (complex involution).
quency wave propagation calculations are presented in order to demonstrate the versatility of the present approach.

2. A Hamiltonian Schur complement approach

Following [2,9] we obtain an explicitly self-adjoint expression for $\mathcal{Y}$ by adjoining to (4) the derived integral equation

$$\frac{1}{2}E_n(r) = \int_c \left[ \left( \frac{\partial^2}{\partial n \partial n} g(r - r') \right) E(r') - \left( \frac{\partial}{\partial n} g(r - r') \right) E_n(r') \right] ds'$$

(10)

which can formally be written as

$$\frac{1}{2}E_n = g_{nn}E - g_nE_n$$

(11)

By construction, it is seen that $g_{nn}$ is self-adjoint. Eqs. (5) and (11) together can be written in block format as

$$\begin{bmatrix} E \\ E_n \end{bmatrix} = \begin{bmatrix} K & -G \\ J & -K' \end{bmatrix} \begin{bmatrix} E \\ E_n \end{bmatrix}$$

$$= \mathcal{H} \begin{bmatrix} E \\ E_n \end{bmatrix}$$

(12)

with $G = G', K = 2g_n, K' = 2g_n$ and $J = J' = 2g_{nn}$. The operator $\mathcal{H}$ thus defined exhibits a Hamiltonian structure [10], i.e., we have

$$\mathcal{H} = \begin{bmatrix} J & -K' \\ -K & G \end{bmatrix} = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \mathcal{H}^\prime$$

(13)

We know that $E_n = \mathcal{Y}E$ with $\mathcal{Y} = \mathcal{Y}$. From Eq. (12) it is also clear that $\mathcal{Y}$ satisfies the operator equations

$$I = K - G\mathcal{Y}$$

(14)

$$\mathcal{Y} = J - K'\mathcal{Y}$$

(15)

Furthermore, the square of the operator $\mathcal{H}$ is

$$\mathcal{H}^2 = \begin{bmatrix} K^2 - GJ & -KG + GK' \\ JK - K'J & (K^2 - GJ)' \end{bmatrix}$$

(16)

From Eq. (14) we obtain $G = KG - G\mathcal{Y}G$, and from the adjoint of Eq. (14), i.e., $I = K' - \mathcal{Y}G$, we obtain $G = GK' - G\mathcal{Y}G$, implying that $KG - GK' = 0$. Also, pre-multiplying Eq. (14) with $\mathcal{Y}$ we obtain $\mathcal{Y} = \mathcal{Y}K - \mathcal{Y}G\mathcal{Y}$, thereby showing that $K'\mathcal{Y} = \mathcal{Y}K$. Similarly, from Eq. (15) we obtain $\mathcal{Y}K = JK - K'\mathcal{Y}K$, and from the adjoint of Eq. (15), i.e., $\mathcal{Y}' = J - \mathcal{Y}K$, we obtain $K'\mathcal{Y} = K'J - K'\mathcal{Y}K$, implying that $JK - K'J = 0$. Hence

$$\mathcal{H}^2 = \begin{bmatrix} K^2 - GJ & 0 \\ 0 & (K^2 - GJ)' \end{bmatrix}$$

(17)

Eqs. (14) and (15) can be written in block format as:

$$\begin{bmatrix} I \\ \mathcal{Y} \end{bmatrix} = \mathcal{H} \begin{bmatrix} I \\ \mathcal{Y} \end{bmatrix}$$

(18)

Hence, applying $\mathcal{H}$ twice we obtain

$$\begin{bmatrix} I \\ \mathcal{Y} \end{bmatrix} = \mathcal{H}^2 \begin{bmatrix} I \\ \mathcal{Y} \end{bmatrix} = \begin{bmatrix} K^2 - GJ & 0 \\ 0 & (K^2 - GJ)' \end{bmatrix} \begin{bmatrix} I \\ \mathcal{Y} \end{bmatrix}$$

(19)
implying that $K^2 - GJ = I$. In other words $\mathcal{H}^2 = I$, i.e., $\mathcal{H}$ is a Hamiltonian square root of the identity, implying that the so-called Calderón operators $\mathcal{P}_\pm = (I \pm \mathcal{H})/2$ are oblique projectors in general\(^2\). The explicitly self-adjoint form of $\mathcal{V}$ can be found as the Schur complement [11,12]:

$$\mathcal{V} = \frac{1}{2} \left( J - (I - K')G^{-1}(I - K) \right)$$

(20)

For $Z = \mathcal{V}^{-1}$ we have a similar self-adjoint Schur complement:

$$Z = \frac{1}{2} \left( -G + (I + K)J^{-1}(I + K') \right)$$

(21)

Note that $\mathcal{V}$ is a self-adjoint solution of the algebraic operator Riccati equation

$$2\mathcal{V} + \mathcal{V}G\mathcal{V} - J = 0$$

(22)

Remark 1. Since $K^2 - GJ = I$ and $KG = GK'$, implying $G^{-1}K = K'G^{-1}$, we easily obtain (see also a similar argument in [13]):

$$J = K'G^{-1}K - G^{-1}$$

(23)

Inserting this in equation (20) we find:

$$\mathcal{V} = \frac{1}{2} \left[ K'G^{-1}K - G^{-1} - (I - K')G^{-1}(I - K) \right] = \frac{1}{2} \left[ (K' - I)G^{-1} + G^{-1}(K - I) \right]$$

(24)

This is exactly the symmetrized form of the solution of equation (14), which is $\mathcal{V} = G^{-1}(K - I)$.

Remark 2. Consider the associated Hamiltonian $\tilde{\mathcal{H}}$, obtained by replacing $K$ with $-K$, i.e.,

$$\tilde{\mathcal{H}} = \begin{pmatrix} -K & -G \\ J & K' \end{pmatrix}$$

(25)

It is clear that we also have $\tilde{\mathcal{H}}^2 = I$. The associated Hamiltonian $\tilde{\mathcal{H}}$ therefore also admits an associated Dirichlet-to-Neumann operator $\tilde{\mathcal{V}}$ defined by the equations:

$$I = -K - G\tilde{\mathcal{V}}$$

(26)

$$\tilde{\mathcal{V}} = J + K'\tilde{\mathcal{V}}$$

(27)

yielding the self-adjoint Schur complement representations:

$$\tilde{\mathcal{V}} = \frac{1}{2} \left( J - (I + K')G^{-1}(I + K) \right)$$

(28)

$$\tilde{Z} = \tilde{\mathcal{V}}^{-1} = \frac{1}{2} \left( -G + (I - K)J^{-1}(I - K') \right)$$

(29)

It is a simple matter to prove the following important identities:

$$-2G^{-1} = \mathcal{V} + \tilde{\mathcal{V}}, \quad 2J^{-1} = Z + \tilde{Z}$$

$$2K = G(\mathcal{V} - \tilde{\mathcal{V}}) = (Z - \tilde{Z})J$$

(30)

Note that, given two self-adjoint invertible operators $\mathcal{V}$ and $\tilde{\mathcal{V}}$, with respective inverses $Z$ and $\tilde{Z}$, the identities (30) imply (31) and are sufficient to define a Hamiltonian $\mathcal{H}$ such that $\mathcal{H}^2 = I$.

Remark 3. If we have the Dirichlet eigenvalues $\lambda_m$ and eigenfunctions $\phi^m(r)$ for the region $D$ at our disposal, we can also write down the integral kernel of $\mathcal{V}$ [5] as:

$$\mathcal{V}(r, r') = \sum_{m=1}^{\infty} \frac{\phi^m(r) \overline{\phi^m(r')}}{k^2 - \lambda_m}$$

(32)

\(^2\) Self-adjoint idempotents are called orthogonal projectors, while non-self-adjoint idempotents are called oblique projectors.
Similarly, with the Neumann eigenvalues \( \tilde{\lambda}_m \) and eigenfunctions \( \tilde{\psi}^m(r) \) for the region \( D \), we can write down the integral kernel of \( Z \):

\[
Z(r, r') = -\sum_{m=1}^{\infty} \frac{\tilde{\psi}^m(r)\tilde{\psi}^m(r')}{k^2 - \tilde{\lambda}_m}
\]

Interestingly enough, the representations (32) and (33) are the respective solutions to the algebraic operator Riccati Eq. (22) in the degenerate cases \( G = 0 \) (Dirichlet Green’s function) and \( J = 0 \) (Neumann Green’s function).

3. TM scattering by a dielectric cylinder

As an application, we consider the TM scattering problem of a lossy dielectric cylinder with wavenumber \( k \) and cross-section \( D \), in an incoming field \( E'(r) \). The pertinent integral equations are [8]:

\[
\frac{1}{2}E(r) = g_0E - gE_a
\]

\[
E'(r) - \frac{1}{2}E(r) = \int_c \left[ \left( \frac{\partial}{\partial n}g_0(r - r') \right) E'(r') - g_0(r - r')E_a(r') \right] ds'
\]

(34)\hspace{1cm}(35)

where \( g_0(r - r') = \frac{1}{2}H_0^1(k_0|r - r'|) \) with \( k_0 \) the wavenumber outside the cylinder. The integral equations (34) and (35) can be written in an easily understood shorthand notation:

\[
\frac{1}{2}E = g_0E - gE_a
\]

\[
E' - \frac{1}{2}E = g_0E - g_0E_a
\]

\[
-\frac{1}{2}E^s = g_0E^s - g_0E^s_a
\]

(36)\hspace{1cm}(37)\hspace{1cm}(38)

where the scattered field \( E^s = E - E' \). Note that we have used the fact:

\[
\frac{1}{2}E^s = g_0E - g_0E^s_a
\]

(39)

which is equivalent with \( E^s_n = \gamma_0E' \). The scattered field \( E^s \) can be written as a single layer potential \( E^s = g_0\zeta \), yielding the single integral equation for \( \zeta \):

\[
\frac{1}{2}E^s - g_0E^s + gE^s_a = \left[ -\frac{1}{2}g_0 - \frac{1}{2}g + g_0g_0 - gg_0 \right] \zeta
\]

(40)

Inside the scatterer we can write the single layer potential \( E = g\zeta \), yielding the single integral equation for \( \zeta \):

\[
E' = \left[ \frac{1}{2}g_0 + \frac{1}{2}g + g_0g_0 - g_0g_0 \right] \zeta
\]

(41)

The integral equations (40) and (41), which were first introduced in [8] and later also documented in [14], can be further reduced to a simpler form. With the notations of Section 2, the integral equations (36) and (37) can be written as

\[
E = KE - GE_a
\]

\[
2E' - E = K_0E - G_0E_a
\]

(42)\hspace{1cm}(43)

The integral equation (42) can be replaced with \( E_a = \gamma E \), which inserted in (43) yields

\[
E^s = g_0[\gamma_0 + \gamma]E
\]

(44)

The simple integral equation (44) allows us to find \( E \) on \( c \) directly. The relationships \( E = E^s + g_0\zeta \) and \( E = g\zeta \) (7) then yield \( \zeta \) and \( \zeta \) and therefore the complete solutions inside and outside the scatterer. The integral equa-
tion (44) presents an interesting twist: since the first identity of (30) tells us that \( \mathcal{Y}_0 + \mathcal{Y}'_0 = -g_0^{-1} \), Eq. (44) can be written as

\[
E^i = E + g_0[\mathcal{Y}_0 - \mathcal{Y}]E
\]

which is a Fredholm equation of the second kind. Eq. (45), which exhibits the differential Dirichlet-to-Neumann operator [5] \( \mathcal{Y}_0 - \mathcal{Y} \), can also be found by another means, for instance by introducing the additional 'phantom' integral equation:

\[
\frac{1}{2}E = g_0E - g_0\tilde{E}_n
\]

We can always do so provided \( \tilde{E}_n = \mathcal{Y}_0E \). Subtracting (46) from (37) we obtain

\[
E^i - E = g_0[\tilde{E}_n - E_n]
\]

which is precisely integral equation (45). Note that Eq. (45) implies that \( E^sc = g_0[\mathcal{Y}_0 - \mathcal{Y}]E \)

resulting in \( \xi = [\mathcal{Y} - \mathcal{Y}_0]E \). Finally, let us effectively prove that the formidable integral equations (40) and (41) can be reduced to the very simple integral equation (44). Regarding integral equation (41), it is relatively easy to show that

\[
\frac{1}{2}g_0 + \frac{1}{2}g + g_0 \epsilon g - g_0 g_n = -g_0[\mathcal{Y}_0 + \mathcal{Y}]g
\]

which is consistent with integral equation (44). We can also find an explicit expression for \( \xi \), i.e.,

\[
\xi = -[\mathcal{Y} + \mathcal{Y}_0]E^i - [\mathcal{Y}_0 - \mathcal{Y}]E^{sc}
\]

The case of integral equation (40) is more difficult; however, it is not too hard to prove that

\[
\frac{1}{2}E^i - g_0E^i + gE_n = g[\mathcal{Y}_0 - \mathcal{Y}]E^i
\]

and

\[
-\frac{1}{2}g_0 + \frac{1}{2}g + g_0 \epsilon g - gg_0 g_n = g[\mathcal{Y}_0 + \mathcal{Y}]g_0
\]

With the proviso that \( \text{nullspace}(g) = \{0\} \), integral equation (40) is equivalent with

\[
[\mathcal{Y}_0 - \mathcal{Y}]E^i = [\mathcal{Y}_0 + \mathcal{Y}]E^{sc}
\]

which is easily transformed into Eq. (48). The above derivations also show the conceptual superiority of the Dirichlet-to-Neumann approach as compared to the usual integral equation techniques.

4. The projected Hamiltonian matrix

As was said in Section 1, \( \mathcal{Y} \) is a self-adjoint pseudo-differential operator of order 1 mapping \( H_{1/2}(c) \) to \( H_{-1/2}(c) \), where \( c \) is the boundary contour of the relevant region \( D \). It should be noted that \( H_{1/2}(c) \) is a Sobolev–Hilbert space with norm [15] p. 208:

\[
\|E\|_{1/2} = \left( \int_c |E(s)|^2 ds + \ell \int_c \int_c \frac{|E(s) - E(s')|^2}{R^2} ds ds' \right)^{\frac{1}{2}}
\]

In Eq. (54) \( R \) stands for the Euclidian distance between the two points parametrized by \( s \) and \( s' \) on the contour \( c \), and \( \ell \) is a positive parameter proportional to the length of the contour \( c \) in order to make formula (54) dimensionally correct. The dual norm \( \|E\|_{-1/2} \) is defined via the usual procedure (see [4] p. 320), but is virtually impossible to compute in any practical situation. Fortunately, we know [3] that
with $H_{1/2}(c)$ dense in $L_2(c)$. For instance, as a consequence of the proper subset equation (55), there are functions in $L_2(c)$ that are not in $H_{1/2}(c)$, and functions in $H_{-1/2}(c)$ that are not in $L_2(c)$.

In the context of a Galerkin procedure for obtaining an approximation to $\gamma$, this is important, since we have to develop $E$ into basis functions in $H_{1/2}(c)$ and $E_n$ into basis functions in $H_{-1/2}(c)$. Note that the second integral in formula (54) is a so-called hypersingular integral, which diverges for piecewise constant functions $E$ but converges for piecewise linear functions $E$ [16]. This having been specified, recall that our pertinent equations are

$$E = KE - GE_n$$  \hspace{1cm} (56)
$$E_n = J E - K' E_n$$  \hspace{1cm} (57)
$$E_n = \gamma E$$  \hspace{1cm} (58)

The fields $E$ and $E_n$ are expanded as

$$E = \sum_{k=1}^{\infty} \alpha_k b_k(s)$$  \hspace{1cm} (59)
$$E_n = \sum_{k=1}^{\infty} \beta_k t_k(s)$$  \hspace{1cm} (60)

where the set of real basis functions $\{b_k(s)\}$ and $\{t_k(s)\}$ are complete, respectively, in $H_{1/2}(c)$ and $H_{-1/2}(c)$. Inserting this in Eqs. (56) and (58) we obtain

$$\sum_{k=1}^{\infty} \alpha_k b_k = \sum_{k=1}^{\infty} \alpha_k K b_k - \sum_{k=1}^{\infty} \beta_k G t_k$$  \hspace{1cm} (61)
$$\sum_{k=1}^{\infty} \beta_k t_k = \sum_{k=1}^{\infty} \alpha_k J b_k - \sum_{k=1}^{\infty} \beta_k K' t_k$$  \hspace{1cm} (62)
$$\sum_{k=1}^{\infty} \beta_k t_k = \sum_{k=1}^{\infty} \alpha_k \gamma b_k$$  \hspace{1cm} (63)

A self-consistent Galerkin procedure is obtained by testing Eq. (61) with the set $\{t_k\}$, while testing Eqs. (62) and (63) by means of the set $\{b_k\}$, resulting in

$$\sum_{k=1}^{\infty} \alpha_k \langle t_1, b_k \rangle = \sum_{k=1}^{\infty} \alpha_k \langle t_1, K b_k \rangle - \sum_{k=1}^{\infty} \beta_k \langle t_1, G t_k \rangle$$  \hspace{1cm} (64)
$$\sum_{k=1}^{\infty} \beta_k \langle b_1, t_k \rangle = \sum_{k=1}^{\infty} \alpha_k \langle b_1, J b_k \rangle - \sum_{k=1}^{\infty} \beta_k \langle b_1, K' t_k \rangle$$  \hspace{1cm} (65)
$$\sum_{k=1}^{\infty} \beta_k \langle b_1, t_k \rangle = \sum_{k=1}^{\infty} \alpha_k \langle b_1, \gamma b_k \rangle$$  \hspace{1cm} (66)

Note that, the operator $J$ being a hypersingular operator [16], the self-patch elements $\langle b_k, J b_l \rangle$ are finite if and only if the basis functions $b_k$ belong to $H_{1/2}(c)$, since the hypersingular integral present in the norm (54) exhibits the same singularity as $J$. In the same context, it is known that operator $J$ can alternatively be written as an integro-differential operator [9], i.e.,

$$J = k^2 \mathbf{n}(r) \cdot \mathbf{n}(r') g(r - r') + \frac{\partial g(r - r')}{\partial \mathbf{s'}} \frac{\partial}{\partial \mathbf{s}}$$  \hspace{1cm} (67)

resulting in the Galerkin elements:

$$\langle b_k, J b_l \rangle = k^2 \int_c \int_c b_k(s) b_l(s') \mathbf{n}(r) \cdot \mathbf{n}(r') g(r - r') ds ds' - \int_c \int_c b_k'(s) b_l'(s') g(r - r') ds ds'$$  \hspace{1cm} (68)
Of course, the derivation of formula (68) requires the slightly more stringent assumption that the basis functions \{b_k\} belong to \(H_1(c)\), which is, e.g., the case when the \{b_k\} are piecewise boundedly differentiable, say in practice when one uses the well-known linear rooftop functions [16].

Eqs. (64)–(66) can be written in the easily understood infinite matrix format

\[
\begin{align*}
T_x &= Kx - G\beta \\
T^T\beta &= Jx - K^T\beta \\
T^T\beta &= Yx
\end{align*}
\] (69) (70) (71)

where

\[
T_{kl} = \langle t_k, b_l \rangle \quad K_{kl} = \langle t_k, Kb_l \rangle \quad G_{kl} = \langle t_k, Gt_l \rangle \quad J_{kl} = \langle b_k, Jb_l \rangle \quad Y_{kl} = \langle b_k, Yb_l \rangle
\] (72)

Eliminating the unknowns \(x\) and \(\beta\), we obtain the projected infinite block matrix equations

\[
\begin{pmatrix}
1 \\
Y
\end{pmatrix} = H \begin{pmatrix}
1 \\
Y
\end{pmatrix}
\] (73)

with projected Hamiltonian matrix

\[
H = \begin{pmatrix}
T^{-1}K & -T^{-1}GT^{-T} \\
J & -K^T T^{-T}
\end{pmatrix} = \begin{pmatrix}
\hat{K} & -\hat{G} \\
\hat{J} & -\hat{K}
\end{pmatrix}
\] (74)

The explicitly symmetric form of \(Y\) can be found as the Schur complement:

\[
Y = \frac{1}{2} \left[ \hat{J} - (I - \hat{K}^T)\hat{G}^{-1}(I - \hat{K}) \right] = \frac{1}{2} \left[ J - (T - K)^T G^{-1}(T - K) \right]
\] (75)

It is seen that, exactly in parallel with the operator formalism of Section 2, the requirement \(H^2 = I\) is needed, implying that \(\hat{K} \hat{G} = \hat{G} \hat{K}^T\) and \(\hat{K} \hat{J} = \hat{J} \hat{K}^T\). Also, following Remark 1 of Section 2, it follows that \(Y\) can similarly be written in the symmetrized form

\[
Y = \frac{1}{2} \left[ (\hat{K}^T - I)\hat{G}^{-1} + \hat{G}^{-1}(\hat{K} - I) \right] = \frac{1}{2} \left[ (K - T)^T G^{-1}T + T^T G^{-1}(K - T) \right]
\] (76)

and hence the hypersingular Galerkin matrix \(J = \hat{J}\) can be written as

\[
J = \hat{K}^T \hat{G}^{-1} \hat{K} \hat{G}^{-1} - \hat{K} \hat{G}^{-1} = K^T G^{-1}K - T^T G^{-1}T
\] (77)

A similar (although in a different context) expression for \(J\) was found in [13]. This means that we only have to calculate the entries of the matrices \(G\), \(K\) and \(T\). A still ‘cheaper’ approach can be found in the Theorems A and B of the Appendix, where it is shown that one only needs the eigen-decomposition of the matrix \(K\) and the diagonal entries of one of the matrices \(G\) or \(J\). Of course, it should be noted that all this will only be approximately valid when the bases \(\{b_k\}\) and \(\{t_k\}\) are truncated, i.e., when we have \(1 \leq k \leq M\) for some sufficiently large, but finite \(M\).

5. Verification and numerical simulations

The different expressions for the discretized Dirichlet-to-Neumann operator \(Y\) will be constructed for a number of two-dimensional examples, where the cross-section \(D\) of the cylinder is a rectangle. The parameters of the lossy cylinder are \(\epsilon\), \(\mu_0\), \(\sigma\) and the working frequency is \(f = \omega / 2\pi\), resulting in the wavenumbers \(k_0 = \omega / c = 2\pi / \lambda\) and \(k = \sqrt{-\omega \mu_0 (\sigma + j\omega \epsilon)}\). From the derivation of formula (68) we need \(\{b_k\} \subset H_1(c)\), and for all practical purposes this means that one may use the well-known linear rooftop functions [16]. In order to avoid unnecessary complications we also consider the ‘full’ Galerkin case \(\{t_k\} = \{b_k\}\). The linear rooftop basis \(\{b_k\}\) is shown in Fig. 1. It is seen that the boundary of the cross-section of the cylinder is divided into 32 overlapping segments of width \(2d\), where \(d = d_x = d_y\) is the discretization step. The number of discretizations in the \(x\)- and \(y\)-directions are \(n_x = 12\) and \(n_y = 4\) for the configuration shown in Fig. 1.
In this section, we shall first calculate a number of projected Dirichlet-to-Neumann operators and verify the symmetry and convergence properties. The entries of these Dirichlet-to-Neumann operators are subsequently compared with the results obtained from the Dirichlet eigenfunction expansion method [5]. Finally, we will discuss the performance of the different methods with respect to the modelling of low frequency waves. The methods presented in the previous sections, that will be applied below, will be referred to as the Schur complement method (see Eq. (75)), the symmetrization approach (see Eq. (76)), the asymmetric description (utilizing only the two Eqs. (69) and (71))) and the eigen-decomposition method (see Theorems A and B of the Appendix).

5.1. Comparison of the projected operators with results from other methods

In this subsection, we compare the different $Y$ matrices, obtained by applying a Galerkin projection in the case of a rectangular cylinder with dimensions $a = 6$ mm and $b = 3$ mm. The lossless ($\sigma = 0$) cylinder has a permittivity of $\varepsilon_r = 6$. The results obtained with the Schur complement approach (75) are first compared with those resulting from the Dirichlet method [5] and with those obtained from the asymmetric approach (76). The interactions with a rooftop in the upper right corner (row 19 of the admittance matrix) of the cylinder are plotted as a function of frequency in Fig. 2 (imaginary part) and in Fig. 3 (real part). Figs. 2 and 3 indicate that the Schur complement method matrix elements coincide with the matrix entries obtained with the Dirichlet method [5]. The asymmetric approach yields mostly correct results, although the self-interaction (located at the 19th coordinate) is not truly accurate. When observing the real part (Fig. 3) of the three methods under scrutiny, which should be zero ($\sigma = 0$), the result obtained with the asymmetric approach is largely unsatisfactory. The real part is small, but non-negligible. The overall impact could be unacceptable, should an admittance model be used in a global simulation.

The interactions of a rooftop in the middle of the upper edge of the cylinder (10th row of the $Y$ matrix) are shown in Fig. 4 (imaginary part) and in Fig. 5 (real part). All methods now yield correct results with respect to the imaginary part, but the discrepancies in the real part are still important. The other non-Schur methods result in comparable discrepancies of the real part. In Fig. 6, the real parts of the corner interactions (19th row of the $Y$ matrix) are presented, for three non-Schur approaches: the asymmetric method, the symmetrization approach and the eigen-decomposition algorithm. For this particular example, the symmetrization approach performs better than the other two methods. The residual dissipation is more or less equal for the three examples.

In Fig. 7, the real parts of the interactions with a rooftop in the middle of the upper edge (row 19) are shown, for the three non-Schur approaches discussed above. Comparing with the corner case, we can conclude that the behavior is similar, whereas the residual dissipation is somewhat smaller on the edges than on the corners. In the next subsection, it will be shown that the residual dissipation resulting from the non-Schur approaches significantly alters the results when a conductive material is used.
5.2. Verification of the DC resistance

When a low frequency transverse magnetically (TM) polarized wave impinges on a homogeneous conducting cylinder or when a low frequency signal propagates through the cylinder, a uniform current distribution pattern develops inside the cylinder. The associated DC resistance per unit of length (p.u.l.) is given by Pouillet’s law:

\[ R = \frac{2\pi \sigma L}{\delta} \]

where:
- \( R \) is the DC resistance per unit of length (p.u.l.),
- \( \sigma \) is the conductivity of the material inside the cylinder,
- \( L \) is the length of the cylinder, and
- \( \delta \) is the characteristic length of the wave propagation.

Fig. 2. Imaginary part of the 19th row (corner interaction) of the Schur complement, Dirichlet-based and symmetrization \( Y \) matrices.

Fig. 3. Real part of the 19th row (corner interactions) of the Schur complement, eigenfunction-based and symmetrization \( Y \) matrices.
where $a$ and $b$ are the dimensions of the rectangular cylinder. The calculation of the DC p.u.l. resistance from the admittance matrix is straightforward:

$$R_{DC} = \frac{1}{\sigma \, ab} \quad (78)$$
It is of course very important that $R_{DC}$ is accurately predicted by any numerical method. We will now take a look at the performance of the various methods discussed above with regard to this DC resistance. We con-

$$R_{DC} = \Re \left\{ \sum_i \sum_j Y_{ij} \right\}^{-1}$$ (79)

Fig. 6. Real part of the 19th row (corner interactions) of three non-Schur-based $Y$ matrices.

Fig. 7. Real part of the 10th row (middle of upper edge) of three non-Schur-based $Y$ matrices.

It is of course very important that $R_{DC}$ is accurately predicted by any numerical method. We will now take a look at the performance of the various methods discussed above with regard to this DC resistance. We con-
sider a copper cylinder ($\sigma = 5.72 \times 10^7$ S/m) with aspect ratio $r = a/b = 3/2$. The number of discretizations in the $x$, resp. $y$-direction, is $n_x$, resp. $n_y$.

In Table 1, the theoretical DC resistance (in $\Omega$/m) is shown for five simulations with subsequent mesh refinements, together with the results obtained with the Schur complement method and with those obtained with three non-Schur methods. These are the asymmetric approach, the symmetrized approach and the eigen-decomposition method, which turn out to be equivalent when calculating DC resistances. This explains why only a single value is given in the last column of Table 1. It should be noted that the DC resistances of Table 1 are remarkably close to the theoretical values given by Eq. (78). The non-Schur results deviate only slightly for some simulations. When simulating semiconductor type cylinders, the conclusions are very different.

In Table 2, the admittances $Y_{DC} = 1/R_{DC}$ of a $14.4 \mu$m ($n_x = 12$) by $9.6 \mu$m ($n_y = 8$) cylinder are shown for a total of 20 different $\sigma$ values. $Y_{DC}$ is in units of $10^{-12}$ S/m. Only the Schur results are displayed; the admittances obtained from the non-Schur methods were several orders of magnitude too large and negative, i.e., $Y_{DC}$ (non-Schur) in the range $[-0.3283 \times 10^{-9}, -0.1442 \times 10^{-9}]$ S/m for all non-Schur simulations. The results obtained with the Schur complement method are correct when a sufficient number of basis functions is chosen.

The results for the lower conductivity values are slightly less accurate, probably due to the residual dissipation which starts to play a role at these low conductivity values.

### 5.3. Numerical verification of symmetry

In order to verify the accuracy of the expressions (75) and (76) in a realistic context, we consider how the $Y$ matrices of a rectangular cylinder evolve as a function of frequency, the number of basis functions and the material parameters. We use the same notation as in the previous example for the dimensions and discretizations.

Here we consider good conductors, semiconductors and dielectric materials: copper [Cu] ($\sigma = 5.72 \times 10^7$ S/m, $\varepsilon_r = 1.0$), silicon [Si] ($\sigma = 1.6 \times 10^{-3}$ S/m, $\varepsilon_r = 11.0$) and PECVD Silicon Nitride [SiN] ($\sigma = 10^{-10}$ S/m, $\varepsilon_r = 7.0$). The material name abbreviations between square brackets are used in Table 3, where the relevant parameters for the subsequent simulations are shown.

For the simulations with Si and SiN, a frequency sweep between $f_l = 1$ MHz and $f_h = 1$ THz is performed. For the copper example, the simulation bandwidth is chosen such that $\rho = 0.5(a + b)/\delta \in [10^{-2}, 10^4]$, where the skin depth $\delta$ is defined as:

$$\delta = \sqrt{\frac{2}{2\pi f \sigma \mu_0}}$$

Because of this particular choice of a set of frequency points, the transition region between the low frequency situation (the current flows uniformly in the longitudinal direction) and the high frequency case (the current is forced to the border of the cylinder), is completely covered. The numerical symmetry of the Schur complement formulation is compared with the results of the asymmetric and eigen-decomposition formulations. In order to measure the departure from symmetry, we take the relative 2-norm of the asymmetric part: $\alpha(f) = \|Y - Y^T\|_2/\|Y\|_2$ as a function of frequency. The maximum and minimum values over the chosen frequency range for the Schur approach are listed in Table 3 as $\varepsilon_{\text{max}}$ and $\varepsilon_{\text{min}}$ for a total of twelve simulations. For the asymmetric and eigen-decomposition formulations, $\alpha(f)$ as a function of frequency remains acceptable at the higher part of the spectrum, but very rapidly increases for the lower frequencies to reach values of the order of 0.5.

<table>
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<th>$a$</th>
<th>$b$</th>
<th>$n_x$</th>
<th>$n_y$</th>
<th>$R_{DC}$ (Pouillet)</th>
<th>$R_{DC}$ (Schur)</th>
<th>$R_{DC}$ (non-Schur)</th>
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<td>4</td>
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<td>8</td>
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</tbody>
</table>
minimum values $\epsilon_{\text{min}}$ are also given in Table 3. These values clearly show that the Schur approach is the only one assuring that the physically required symmetry property of the Dirichlet-to-Neumann operator is well-preserved in its discretized version.

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**Appendix A**

**Theorem A.** Let the complex matrices $G = G^T$, $J = J^T$ and $K$ be such that

1. $K$ is diagonalizable with all its eigenvalues different.\(^3\)

Then, $K$, $G$ and $J$ can be written as

$$K = PA_K P^{-1} \quad G = PA_G P^T \quad J = P^{-T} A_J P^{-1}$$

(A.1)


**Proof.** $K = PA_K P^{-1}$ is simply the eigen-decomposition of $K$ where supposedly $\lambda_K = \text{diag}\{\lambda_k\}$ with all $\lambda_k$ different. Since $P$ is non-singular, the symmetric matrix $G$ can be written uniquely as $G = P WP^T$, where $W$ symmetric is given by $W = P^{-1} GP^T$. Since $KG = PA_K WP^T$ has to be symmetric, it is necessary that $A_K W$ is symmetric. Hence we need

$$(\lambda_i - \lambda_j) W_{ij} = 0 \quad \forall i, j$$

(A.2)

implying that $W$ must be a diagonal matrix. Regarding $J$, the same reasoning applied to the matrix $V = P^{-T} J P$ results in $V$ being diagonal, and the proof is complete. \(\square\)

Note that if we put $A_G = \text{diag}\{\mu_k\}$, the matrix $G$ can be written as

$$G_{ij} = \sum_k P_{ik} P_{jk} \mu_k$$

(A.3)

implying that the diagonal entries $G_{ii}$ are sufficient to obtain the values $\mu_k$ by solving the linear equations

$$G_{ii} = \sum_k P_{ik}^2 \mu_k$$

(A.4)

Obtaining $A_J = \text{diag}\{\tau_k\}$, is then simply a matter of substitution (if none of the $\mu_k = 0$) in the equation

$$\lambda_k^2 - \mu_k \tau_k = 1$$

(A.5)

Similarly, putting $Q = P^{-T}$, the values $\tau_k$ can be obtained by solving the linear equations

$$J_{ii} = \sum_k Q_{ik}^2 \tau_k$$

(A.6)

and the $\mu_k$ follow from Eq. (A.5). The matrix $Y = G^{-1} (K - I)$ is also symmetric, and can be written as

$$Y = Q A_G^{-1} (A_K - I) Q^T = Q A_J (A_K + I)^{-1} Q^T$$

(A.7)

In the case where the eigenvalues of $K$ are algebraically degenerate, the following weaker theorem can be used.

**Theorem B.** Let the complex matrices $G = G^T$, $J = J^T$ and $K$ be such that

1. $K$ is diagonalizable.

Then the matrix $Y = G^{-1} (K - I)$ is symmetric and can be constructed from the matrices $K$ and $\Theta_G$ alone, or, equivalently, the matrices $K$ and $\Theta_J$ alone, where

$$K = PA_K P^{-1} \quad G = P \Theta_G P^T \quad J = P^{-T} \Theta_J P^{-1}$$

(A.8)

\(^3\) No similar or other restrictions are necessary regarding the eigenvectors.
Proof. $K = PA_KP^{-1}$ is again the eigen-decomposition of $K$, but here we do not require that all eigenvalues are different. $G$ can be written as $G = P\Theta_GP^T$, where the symmetric matrix $\Theta_G = P^{-1}GP^{-T}$. Similarly, for $J$, we obtain the symmetric matrix $\Theta_J = P^TJP$. Substituting this in $K^2 - GJ = I$, we obtain $A_K^2 - \Theta_G\Theta_J = I$. Putting $Q = P^{-T}$, the matrix $Y = G^{-1}(K - I)$ can be written as

$$Y = Q\Theta^{-1}_G(A_K - I)Q^T = Q\Theta_J(A_K + I)^{-1}Q^T$$

(A.9)

From the premises $KG = GK^T$ and $JK = K^TJ$ it is clear that the matrices $A_K\Theta_G$ and $\Theta_JA_K$ are symmetric and hence also the matrix

$$\Theta^{-1}_G A_K = A_K(\Theta_GA_K)^{-1}A_K$$

(A.10)

implying that $Y$ is symmetric. \qed

References