A Residual Based Error Formula for a Class of Transport Equations

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Abstract

We present an exact residual based error formula in natural norms for a class of transport equations. The derivation of the error formula relies on an abstract formulation in a general Hilbert space setting. The key role is played by the validity of an inversion formula. Its verification is for particular radiative transfer equations equivalent to the identification strong and weak traces. The residual based error formula can be used in the design of efficient and accurate simulations of the cooling process of high quality glass [5].

Key words. heat equation; stationary radiative transfer equation; residual based error formula; frequency bands; cooling processes.

AMS(MOS) subject classification. 35F15, 35Q60.

1 Introduction

We are concerned with a residual based error formula for a class of transport equations representable in the form

$$u + Au = f, \quad B^{-}u = g, \tag{1}$$

where A and B^{-} are linear operators whose domain is a Hilbert space H and whose ranges are contained in Hilbert spaces $H_0 \subseteq H$ and H_∂, respectively. In applications we have in mind the operator B^{-} is the "negative part" of a linear operator $B : H \to H_\partial$, i.e. B has a canonical representation $B = B^{+} - B^{-}$ where $B^{+} : H \to H_\partial$ is linear. The source function f of (1) is in H and the boundary value function g is in H_∂.

The operators A, B^{-} of (1) and the inner products of H, H_0, H_∂ are assumed to satisfy several compatibility conditions whose precise formulation is postponed for the moment.

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The need for an residual based error formula of (1) originates from numerical treatments. If distinct algorithms are applicable, one will wish to decide which of the approximate solutions is preferable. A most natural strategy to decide is to compare the distances of the approximate solutions from the (assumed to be unique) solution u of (1). Obviously, this strategy can not be followed in a *naive* manner: in order to calculate this distance the solution u has already to be known.

However, we will prove that for a canonical norm - the norm of H indeed - the distance equals a normed residuum. More precisely, we are heading to a proof of the residual based error formula

$$\|u-\overline{u}\|_H = \|\overline{u}+A\overline{u}-f\|_{H_0} + 2\|B^-\overline{u}-g\|_{H_\partial}, \quad \overline{u}\in H. \tag{2}$$

In (2) one can calculate the distance of an approximate solution $\overline{u}$ from u *without referring to* u. Only normed residua - one residuum for the operator term, the other one for the boundary term - have to be evaluated and summed up.

This paper's investigations originate from simulations used in glass industry. In particular, the design of cooling processes for high quality glass has to observe two incompatible aspects and is, thus, a challenging task. If the cooling is too slow, the production will be time and energy consuming and will thus be too expensive for the glass producer.

In other words, for quality and for economical reasons, the cooling process should be as short as possible but as careful as necessary.

The design of cooling processes meeting both aspects is nowadays strongly supported by efficient and reliable numerical simulations, see [1].

To fix ideas let us give a brief description of the mathematical model (further details can be found in [5]).

The cooling process of high quality glass is described by the spatio-temporal evolution of the temperature $T(t,x)$, $t\in\mathbb{R}^+$, $x\in G\subset\mathbb{R}^3$, at time t at position x in the glass.

Typically the heat transfer is induced by conduction and radiation. The radiation field inside the glass is generated by temperature depending sources. Temperature usually changes on a time scale much slower than radiation transport. Thus, it is appropriate to employ the stationary radiative transfer equation (RTE) with time depending sources.

As a consequence, the simulation of T consists in solving the heat equation where in each time step the radiative heat sources are solutions of the RTE.

The basic idea of the hybrid approach developed in [5] is to couple two fast methods originally designed for high and low absorption rates, respectively. A switching mechanism dynamically selects the more accurate method in each frequency band. The selection relies on the residual based error formula (2) which allows for the calculation of the distance $\|\overline{u}-u\|_H$ between an approximative solution $\overline{u}$ and the exact (but unavailable) solution u of the RTE, see [2].

Thus, we can assign to $\overline{u^{high}}$ (approximative solution of the RTE in the high absorption regime) and to $\overline{u^{low}}$ (approximative solution of the RTE in the low absorption regime) the respective distances $\|\overline{u^{high}} - u\|_H$ and $\|\overline{u^{low}} - u\|_H$. The selection mechanism will pick $\overline{u^{high}}$ if $\|\overline{u^{high}} - u\|_H \le \|\overline{u^{low}} - u\|_H$, and the mechanism will pick $\overline{u^{low}}$ if $\|\overline{u^{low}} - u\|_H < \|\overline{u^{high}} - u\|_H$.

The paper is organized as follows. In section 2 we present the residual based error formula for a (integrated) RTE. We formulate the two most important, yet unanswered questions concerning the validity of the derivation. Then we are concerned with a rigorous justification of the residual based error formula and, in particular, with giving answers to the two open questions.

It is convenient to give the proof a hierarchical structure. We begin with a very abstract formulation, perform intermediate steps on a less abstract level and finish the proof in a final step. On the most abstract level "G-pairs of operators" are introduced and the verification of the residual based error formula is rather immediate, see section 3. However, it is a long way to pass from this abstract result to real-life applications. Two intermediate step in Hilbert space theory (sections 4 and 5) are necessary before we can perform the proof's last step (section 6).

In comparison with the previous steps the argumentation of section 6 is rather technical. It is convenient to illustrate the strategy of the proof at hand of a toy problem.

We consider the operator $A_\circ u = \boldsymbol{\xi}_0 \cdot \nabla u = \nabla \cdot (\boldsymbol{\xi}_\circ u)$, where $\boldsymbol{\xi}_0$ is a fixed unit vector in $\mathbb{R}^3$ and $u \in H^1(G)$. Assuming a sufficiently smooth boundary of G, there is a "strong" trace operator $T_\circ : H^1(G) \to L^2(\partial G)$ such that

$$\forall \phi \in C^\infty(\overline{G}) :$$
$$\int_G (\nabla \cdot (\boldsymbol{\xi}_\circ u))(x)\phi(x)dx + \int_G u(x)(\boldsymbol{\xi}_\circ \cdot \nabla\phi)(x)dx = \int_{\partial G} (T_\circ(u)\phi)(\boldsymbol{\zeta})\ (\boldsymbol{\xi}_\circ \cdot \boldsymbol{n}(\boldsymbol{\zeta}))d\mathsf{s}(\boldsymbol{\zeta}), \quad (3)$$

where $\mathsf{s}(\boldsymbol{\zeta})$ is the surface measure on ∂G and $\boldsymbol{n}(\boldsymbol{\zeta})$ is the outer unit normal vector at $\boldsymbol{\zeta} \in \partial G$.

The Gauss-like integration by parts formula (3) allows to define a "weak" trace of a function $u \in H^1(\Omega)$: We say that $v \in L^2(\Omega)$ is a "weak trace of u" iff

$$\forall \phi \in C^\infty(\overline{G}) :$$
$$\int_G (\nabla \cdot (\boldsymbol{\xi}_\circ u))(x)\phi(x)dx + \int_G u(x)(\boldsymbol{\xi}_\circ \cdot \nabla\phi)(x)dx = \int_{\partial G} (v\phi)(\boldsymbol{\zeta})\ (\boldsymbol{\xi}_\circ \cdot \boldsymbol{n}(\boldsymbol{\zeta}))d\mathsf{s}(\boldsymbol{\zeta}). \quad (4)$$

What has to be shown in section 6 reads in the present context: If v is a weak trace of u, then v is the strong trace of u, i.e. $v = T_\circ u$.

It is quite clear how to prove this for (3) and (4): One has to prove that it is possible to extend any function in $C_0^\infty(\partial^+ G \cup \partial^- G)$ to a smooth function defined on G, where $\partial^\pm G = \{\boldsymbol{\zeta} \in \partial G : \pm \boldsymbol{\xi}_\circ \cdot \boldsymbol{n}(\boldsymbol{\zeta}) > 0\}$.

Although the coupling of the (differential) operator A and the boundary operator B^- of (1) is in the interesting situations much more complicated - for example, the boundary operator is $\boldsymbol{\xi}$-dependent, where $\boldsymbol{\xi}$ ranges in the unit sphere of $\mathbb{R}^3$ - the strategy of the proof is the same. We specify assumptions on ∂G such that an apropriate extension of certain, smooth boundary functions is possible and apply Gauss-like integration by parts formulae then to identify boundary functions with respective strong traces.

2 The Residual Based Error Formula

The hybrid algorithm [5] switches between approximative solutions of RTEs in several frequency bands. The RTEs are in each frequency band of the form

$$\frac{1}{\sigma}\,\boldsymbol{\xi} \cdot \nabla u + u = f, \quad \text{on } S^2 \times G, \tag{5}$$

$$u - \hat{\rho} u'' = g = (1 - \hat{\rho})\ h, \quad \text{for } (\boldsymbol{\xi}, \boldsymbol{\zeta}) \in S^- \tag{6}$$

where σ is the positive, constant absorption coefficient, ξ ranges in the unit sphere $S^2 = \{\boldsymbol{\xi} \in \mathbb{R}^3 : \boldsymbol{\xi} \cdot \boldsymbol{\xi} = 1\}$ of $\mathbb{R}^3$, $u = u(\boldsymbol{\xi}, \boldsymbol{x})$ is the unknown (integrated) radiation intensity in direction $\boldsymbol{\xi}$ at position $\boldsymbol{x} \in G$, where $G \subset \mathbb{R}^3$ is the glass' domain and f is a smooth, temperature dependent source function. Equation (6) is a modified Fresnel boundary condition for u which applies on the subset $S^- := \{(\boldsymbol{\xi}, \boldsymbol{\zeta}) \in S^2 \times \partial G : \boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta}) < 0\}$ (where $\boldsymbol{n}(\boldsymbol{\zeta})$ is the outer unit normal vector of G at $\boldsymbol{\zeta} \in \partial G$) of the boundary $S^2 \times \partial G$. The reflection coefficient function $\hat{\rho} : [0,1] \to [0,1]$ is determined by a Fresnel–type law and is evaluated at $|\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|$, h is a smooth temperature dependent source function and u'' is the intensity $u(\boldsymbol{\xi}'', \boldsymbol{\zeta})$ in the reflected direction

$$\boldsymbol{\xi}'' = \boldsymbol{\xi}''(\boldsymbol{\xi}, \boldsymbol{n}(\boldsymbol{\zeta})) = \boldsymbol{\xi} - 2\,(\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})) \cdot \boldsymbol{n}(\boldsymbol{\zeta}).$$

For the hybrid method [5] approximate solutions $\overline{u}$ of (5), (6) are computed. To decide which of the approximative solutions is closer to the (unique) solution u, the following residual based error formula is formally derived in [5],

$$\|u - \overline{u}\|^2 = \left\| \overline{u} + \frac{1}{\sigma}\,\xi \cdot \nabla \overline{u} - f \right\|^2_{\mathbb{L}^2(S^2 \times G)} + 2\|B^- \overline{u} - g\|^2_\partial, \tag{7}$$

where $\|.\|_{\mathbb{L}^2(S^2 \times G)}$ is the standard norm on $\mathbb{L}^2(S^2 \times G)$,

$$\|u - \overline{u}\|^2 = \|u - \overline{u}\|^2_{\mathbb{L}^2(S^2 \times G)} + \int_{S^2 \times G} |\boldsymbol{\xi} \cdot \nabla (u - \overline{u})|^2\, d(\omega(\boldsymbol{\xi}), \boldsymbol{x})$$

$$+ \frac{1}{\sigma} \int_{S^2 \times \partial G} \frac{|(u - \overline{u})(\boldsymbol{\xi}, \boldsymbol{\zeta}) - \hat{\rho}(|\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|)\,(u - \overline{u})(\boldsymbol{\xi}'', \boldsymbol{\zeta})|^2}{1 - \hat{\rho}^2(|\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|}\, |\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|\, d(\omega(\boldsymbol{\xi}), \mathsf{s}(\boldsymbol{\zeta})),$$

where ω is the standard surface measure on S^2, s is the standard surface measure on the 2-manifold ∂G in $\mathbb{R}^3$,

$$B^{-}\overline{u} : S^2 \times \partial G \to \mathbb{R},$$

$$B^{-}\overline{u}(\boldsymbol{\xi}, \boldsymbol{\zeta}) = \begin{cases} \overline{u}(\boldsymbol{\xi}, \boldsymbol{\zeta}) - \hat{\rho}(|\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|)\, \overline{u}(\boldsymbol{\xi}'', \boldsymbol{\zeta}) & , \quad \boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta}) < 0 \\ 0 & , \quad \boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta}) \geq 0 \end{cases}$$

and

$$\begin{aligned} &\|B^{-}u - g\|_{\partial}^{2} \\ &\quad = \frac{1}{\sigma} \int_{S^2 \times \partial G} \frac{|(B^{-}u - g)(\boldsymbol{\xi}, \boldsymbol{\zeta}) - \hat{\rho}(|\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|)\,(B^{-}u - g)(\boldsymbol{\xi}'', \boldsymbol{\zeta})|^2}{1 - \hat{\rho}^2(|\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|} \\ &\qquad\qquad\qquad \times\, |\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|\, d(\omega(\boldsymbol{\xi}), \mathsf{s}(\boldsymbol{\zeta})). \end{aligned}$$

The formal derivation of (7) leaves the following questions open.

Q1. For which functions $\overline{u}$ does (7) hold ?

Q2. Some of the integrals of (7) involve traces on $S^2 \times \partial G$. Which smoothness requirements on ∂G are actually required that such traces exist with reasonable domains and ranges ?

The answers two both questions are of distinctive importance for the reliability of the hybrid method. Concerning Q1. it is important to recall that the approximative solutions $\overline{u}$ are constructed via formal asymptotic methods. Thus, it is a priori not clear which minimal regularity properties ensure the validity of (7). Concerning Q2. it is important to recall that in real-life applications the hybrid method must perform well for very different shapes G of high quality glass. Hence, the existence of reasonable trace operators for geometries arising in these real-life situations is vital for the reliability of the hybrid method.

It is the aim of the subsequent sections to derive (7) rigorously and, in particular, to address to the questions Q1. and Q2.

3 G-Pairs of Operators

In this section we prove an auxiliary result which will be needed later on. The point of view is rather abstract and the connection with the original RTE (5), (6) is hardly visible. We give

Definition 1. *Let X, Y be Hilbert spaces with respective inner products $\langle .,. \rangle_X$ and $\langle .,. \rangle_Y$. Let $L_1, L_2 : X \to Y$ be linear and bounded. The pair (L_1, L_2) is a "G–pair", iff*

(a) *L_1 and L_2 are isometries,*

(b) *there exist closed subspaces* Y_1, Y_2 *of* Y *such that* $\mathrm{im}(L_1) \subseteq Y_1$, $\mathrm{im}(L_2) \subseteq Y_2$, *and for any pair* $(y_1, y_2) \in Y_1 \times Y_2$, *the relation*

$$\forall x \in X : \qquad \langle L_1 x, y_1 \rangle_Y = \langle L_2 x, y_2 \rangle_Y$$

implies that there is $z \in X$ *with* $L_1 z = y_1$ *and* $L_2 z = y_2$.

The subspace Y_1 *(*Y_2*) of* (b) *is the "G–range of* L_1 *(of* L_2*)".*

Remark 1. *The notion "G–pair" is motivated by the fact that, in the case of radiative transfer problems, properties* (a) *and* (b) *in Definition 1 are closely related to a Gauss-like integration-by-parts formula and its inversion.*

For G–pairs, we have the following result.

Theorem 1. *Let* X, Y *be Hilbert spaces with respective inner products* $\langle .,. \rangle_X$ *and* $\langle .,. \rangle_Y$. *Let* (L_1, L_2) *be G–pair with respective G–ranges* Y_1 *and* Y_2. *Then*

1. $Y_1 = \mathrm{im}(L_1)$ *and* $Y_2 = \mathrm{im}(L_2)$.
2. *For each* $y_1 \in Y_1$, *the equation* $L_1 x = y_1$ *has a unique solution* $x \in X$. *Moreover,* $\|x\|_X = \|y_1\|_Y$ *and one has the residual based error formula*

$$\forall \bar{x} \in X : \qquad \|x - \bar{x}\|_X = \|L_1 \bar{x} - y_1\|_Y.$$

3. *Respective conclusions apply to the equation* $L_2 x = y_2$, *where* $y_2 \in Y_2$.

Proof. The proof is carried out for L_1 (due to the symmetry in the definition of G–pairs, the same arguments can be applied to L_2). We start by showing that $\mathrm{im}(L_1)$ is dense in Y_1. Let $x \in X$. If we assume that $\langle L_1 x, y_1 \rangle_Y = 0$ for all $x \in X$ we obtain with $y_2 = 0$

$$\forall x \in X : \qquad \langle L_1 x, y_1 \rangle_Y = \langle L_2 x, y_2 \rangle_Y \, .$$

Thus, there exists $z \in X$ such that $L_1 z = y_1$ and $L_2 z = y_2$. In particular, $L_2 z = 0$ which implies $z = 0$ because L_2 is an isometry and thus injective. We also conclude $y_1 = L_1 0 = 0$ which shows that the orthogonal complement of $\mathrm{im}(L_1)$ in Y_1 is the zero space which is equivalent to density of $\mathrm{im}(L_1)$ in Y_1. Using the fact that L_1 is an isometry, $\mathrm{im}(L_1)$ is closed in Y_1, so that $\mathrm{im}(L_1) = Y_1$. Consequently, the problem $L_1 x = y_1$ has a solution for any $y_1 \in Y_1$ which is unique since L_1 is one-to-one. Using again that L_1 is an isometry, we get $\|y_1\|_Y = \|L_1 x\|_Y = \|x\|_X$ and

$$\|L_1 \bar{x} - y_1\|_Y^2 = \|L_1(\bar{x} - x)\|_Y^2 = \|\bar{x} - x\|_X^2.$$

□

4 An Abstract Operator Equation

In this section we reconsider (5), (6) from a "medium" abstract point of view. The core of the approach is Hilbert space theory. In particular, we assume

- H1 $(H, \langle\cdot,\cdot\rangle)$ and $(H_0, \langle\cdot,\cdot\rangle_0)$ and $(H_\partial, \langle\cdot,\cdot\rangle_\partial)$ are Hilbert spaces.
- H2 $A : H \to H_0$ and $B^+ : H \to H_\partial$ and $B^- : H \to H_\partial$ are bounded linear operators.
- H3 ${H_\partial}^- := B^-(H)$ and ${H_\partial}^+ := B^+(H)$ are closed subspaces of H_∂.

For given $f \in H_0$ and $g \in {H_\partial}^-$ let us consider the prototype operator equation emerging from (5), (6),

$$u + Au = f, \qquad B^-u = g, \tag{8}$$

with unknown $u \in H$. We are concerned with the question of unique solvability of (8) and the derivation of a residual based error formula. It turns out that, whenever the operators $A, B^\pm$ and the Hilbert spaces H, H^0, H_∂ satisfy certain compatibility conditions (see G0, G1, G2 below), a rather complete analysis follows from Theorem 1. The main result is

Theorem 2. *Assume* H1, H2, H3. *Let $f \in H_0$ and $g \in H_\partial^-$. Furthermore assume*

- G0 *$H \subseteq H_0$ and for all $u, v \in H$,*

$$\langle u,v\rangle = \langle u,v\rangle_0 + \langle Au,Av\rangle_0 + \left\langle B^-u,B^-v\right\rangle_\partial + \left\langle B^+u,B^+v\right\rangle_\partial. \tag{9}$$

- G1 *For all $u, v \in H$,*

$$\langle u,Av\rangle_0 + \langle Au,v\rangle_0 + \left\langle B^-u,B^-v\right\rangle_\partial - \left\langle B^+u,B^+v\right\rangle_\partial = 0. \tag{10}$$

- G2 *For all $u, \bar{u} \in H_0$, $u^+ \in H_\partial^+$, and $u^- \in H_\partial^-$: If*

$$\forall v \in H : \qquad \langle u,Av\rangle_0 + \langle \bar{u},v\rangle_0 + \left\langle u^-,B^-v\right\rangle_\partial - \left\langle u^+,B^+v\right\rangle_\partial = 0, \tag{11}$$

  then $u \in H$, $\bar{u} = Au$, and $u^+ = B^+u, u^- = B^-u$.

Then

1. *Problem* (8) *has a unique solution $u \in H$,*
2. $\|u\|^2 = \|f\|_0^2 + 2\|g\|_\partial^2$.
3. *For all $\bar{u} \in H$ one has the residual based error formula*

$$\|u - \bar{u}\|^2 = \|\bar{u} + A\bar{u} - f\|_0^2 + 2\|B^-\bar{u} - g\|_\partial^2.$$

4. The solution u is characterized by

$$\forall v \in H: \qquad \langle u + Au, v + Av \rangle + 2 \left\langle B^- u, B^- v \right\rangle_\partial = \langle f, v + Av \rangle + 2 \left\langle g, B^- v \right\rangle_\partial .$$

Proof. In order to relate (8) to the general result for G-pairs of operators, we set

$$X := H, \quad Y := H_0 \times H_\partial,$$

where we equip Y with the scalar product

$$\langle \boldsymbol{y}, \boldsymbol{z} \rangle_Y := \langle y, z \rangle_0 + 2 \langle y_\partial, z_\partial \rangle_\partial, \qquad \boldsymbol{y} = (y, y_\partial) \in Y, \ \boldsymbol{z} = (z, z_\partial) \in Y.$$

We combine the equations $u + Au = f$ and $B^- u = g$ into a single equation via

$$L_1 := \begin{pmatrix} I + A \\ B^- \end{pmatrix} : X \to Y.$$

Note that $\mathrm{im}(L_1) \subset H_0 \times H^- =: Y_1$, which is a closed subspace of Y. Now, (8) has the simple form: given $y_1 \in Y_1$ find $x \in X$ such that $L_1 x = y_1$.
The mapping $L_1 : X \to Y$ is an isometry, because for all $x, \bar{x} \in X$ we have

$$\begin{aligned} \langle L_1 x, L_1 \bar{x} \rangle_Y &= \langle (I + A)x, (I + A)\bar{x} \rangle_0 + 2 \left\langle B^- x, B^- \bar{x} \right\rangle_\partial \\ &= \langle x, \bar{x} \rangle_0 + \langle Ax, A\bar{x} \rangle_0 + \langle Ax, \bar{x} \rangle_0 + \langle x, A\bar{x} \rangle_0 + 2 \left\langle B^- x, B^- \bar{x} \right\rangle_\partial \end{aligned}$$

such that by (10), (9) the scalar product in $X = H$ is recovered. In the next step, we show that (L_1, L_2) is a G–pair, where L_2 is the operator complementary to L_1,

$$L_2 := \begin{pmatrix} I - A \\ B^+ \end{pmatrix}$$

which maps X into the closed subspace $Y_2 = H_0 \times H^+$ of Y. With a similar argument as above, one verifies that L_2 is an isometry.
While (10) is necessary to show this isometry property, the converse relation (11) is required to obtain the second condition for G–pairs. To see this, let $\boldsymbol{y}_1 = (y_1, y_{1\partial})^T \in Y_1$, $\boldsymbol{y}_2 = (y_2, y_{2\partial})^T \in Y_2$, and assume that

$$\forall x \in X: \qquad \langle L_1 x, \boldsymbol{y}_1 \rangle_Y = \langle L_2 x, \boldsymbol{y}_2 \rangle_Y .$$

Then, for all $x \in X$

$$\langle x, y_1 - y_2 \rangle_0 + \langle Ax, y_1 + y_2 \rangle_0 + \left\langle B^- x, 2y_{1\partial} \right\rangle_\partial - \left\langle B^+ x, 2y_{2\partial} \right\rangle_\partial = 0$$

from which we deduce with (11) that

$$z = \frac{1}{2}(y_1 + y_2) \in X, \qquad y_1 - y_2 = 2Az, \qquad y_{1\partial} = B^- z, \qquad y_{2\partial} = B^+ z.$$

We note $z + Az = y_1$ and $z - Az = y_2$ so that $y_1 = L_1 z$ and $y_2 = L_2 z$. Having checked the properties of (L_1, L_2) being a G–pair, an application of Theorem 1 yields statements 1, 2, and 3. For the last statement, we just note that the solution u is clearly the minimizer of the quadratic functional $\bar{u} \mapsto \|u - \bar{u}\|^2$. The necessary and sufficient condition of vanishing directional derivatives gives rise to the weak formulation. $\square$

5 Assumptions H1-H3, G0-G2 Revisited

If one tries to prove the residual based error formula (7) by means of theorem (2) one will immediately realize that the verification of H1-H3, G0-G2 requires more or less subtle combinations of abstract Hilbert space theory and data-dependent arguments (like integrations by parts formulae and trace operators).

In order to separate these different aspects (and, thus, to improve readability) we have to reformulate assumptions H1-H3, G0-G2 in such a way that the new assumptions allow for a more direct verification in case of the RTE (5), (6).

The assumptions are as follows.

B0 $(H_0, \langle .,. \rangle_0)$ is a Hilbert space.

B1 H^{aux} is a linear subspace of H_0. $A_1 : H^{aux} \to H_0$ is a closed linear operator.

Remark 2. *a) For the RTE we have $H_0 = \mathbb{L}^2(S^2 \times G)$ (equipped with the canonical inner product) and $A_1 u = \frac{1}{\sigma}\boldsymbol{\xi} \cdot \nabla u$.*
b) We shall put $A = A_1 \downharpoonright H$ after having defined $H \subseteq H_0$.
c) For the RTE the space H^{aux} is the set of all $u \in \mathbb{L}^2(S^2 \times G)$ with $\boldsymbol{\xi} \cdot \nabla u \in \mathbb{L}^2(S \times G)$.
d) In B1 the space H^{aux} is equipped with the trace inner product of H_0. Later on we will introduce the "canonical" inner product $\langle .,. \rangle_{aux}$ on H^{aux} via

$$\langle u, v \rangle_{aux} := \langle u, v \rangle_0 + \langle A_1 u, A_1 v \rangle_0 .$$

*e) Since A_1 is a closed operator we can follow [3] to deduce from **B0**, **B1** that $(H^{aux}, \langle .,. \rangle_{aux})$ is a Hilbert space.*

We require a "trace" operator T.

B2 Z is a vector space.

B3 $T : H^{aux} \to Z$ is linear.

Remark 3. *For the RTE we have $Z = \mathbb{L}^1_{loc}(d|o|)$, where $d|o|$ is the measure density $|(\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|\, d(\omega(\boldsymbol{\xi}), \mathsf{s}(\boldsymbol{\zeta}))$ on the set of all Borel measurable subsets of $S^2 \times \partial G$.*

We assume

B4 $(V, \langle .,. \rangle_V)$ is a Hilbert space and $V \subseteq Z$.

Remark 4. *For the RTE we will have $V = \mathbb{L}^2(d|o|)$.*

We introduce the set

$$H := T^{-1}[V], \tag{12}$$

and assume

B5 $T_V : H \to V,\ T_V(v) = T(v)$ is closed.

Remark 5. *a) In* **B5***, H is equipped with the trace inner product of H^{aux}. The "canonical" inner product $\langle .,. \rangle$ will be introduced in* (14)*.*
b) For the RTE, H is the set of all functions of H^{aux} whose trace in $S^2 \times \delta G$ belongs to $\mathbb{L}^2(S^2 \times \delta G)$.
c) As we shall see later on, **B5** *is a rather weak assumption for the RTE. In particular in* **B5** *it is* not required *that the trace operator maps H^{aux} continuously into a space $L^p(S^2 \times \delta G)$, $p \in [1, \infty)$.*

The Hilbert space H_∂ is introduced by means of the operator D.

B6 $D : V \to V$ is linear, self-adjoint with operator norm $\|D : V \to V\| < 1$.

Remark 6. *For the RTE, D represents the Fresnel reflection operator of the boundary conditions* (6)*.*

In the sequel we make use of the linear, bounded, self adjoint operator

$$F := \left(\mathsf{id} - D^2\right)^{-1/2},$$

where id is the identity on V. We put

$$H_\partial := V, \qquad \langle w_1, w_2 \rangle_\partial := \langle F w_1, F w_2 \rangle_V, \quad w_1, w_2 \in H_\partial. \tag{13}$$

It is quite obvious that $(H_\partial, \langle .,. \rangle_\partial)$ is a Hilbert space which is isometrically isomorphic to $(V, \langle .,. \rangle_V)$. We put

$$\langle u, v \rangle := \langle u, v \rangle_{aux} + \langle (\mathsf{id} - D) T u, (\mathsf{id} - D) T v \rangle_\partial . \tag{14}$$

Now we can prove

Lemma 3. *Assume* **B1***, ... ,***B6***. Then $(H, \langle .,. \rangle)$ is a Hilbert space.*

Proof. $\langle .,. \rangle$ is obviously an inner product on H. Let $(u_n)_{n\in\mathbb{N}}$ be Cauchy sequence in H with respect to $\langle .,. \rangle$. Then $(u_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in H^{aux} as well. Hence there is $u_\infty \in H^{aux}$ with $\lim_{n\to\infty} \|u_\infty - u_n\|_{aux} = 0$. Furthermore, the mapping $\mathsf{id} - D : V \to V$ is invertible with bounded inverse. Thus the sequence $(Tu_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in V. Therefore, there is $w_\infty \in V$ with $\lim_{n\to\infty} \|w_\infty - Tu_n\|_V = 0$. Due to closedness of T (assumption B5), we have $w_\infty = Tu_\infty$. Hence $\lim_{n\to\infty} \|Tu_\infty - Tu_n\|_V = 0$. This implies $u_\infty \in H$ and

$$\lim_{n\to\infty} \|F(\mathsf{id} - D)T(u_\infty - u_n)\|_V = 0.$$

Thus $\lim_{n\to\infty} \|u_\infty - u_n\| = 0$. ∎

Now let us introduce the operators $B^\pm$. We require

B7 U^+ is a closed subspace of V.

Remark 7. *For the RTE, U^+ will be the set of all functions of V vanishing on the set $\{(\boldsymbol{\xi}, \boldsymbol{\zeta}) \in S^2 \times \partial G : \boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta}) \le 0\}$.*

Let

$$P^+ : V \to U^+, \quad P^- := \mathsf{id} - P^+, \tag{15}$$

be the projection onto U^+ and onto the orthogonal complement U^- of U^+, respectively. We assume the commutation relation

B8 $DP^+ = P^- D$.

Remark 8. **B8** *is equivalent with* $DP^- = P^+ D$.

We note for later reference

Proposition 4. *Assume* **B1**, ... ,**B8**. *Then for all* $w_1, w_2 \in H_\partial$,

$$\langle w_1, w_2 \rangle_\partial = \left\langle P^+ w_1, P^+ w_2 \right\rangle_\partial + \left\langle P^- w_1, P^- w_2 \right\rangle_\partial , \tag{16}$$

and

$$\left\langle P^+ w_1, w_2 \right\rangle_\partial = \left\langle P^+ w_1, P^+ w_2 \right\rangle_\partial , \quad \left\langle P^- w_1, w_2 \right\rangle_\partial = \left\langle P^- w_1, P^- w_2 \right\rangle_\partial . \tag{17}$$

Proof. Due to **B8** and due to Remark 8 we have $D^2 P^+ = D(DP^+) = D(P^- D) = (DP^-)D = (P^+ D)D = P^+ D^2$ and $D^2 P^- = P^- D^2$. As a consequence, $FP^+ = P^+ F$ and $FP^- = P^- F$. Now we deduce from (13) since $P^+ + P^- = \mathsf{id}$ and $P^+ P^- = P^- P^+ = 0$, the zero operator on V,

$$\begin{aligned}
\langle w_1, w_2 \rangle_\partial = \langle F w_1, F w_2 \rangle_V \\
&= \left\langle P^+ F w_1, P^+ F w_2 \right\rangle_V + \left\langle P^- F w_1, P^- F w_2 \right\rangle_V \\
&= \left\langle F P^+ w_1, F P^+ w_2 \right\rangle_V + \left\langle F P^- w_1, F P^- w_2 \right\rangle_V \\
&\qquad = \left\langle P^+ w_1, P^+ w_2 \right\rangle_\partial + \left\langle P^- w_1, P^- w_2 \right\rangle_\partial .
\end{aligned}$$

The relations in (17) follow in analogy. □

We set

$$B^+ := P^+ (\mathsf{id} - D) T, \quad B^- := P^- (\mathsf{id} - D) T. \tag{18}$$

As in the previous section we put

$$H_\partial^+ := B^+(H), \quad H_\partial^- := B^-(H).$$

Finally, we require an integration-by-parts formula of Gauss' type and its inversion.

B9 For all $u, v \in H$,

$$\langle u, Av \rangle_0 + \langle Av, u \rangle_0 = \left\langle P^+ T u, T v \right\rangle_V - \left\langle P^- T u, T v \right\rangle_V .$$

B10 For all $u, \bar{u} \in H_0$, $u^+ \in H^+$, and $u^- \in H^-$: If

$$\langle u, Av \rangle_0 + \langle \bar{u}, v \rangle_0 + \left\langle u^-, B^- v \right\rangle_\partial - \left\langle u^+, B^+ v \right\rangle_\partial = 0 \qquad \forall v \in H, \tag{19}$$

then $u \in H$, $\bar{u} = Au$, and $u^\pm = B^\pm u$.

Having revisited assumptions G0, G1, G2 we can formulate the main result of this section.

Theorem 5. *Assume* **B0**, ... ,**B10** *and let* $A = A_1 \downharpoonright H$. *Furthermore, let* $f \in H_0$ *and* $g \in H^-$. *Then*

1. *Problem* (8) *has a unique solution* $u \in H$,
2. $\|u\|^2 = \|f\|_0^2 + 2\|g\|_\partial^2$.
3. *For all* $\bar{u} \in H$ *one has the residual based error formula*
$$\|u - \bar{u}\|^2 = \|\bar{u} + A\bar{u} - f\|_0^2 + 2\|B^-\bar{u} - g\|_\partial^2.$$
4. *The solution* $u \in H$ *is characterized by the weak formulation*
$$\langle u + Au, v + Av\rangle + 2\left\langle B^-u, B^-v\right\rangle_\partial = \langle v + Av, f\rangle + 2\left\langle B^-v, g\right\rangle_\partial \quad \forall v \in H.$$

Proof. We have to check H0, H1, H2 and G0, G1, G2.

<u>H1:</u> $(H_0, \langle .,. \rangle_0)$ is by **B0** a Hilbert space. As discussed in the context of (13), $(H_\partial, \langle .,. \rangle_\partial)$ is a Hilbert space, too. $(H, \langle .,. \rangle)$ is a Hilbert space due to Lemma 3.

<u>H2:</u> The operator $A_1 : H^{aux} \to H_0$ is due to remark 2 e) a linear, bounded operator. Since the norm of $H \subseteq H^{aux}$ is stronger than the norm of H^{aux}, the operator $A = A_1 \downharpoonright H$ is bounded, too. Since $\mathsf{id} - D$ is invertible on V, the norm $\langle .,. \rangle$ is equivalent to the norm

$$\langle .,. \rangle' := \langle .,. \rangle_{aux} + \langle T.,T. \rangle_\partial .$$

With respect to the corresponding norm on H, the operator $T : H \to V$ is by B5 continuous. Hence, also in case H is equipped with the inner product $\langle .,. \rangle$, the operator $T : H \to V$ is continuous. Since $\mathsf{id} - D$ and $P^\pm$ are continuous mappings of V into V and since the norm on V is equivalent to the norm $\|.\|_\partial$, the operators $B^\pm = P^\pm(\mathsf{id} - D)T : H \to H_\partial$ are linear and bounded.

<u>H3:</u> Since $\mathsf{id} - D$ is invertible, we have $(\mathsf{id} - D)TH = H_\partial = V$. Hence $B^\pm(H_\partial) = U^\pm$, which are closed subspaces of V. Since the norms $\|.\|_V$ and $\|.\|_\partial$ are equivalent, $U^\pm$ are closed subspaces of H_∂ as well.

<u>G0:</u> Since $V \subseteq Z$ (due to **B4**) and since $T : H^{aux} \to Z$, we have $H = T^{-1}[V] \subseteq H^{aux}$. Furthermore, due to B1, we have $H^{aux} \subseteq H_0$. Thus $H \subseteq H_0$ and it remains to verify (9). According to the definition of $\langle .,. \rangle$, see (14), due to the definition of $\langle .,. \rangle_{aux}$ in remark 2, and due to $A = A_1 \downharpoonright H$, it suffices to prove:

$$\langle (\mathsf{id} - D)Tu, (\mathsf{id} - D)Tv \rangle_\partial = \left\langle B^-u, B^-v\right\rangle_\partial + \left\langle B^+u, B^+v\right\rangle_\partial, \quad \forall u, v \in H. \qquad (20)$$

We recall $B^\pm = P^\pm(\mathsf{id} - D)T$, see (18), in particular $B^+ + B^- = (\mathsf{id} - D)T$ and $\langle B^+u, B^-v \rangle_\partial = 0$ for all $u, v \in H$. This proves (20).

G1: We have to verify (10) for all $u,v \in H$. Comparing (10) with **B9**, it suffices to prove

$$\langle P^+Tu, Tv\rangle_V - \langle P^-Tu, Tv\rangle_V = \langle B^+u, B^+v\rangle_\partial - \langle B^-u, B^-v\rangle_\partial . \tag{21}$$

Setting $\bar{u} = Tu$, $\bar{v} = Tv$ and employing (13) and the self-adjointness of F^{-1} (which follows from **B6**), we calculate

$$\begin{aligned}\langle P^+\bar{u}, \bar{v}\rangle_V - \langle P^-\bar{u}, \bar{v}\rangle_V &= \langle (P^+ - P^-)\bar{u}, \bar{v}\rangle_V \\ &= \langle F^{-1}(P^+ - P^-)\bar{u}, F^{-1}\bar{v}\rangle_\partial = \langle F^{-2}(P^+ - P^-)\bar{u}, \bar{v}\rangle_\partial .\end{aligned}$$

Using the identity $\mathsf{id} - D^2 = (\mathsf{id} - D)(\mathsf{id} + D)$ and the self-adjointness of $\mathsf{id} - D$ (which again follows from **B6**), we obtain

$$\begin{aligned}&\langle F^{-2}(P^+ - P^-)\bar{u}, \bar{v}\rangle_\partial = \langle (\mathsf{id} - D^2)(P^+ - P^-)\bar{u}, \bar{v}\rangle_\partial \\ &\quad = \langle (\mathsf{id} - D)(\mathsf{id} + D)(P^+ - P^-)\bar{u}, \bar{v}\rangle_\partial = \langle (\mathsf{id} + D)(P^+ - P^-)\bar{u}, (\mathsf{id} - D)\bar{v}\rangle_\partial .\end{aligned}$$

Finally, the identity $(\mathsf{id} + D)(P^+ - P^-) = (P^+ - P^-)(\mathsf{id} - D)$ (which follows from **B8**) yields in connection with proposition 4

$$\begin{aligned}&\langle (\mathsf{id} + D)(P^+ - P^-)\bar{u}, (\mathsf{id} - D)\bar{v}\rangle_\partial = \langle (P^+ - P^-)(\mathsf{id} - D)\bar{u}, (\mathsf{id} - D)\bar{v}\rangle_\partial \\ &\qquad = \langle (P^+(\mathsf{id} - D)\bar{u}, (\mathsf{id} - D)\bar{v}\rangle_\partial - \langle (P^-(\mathsf{id} - D)\bar{u}, (\mathsf{id} - D)\bar{v}\rangle_\partial \\ &\qquad = \langle P^+(\mathsf{id} - D)\bar{u}, P^+(\mathsf{id} - D)\bar{v}\rangle_\partial - \langle (P^-(\mathsf{id} - D)\bar{u}, P^-(\mathsf{id} - D)\bar{v}\rangle_\partial \\ &\qquad = \langle B^+u, B^+v\rangle_\partial - \langle B^-u, B^-v\rangle_\partial .\end{aligned}$$

G2: Follows from **B10**. □

6 The Rigorous Global Error Estimator

In this section we give a rigorous proof for the residual based error formula (7). The argumentation is settled on the verification of assumptions **B0**, ... ,**B10** of theorem 5 in terms of the following geometrical assumptions.

A.1 $G \subseteq \mathbb{R}^3$ is a bounded, non-void domain.

A.2 $\partial G = \Gamma_{sing} \cup \delta G$, where $\Gamma_{sing} \cap \delta G = \emptyset$ and $\delta G = \Gamma_1 \cup \ldots \cup \Gamma_N$, $N \in \mathbb{N}$, where $\Gamma_1, \ldots, \Gamma_N$ are relatively open in ∂G, pairwise disjoint and nonempty.

A.3 There are for each $j \in \{1, \ldots, N\}$ mappings $\boldsymbol{p}_j : O_j \to \Gamma_j$, $\boldsymbol{n}_j : O_j \to S^2$, $O_j \subseteq \mathbb{R}^{d-1}$ is a non-void, bounded domain, such that

(a) $\boldsymbol{n}_j, \boldsymbol{p}_j \in C^k(\overline{O_j})$, for all $k \in \mathbb{N}_0$.

(b) $\boldsymbol{p}_j$ is a homeomorphism whose partial derivatives are linearly independent at each $(t_1, \ldots, t_{d-1}) \in O_j$.

(c) For all $(t_1, \ldots, t_{d-1}) \in O_j$ and for all $\kappa \in \{1, \ldots, d-1\}$, the vector $\boldsymbol{n}_j(t_1, \ldots, t_{d-1})$ is orthogonal to $(\partial_\kappa \boldsymbol{p}_j)(t_1, \ldots, t_{d-1})$.

(d) There is for each compact set $K \subseteq O_j$ a positive number $\varepsilon(K;j)$ with

$$\left\{ \left(\boldsymbol{p}_j - \tau \boldsymbol{n}_j\right)(t_1, \ldots, t_{d-1}) : (t_1, \ldots, t_{d-1}) \in K, \tau \in (0, \varepsilon(K;j)) \right\} \subseteq G.$$

A.4 There is for each $j \in \{1, \ldots, N\}$, for each compact $K \subset \Gamma_j$ and for each $\varepsilon \in \mathbb{R}^+$ a real number $\mathsf{m}_j(K;\varepsilon) \in \mathbb{R}^+$ such that for all $\boldsymbol{\xi} \in S^2$,

$$(\Gamma_j \cap D_\varepsilon^+(K, \boldsymbol{\xi})) - (0, \mathsf{m}_j]\boldsymbol{\xi} \subseteq G, \quad (\Gamma_j \cap D_\varepsilon^-(K, \boldsymbol{\xi})) + (0, \mathsf{m}_j]\boldsymbol{\xi} \subseteq G,$$

where $D_\varepsilon^\pm(K, \boldsymbol{\xi}) := \{\boldsymbol{\zeta} \in K : \pm\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta}) \geq \varepsilon\}$.

Remark 9. *a) In* **A.2** *only* local *smoothness properties of G are required, that is,* **A.2** *does not apply to Γ_{sing} representing the "singular" parts (edges, corners, boundaries of smooth parameterizations) of ∂G.*
b) The singular part Γ_{sing} of ∂G will play no explicit role in the sequel. Nevertheless Γ_{sing} is *important: The set $\delta G = \partial G \setminus \Gamma_{sing}$ has to be "almost all of ∂G" in the sense that the Gauss integration formula holds for δG replacing ∂G, see assumption* **A.6** *below.*
c) Loosely speaking, assumption **A.3** *expresses the fact that Γ_j, $j \in \{1, \ldots, N\}$, is a regular, uniformly smooth part of ∂G, parameterized by $\boldsymbol{p}_j$, equipped with a uniformly smooth outer normal vector field $\boldsymbol{n}_j$ such that G lies locally at one side of Γ_j.*
d) For the sake of a simplified notation it is convenient to introduce the outer normal vector field along δG with $\boldsymbol{\zeta}$ as independent variable,

$$\boldsymbol{n} : \delta G \to S^2, \quad \boldsymbol{n}(\boldsymbol{\zeta}) = \boldsymbol{n}_j(\boldsymbol{p}_j^{-1}(\boldsymbol{\zeta})), \text{ if } \boldsymbol{\zeta} \in \Gamma_j.$$

e) Assumption **A.4** *will be needed to define extensions of certain functions with domain in δG.*
f) Assumption **A.4** *is trivially satisfied for smooth boundaries ∂G. However, domains G whose boundary exhibits certain singularities - e.g., cusps - are also allowed.*

Henceforth the variable $\boldsymbol{x}$ ranges in G, the variable $\boldsymbol{\zeta}$ ranges in δG and the variable $\boldsymbol{\xi}$ ranges in S^2. Integration with respect to the standard measure on S^2 is denoted by "$d\omega(\boldsymbol{\xi})$".

Aside from geometrical assumptions on G we shall only be concerned with smooth reflection coefficient functions $\hat{\rho}$ which exclude total reflections at the boundary, i.e. we assume that $\hat{\rho}$ is uniformly bounded away from 1.

A.5 $\hat{\rho} : [0,1] \to [0,1]$ is infinitely many times differentiable and there is $\overline{\rho}$ such that $\hat{\rho}(\mu) \leq \overline{\rho} < 1$ for all $\mu \in [0,1]$.

Remark 10. *The treatment of total reflection requires a more involved analysis (see e.g.* (24)*) which goes beyond the scope of this paper.*

In addition to assumptions **A.1** - **A.5** an integration-by-parts formula is required. Several auxiliary notations have to be introduced.

We set $H_0 := \mathbb{L}^2(S^2 \times G)$, and we identify the inner product $\langle .,. \rangle_0$ with the standard inner product of $\mathbb{L}^2(S^2 \times G)$. Now, we introduce on the family of all Borel subsets of $S^2 \times \delta G$ the signed measure

$$o(\mathsf{B}) = \frac{1}{\sigma} \int_{\mathsf{B}} \boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta}) \; d(\omega(\boldsymbol{\xi}), \mathsf{s}(\boldsymbol{\zeta})), \tag{22}$$

where "$\mathsf{s}(\boldsymbol{\zeta})$" is the standard surface measure on δG. By $\mathcal{M}$ we denote the set of all Borel measurable mappings from $S^2 \times \delta G$ to $\mathbb{R}$. We introduce the equivalence relation

$$\forall w_1, w_2 \in \mathcal{M} : \quad w_1 \sim w_2 \quad \text{iff} \quad |o| \left(\{ w_1(\boldsymbol{\xi}, \boldsymbol{\zeta}) \neq w_2(\boldsymbol{\xi}, \boldsymbol{\zeta}) \} \right) = 0.$$

Let $M(o)$ be the set of all equivalence classes with respect to $\sim$. We set

$$\begin{aligned} &\mathbb{L}^1_{loc}(d|o|) \\ &:= \left\{ w \in M(o) : \text{ for all compact } K \subseteq S^2 \times \delta G\text{: } \int_K |w| \; d|o|(\boldsymbol{\xi}, \boldsymbol{\zeta}) < \infty \right\}, \end{aligned} \tag{23}$$

where $d|o|(\boldsymbol{\xi}, \boldsymbol{\zeta}) = \frac{1}{\sigma} |\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})| \, d(\omega(\boldsymbol{\xi}), \mathsf{s}(\boldsymbol{\zeta}))$.

In a similar (standard) way we introduce the Hilbert space $(\mathbb{L}^2(d|o|), \langle .,. \rangle_{\mathbb{L}^2(d|o|)})$ where

$$\langle w_1, w_2 \rangle_{\mathbb{L}^2(d|o|)} := \int_{S^2 \times \delta G} w_1 \; w_2 \; d|o|(\boldsymbol{\xi}, \boldsymbol{\zeta}), \quad w_1, w_2 \in \mathbb{L}^2(d|o|).$$

Now we define another inner product on $\mathbb{L}^2(d|o|)$ via

$$\langle w_1, w_2 \rangle_\partial := \int_{S^2 \times \delta G} \frac{w_1 \; w_2}{1 - \hat{\rho}^2(|\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|)} \; d|o|(\boldsymbol{\xi}, \boldsymbol{\zeta}), \quad w_1, w_2 \in \mathbb{L}^2(d|o|). \tag{24}$$

Furthermore, let

$$C^{aux} := \left\{ u \in C(\overline{S^2 \times G}) : \boldsymbol{\xi} \cdot \nabla u \in C(\overline{S^2 \times G}) \right\},$$

and we equip

$$H^{aux} := \left\{ u \in \mathbb{L}^2(S^2 \times G) : \boldsymbol{\xi} \cdot \nabla u \in \mathbb{L}^2(S^2 \times G) \right\} \tag{25}$$

with the inner product

$$\langle u_1, u_2 \rangle_{aux} := \langle u_1, u_2 \rangle_{\mathbb{L}^2(S^2 \times G)} + \int_{S^2 \times G} (\boldsymbol{\xi} \cdot \nabla u_1) \, (\boldsymbol{\xi} \cdot \nabla u_2) \; d(\omega(\boldsymbol{\xi}), \boldsymbol{x}). \tag{26}$$

We refer to [4] for

Theorem 6. *Assume* **A.1, A.2, A.3**. *Then there is a continuous, linear trace operator* $T : H^{aux} \to \mathbb{L}^1_{loc}(d|o|)$ *such that*

$$\forall u \in C^{aux} : \quad Tu = u \downharpoonright S^2 \times \delta G.$$

Now we are in the position to formulate

A.6 For all $u_1, u_2 \in H := \{u \in H^{aux} : Tu \in \mathbb{L}^2(d|o|)\}$, we have the integration-by-parts formula

$$\frac{1}{\sigma}\int_{S^2\times G}(\boldsymbol{\xi}\cdot\nabla u_1)\, u_2\; d(\omega(\boldsymbol{\xi}),\boldsymbol{x}) + \frac{1}{\sigma}\int_{S^2\times G}(\boldsymbol{\xi}\cdot\nabla u_2)\, u_1\; d(\omega(\boldsymbol{\xi}),\boldsymbol{x}) = \int_{S^2\times\delta G} Tu_1\, Tu_2\, do(\boldsymbol{\xi},\boldsymbol{\zeta}).$$

In order to present the residual based error formula in a compact form, it is convenient to introduce several operators.
Let "id" be the identity operator on $M(o)$. We introduce for $v \in M(o)$,

$$\rho(v) : S^2 \times \delta G \to \mathbb{R}, \quad \rho(v)(\boldsymbol{\xi},\boldsymbol{\zeta}) = \hat{\rho}(|\boldsymbol{\xi}\cdot\boldsymbol{n}(\boldsymbol{\zeta})|)v(\boldsymbol{\xi},\boldsymbol{\zeta}),$$

where we trivially have $\rho(v) \in M(o)$. Now the operator ρ is defined as

$$\rho : M(o) \to M(o), \quad v \mapsto \rho(v). \tag{27}$$

Furthermore, let

$$\Xi_{refl} : S^2 \times \delta G \to S^2, \quad \Xi_{refl}(\boldsymbol{\xi},\boldsymbol{\zeta}) = \boldsymbol{\xi} - 2(\boldsymbol{n}(\boldsymbol{\zeta})\cdot\boldsymbol{\xi})\boldsymbol{n}(\boldsymbol{\zeta}),$$

where it is easy to see that $\Xi_{refl}(\boldsymbol{\xi},\boldsymbol{\zeta})\cdot\boldsymbol{n}(\boldsymbol{\zeta}) = -\boldsymbol{\xi}\cdot\boldsymbol{n}(\boldsymbol{\zeta})$ and thus

$$\forall(\boldsymbol{\xi},\boldsymbol{\zeta}) \in S^2 \times \delta G : \quad |\Xi_{refl}(\boldsymbol{\xi},\boldsymbol{\zeta})\cdot\boldsymbol{n}(\boldsymbol{\zeta})| = |\boldsymbol{\xi}\cdot\boldsymbol{n}(\boldsymbol{\zeta})|. \tag{28}$$

We introduce the mapping

$$V_{refl} : S^2 \times \delta G \to S^2 \times \delta G, \quad V_{refl}(\boldsymbol{\xi},\boldsymbol{\zeta}) = (\Xi_{refl}(\boldsymbol{\xi},\boldsymbol{\zeta}),\boldsymbol{\zeta})\,.$$

The function V_{refl} is due to the assumed smoothness of $\boldsymbol{n} : \delta G \to S^2$ Lipschitz-continuous. Thus, V_{refl} maps $|o|$-null sets onto $|o|$-null sets and therefore the mapping

$$R : M(o) \to M(o), \quad R(w) = w \circ V_{refl} \tag{29}$$

is well-defined. We write for $w \in M(o)$ and $(\boldsymbol{\xi},\boldsymbol{\zeta}) \in S^2 \times \delta G$,

$$R(w)(\boldsymbol{\xi},\boldsymbol{\zeta}) = w(\Xi_{refl}(\boldsymbol{\xi},\boldsymbol{\zeta}),\boldsymbol{\zeta}) = w(\boldsymbol{\xi} - 2(\boldsymbol{n}(\boldsymbol{\zeta})\cdot\boldsymbol{\xi})\boldsymbol{n}(\boldsymbol{\zeta}),\boldsymbol{\zeta}).$$

We introduce projection operators $P^{\pm} : \mathbb{L}^2(d|o|) \to \mathbb{L}^2(d|o|)$ as follows: since $\{(\boldsymbol{\xi},\boldsymbol{\zeta}) \in S^2 \times \delta G : \boldsymbol{\xi}\cdot\boldsymbol{n}(\boldsymbol{\zeta}) = 0\}$ is an $|o|$-null set we can define $P^{\pm}(v) \in \mathbb{L}^2(d|o|)$ with $v \in \mathbb{L}^2(d|o|)$ for $(\boldsymbol{\xi},\boldsymbol{\zeta}) \in S^2 \times \delta G$ via

$$P^{+}(v)(\boldsymbol{\xi},\boldsymbol{\zeta}) = \begin{cases} v(\boldsymbol{\xi},\boldsymbol{\zeta}) & \text{if} \quad \boldsymbol{\xi}\cdot\boldsymbol{n}(\boldsymbol{\zeta}) > 0 \\ 0 & \text{if} \quad \boldsymbol{\xi}\cdot\boldsymbol{n}(\boldsymbol{\zeta}) \le 0 \end{cases},$$

$$P^{-}(v)(\boldsymbol{\xi},\boldsymbol{\zeta}) = \begin{cases} 0 & \text{if} \quad \boldsymbol{\xi}\cdot\boldsymbol{n}(\boldsymbol{\zeta}) \ge 0 \\ v(\boldsymbol{\xi},\boldsymbol{\zeta}) & \text{if} \quad \boldsymbol{\xi}\cdot\boldsymbol{n}(\boldsymbol{\zeta}) < 0 \end{cases}$$

such that by functional abstraction,

$$P^{\pm} : \mathbb{L}^2(d|o|) \to \mathbb{L}^2(d|o|), \quad v \mapsto P^{\pm}(v). \tag{30}$$

Remark 11. *The operators $P^{\pm}$ are, in fact, orthogonal projections, because due to* **A.1, A.2, A.3** *the sets $U^{\pm} := P^{\pm}[\mathbb{L}^2(d|o|)]$ are closed subspaces of $\mathbb{L}^2(d|o|)$ and $P^{+} + P^{-} = \mathsf{id}_{\mathbb{L}^2(d|o|)}$, $P^{+}P^{-} = P^{-}P^{+} = 0_{\mathbb{L}^2(d|o|)}$ and $P^{+}P^{+} = P^{+}$, $P^{-}P^{-} = P^{-}$, where $\mathsf{id}_{\mathbb{L}^2(d|o|)}$ is the identity operator on $\mathbb{L}^2(d|o|)$ and $0_{\mathbb{L}^2(d|o|)}$ is the zero mapping on $\mathbb{L}^2(d|o|)$.*

We set

$$B := (\mathsf{id} - \rho R)T, \quad B^{\pm} := P^{\pm}(\mathsf{id} - \rho R)T.$$

Now, using (26) and (24), we introduce an inner product on H (see **A.6**),

$$\langle u_1, u_2 \rangle := \langle u_1, u_2 \rangle_{aux} + \langle Bu_1, Bu_2 \rangle_{\partial}.$$

Now we are in the position to formulate the main result.

Theorem 7. *Assume* **A.1** - **A.6**. *Then, for each $f \in \mathbb{L}^2(S^2 \times G)$ and for each $g \in P^{-}\left[\mathbb{L}^2(S^2 \times \delta G)\right]$, the equation*

$$u + Au = f,$$

where $Au = \frac{1}{\sigma}\boldsymbol{\xi} \cdot \nabla u$, subject to the boundary condition

$$B^{-}u = g,$$

has a unique solution u in H, characterized by the weak formulation

$$\langle u + Au, v + Av \rangle + 2\left\langle B^{-}u, B^{-}v \right\rangle_{\partial} = \langle v + Av, f \rangle + 2\left\langle B^{-}v, g \right\rangle_{\partial} \quad \forall v \in H.$$

Furthermore, one has

$$\|u\|^2 = \|f\|^2_{\mathbb{L}^2(S^2 \times G)} + 2\|g\|^2_{\partial},$$

and the global error estimate $\|u - \overline{u}\|^2 = \epsilon(\overline{u})$ with

$$\epsilon(\overline{u}) = \|\overline{u} + A\overline{u} - f\|^2_{\mathbb{L}^2(S^2 \times G)} + 2\|B^{-}\overline{u} - g\|^2_{\partial}, \quad \forall \overline{u} \in H.$$

Proof. (Theorem 7) We shall verify assumptions **B0**, ... ,**B10** of theorem 5.

B0 We set $H_0 := \mathbb{L}^2(S^2 \times G)$, equipped with the canonical inner product $\langle ., . \rangle_{\mathbb{L}^2(S^2 \times G)}$. Thus, $(H_0, \langle ., . \rangle_0)$ is a Hilbert space.

B1 We define H^{aux} as in (25) and we put

$$A_1 : H^{aux} \to H_0, \quad A_1 u = \frac{1}{\sigma}\boldsymbol{\xi} \cdot \nabla u.$$

H^{aux} is a linear subspace of H_0. Closedness of A_1 (with respect to the norm $\|.\|_0$) follows from standard properties of generalized derivatives.

B2 Clearly, $Z := \mathbb{L}^1_{loc}(d|o|)$, see (23), is a linear vector space.

B3 The trace operator $T : H^{aux} \to Z$ of Theorem 6 is linear.

B4 We set $V := \mathbb{L}^2(d|o|)$, equipped with the canonical inner product $\langle .,. \rangle_{\mathbb{L}^2(d|o|)}$. Thus, $(V, \langle .,. \rangle_V)$ is a Hilbert space. Clearly, $V \subseteq Z$.
B5 Let H as in **A.6**, i.e. $H = \{u \in H^{aux} : Tu \in \mathbb{L}^2(d|o|)\}$. We equip for the moment H with the trace inner product of H^{aux}. We have to prove that $T_V : H \to \mathbb{L}^2(d|o|)$, $T_V u = Tu$, is closed. Let us consider a sequence $(u_n)_{n\in\mathbb{N}}$ in H such that

$$\lim_{n\to\infty} \|u_\infty - u_n\|_{aux} + \|w_\infty - Tu_n\|_V = 0$$

for some $u_\infty \in H$ and $w_\infty \in \mathbb{L}^2(d|o|)$. It has to be shown: $Tu_\infty = w_\infty$. Due to Theorem 6, the mapping $T : H^{aux} \to \mathbb{L}^1_{loc}(d|o|)$ is continuous. Hence $Tu_n \to Tu_\infty$ in $\mathbb{L}^1_{loc}(d|o|)$. On the other hand we have $Tu_n \to w_\infty$ in $\mathbb{L}^2(d|o|)$. Since the topology of $\mathbb{L}^2(d|o|)$ is finer than the topology of $\mathbb{L}^1_{loc}(d|o|)$ (in particular: compatible), we can identify the limits, thus $w_\infty = Tu_\infty$.
B6 Let ρ and R be as in (27) and (29), respectively. We immediately obtain

$$\forall w \in M(o) : \quad R^2 w = w. \tag{31}$$

from **A.1**, **A.2**, **A.3** and from (28), i.e. R is a reflection. Furthermore, we readily deduce from **A.1**, **A.2**, **A.3**, **A.5** and from (28) the commutativity of R and ρ, i.e.

$$\forall w \in M(o) : \quad (R\rho)(w) = (\rho R)(w). \tag{32}$$

Now we are in the position to introduce

$$D : V \to V, \quad Du = (\rho R)u, \tag{33}$$

and to prove

Proposition 8. *Assume* **A.1, A.2, A.3, A.5** *and let D as in* (33)*. Then*

1. *D is linear.*
2. *D is self-adjoint.*
3. $\|D : V \to V\| \leq \overline{\rho} < 1$.

Proof. (Proposition (33)) The linearity of D is obvious. Concerning self-adjointness it suffices due to (32) to prove that ρ and R are self-adjoint. The self-adjointness of the multiplication-type operator ρ is clear. The self-adjointness of R follows from the fact that $(\boldsymbol{\xi}, \boldsymbol{\zeta}) \mapsto V_{refl}(\boldsymbol{\xi}, \boldsymbol{\zeta})$ is a (measurable) differentiable bijection on $S^2 \times \partial G$ with determinant one. By a similar argument, we prove $\|R : V \to V\| = 1$. On the other hand, due to **A.5**, we have $\|\rho : V \to V\| \leq \overline{\rho}$. Thus, $\|D : V \to V\| = \|\rho R : V \to V\| \leq \|\rho : V \to V\| \, \|R : V \to V\| \leq \overline{\rho}$. □
B7 We introduce the operators $P^\pm$ as (30) and set $U^+ := P^+[V]$. One can argue as in remark 11 to deduce that U^+ is a closed subspace of V.
B8 It is easy to deduce $RP^+ = P^- R$ from (28). Furthermore, since ρ is a multiplication operator with factor function $\hat{\rho}(|\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})|)$, we have $\rho P^\pm = P^\pm \rho$. Hence $DP^+ = (\rho R)P^+ = \rho(RP^+) = \rho(P^- R) = (\rho P^-)R = (P^-\rho)R = P^-(\rho R) = P^- D$.
B9 Making use of the definitions of $T, P^\pm, B^\pm$ and of the definitions of the inner products $\langle .,. \rangle_V, \langle .,. \rangle_\partial$ we deduce B9 (via **A.1 - A.5**) from **A.6**.
B10 We have to prove the "inversion formula" (19). The core of the proof is the validity of the following extension result.

Lemma 9. *Assume* **A.1** - **A.4**. *Furthermore, let* $w \in C_c(S^2 \times \delta G)$ *such that* $\mathsf{supp}(w) \subseteq \{(\boldsymbol{\xi}, \boldsymbol{\zeta}) \in S^2 \times \delta G : |\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})| > 0\}$. *Then, there is a function* $w^E \in C^{aux}$ *with* $Tw^E = w$.

Proof. (Lemma 9) Due to the linearity of T it suffices to consider $\mathsf{supp}(w) \subseteq S^2 \times \Gamma_j$ for some $j \in \{1, \ldots, N\}$. Since the support $\mathsf{supp}(w)$ of w is a compact subset of $\{(\boldsymbol{\xi}, \boldsymbol{\zeta}) \in S^2 \times \Gamma_j : |\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})| > 0\}$, there is $\varepsilon \in \mathbb{R}^+$ such that $\mathsf{supp}(w) \subseteq \{(\boldsymbol{\xi}, \boldsymbol{\zeta}) \in S^2 \times \Gamma_j : |\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta})| \geq \varepsilon\}$. Due to the linearity of T it suffices to consider the cases $\mathsf{supp}(w) \subseteq \{(\boldsymbol{\xi}, \boldsymbol{\zeta}) \in S^2 \times \Gamma_j : \boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta}) \geq \varepsilon\}$ or $\mathsf{supp}(w) \subseteq \{(\boldsymbol{\xi}, \boldsymbol{\zeta}) \in S^2 \times \Gamma_j : \boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta}) \leq -\varepsilon\}$. We consider only the first case here (the second one can be treated in analogy). Let K be the $\boldsymbol{\xi}$-projection of $\mathsf{supp}(w)$ onto δG. K is a compact subset of Γ_j. By assumption **A.4** there is $\mathsf{m}_j \in \mathbb{R}^+$ such that for all $\boldsymbol{\xi} \in S^2$,

$$
\begin{aligned}
L(\boldsymbol{\xi}) &= \{\boldsymbol{\zeta} \in \delta G : (\boldsymbol{\xi}, \boldsymbol{\zeta}) \in \mathsf{supp}(w)\} - [0, \mathsf{m}_j]\boldsymbol{\xi} \\
&= \{\boldsymbol{\zeta} \in K : (\boldsymbol{\xi}, \boldsymbol{\zeta}) \in \mathsf{supp}(w)\} - [0, \mathsf{m}_j]\boldsymbol{\xi} \subseteq K \cup G.
\end{aligned}
$$

We observe: There is for each $\boldsymbol{\xi} \in S^2$ and for each $\boldsymbol{x} \in L(\boldsymbol{\xi})$ a unique pair $(\boldsymbol{\zeta}(\boldsymbol{\xi}, \boldsymbol{x}), s(\boldsymbol{\xi}, \boldsymbol{x})) \in \Gamma_j \times [0, \mathsf{m}_j]$ with $\boldsymbol{x} = \boldsymbol{\zeta}(\boldsymbol{\xi}, \boldsymbol{x}) - s(\boldsymbol{\xi}, \boldsymbol{x})\boldsymbol{\xi}$. Now let us take $\Phi \in C_c^\infty(\mathbb{R})$ with $\mathsf{supp}(\Phi) \subseteq [-1, \mathsf{m}_j]$ and $\Phi(0) = 1$. For fixed $\boldsymbol{\xi} \in S^2$ and $\boldsymbol{x} \in G$ we define

$$
w^E(\boldsymbol{\xi}, \boldsymbol{x}) = \begin{cases} w(\boldsymbol{\xi}, \boldsymbol{\zeta}(\boldsymbol{\xi}, \boldsymbol{x})).\Phi(s(\boldsymbol{\xi}, \boldsymbol{x})) & \text{if} \quad \boldsymbol{x} \in L(\boldsymbol{\xi}) \\ 0 & \text{else} \end{cases} .
$$

Then the function $w^E : S^2 \times G \to \mathbb{R}, (\boldsymbol{\xi}, \boldsymbol{x}) \mapsto w^E(\boldsymbol{\xi}, \boldsymbol{x})$ belongs to C^{aux} (we note: $\boldsymbol{\xi} \cdot \nabla w^E(\boldsymbol{\xi}, \boldsymbol{x}) = w(\boldsymbol{\xi}, \boldsymbol{\zeta}(\boldsymbol{\xi}, \boldsymbol{x}))\Phi'(s(\boldsymbol{\xi}, \boldsymbol{x}))$ if $\boldsymbol{x} \in L(\boldsymbol{\xi})$ and 0 else) with $w^E \downharpoonright S^2 \times \delta G = w$. $\square$

With the aid of Lemma 9 we can prove B10, i.e. in our context

Theorem 10. *Assume* **A.1** - **A.6**. *Then for all* $u, v \in \mathbb{L}^2(S^2 \times G)$, *for all* $w^- \in H_\partial^-, w^+ \in H_\partial^+$: *If*

$$
\begin{aligned}
&\int_{S^2 \times G} \phi\, v \; d(\omega(\boldsymbol{\xi}), \boldsymbol{x}) + \frac{1}{\sigma} \int_{S^2 \times G} (\boldsymbol{\xi} \cdot \nabla \phi)\, u \; d(\omega(\boldsymbol{\xi}), \boldsymbol{x}) \\
&\qquad = \langle B^+(\phi), w^+ \rangle_{H_\partial} - \langle B^-(\phi), w^- \rangle_{H_\partial},
\end{aligned}
$$

for all $\phi \in H$, *then* $u \in H$, $v = Au$, $w^+ = B^+u$, $w^- = B^-u$.

Proof. Let $\phi \in C_c^\infty(S^2 \times G)$. Then by Theorem 6, $T\phi = 0$, hence $B^+\phi = B^-\phi = 0$ and therefore

$$
\int_{S^2 \times G} \phi\, v \; d(\omega(\boldsymbol{\xi}), \boldsymbol{x}) + \frac{1}{\sigma} \int_{S^2 \times G} (\boldsymbol{\xi} \cdot \nabla \phi)\, u \; d(\omega(\boldsymbol{\xi}), \boldsymbol{x}) = 0,
$$

i.e. $v = \frac{1}{\sigma} \boldsymbol{\xi} \cdot \nabla u = A_1 u$, in particular $u \in H^{aux}$. On the other hand we deduce from Gauss' integration formula **A.6**,

$$
\begin{aligned}
&\int_{S^2 \times G} \phi\, v \; d(\omega(\boldsymbol{\xi}), \boldsymbol{x}) + \frac{1}{\sigma} \int_{S^2 \times G} (\boldsymbol{\xi} \cdot \nabla \phi)\, u \; d(\omega(\boldsymbol{\xi}), \boldsymbol{x}) \\
&\qquad = \left\langle B^+\phi, B^+u \right\rangle_\partial - \left\langle B^-\phi, B^-u \right\rangle_\partial,
\end{aligned}
$$

for all $\phi \in H$, hence

$$\forall \phi \in H : \quad \left\langle B^+\phi, B^+u - w^+ \right\rangle_\partial - \left\langle B^-\phi, B^-u - w^- \right\rangle_\partial = 0.$$

We take $\Psi \in C_c^1(S^2 \times \delta G)$ whose support is contained in $\{\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta}) > 0\}$. Then

$$\Psi' = (\mathsf{id} + D)(\mathsf{id} - D^2)^{-1}\Psi \in C_c^1(S^2 \times \delta G).$$

By Theorem 9 there is $\phi \in H$ with $T\phi = \Psi'$. We certainly have $(\mathsf{id} - D)T\phi = \Psi = B^+\phi$, $B^-\phi = 0$. Hence

$$\forall \Psi \in C_c^1(S^2 \times \delta G) : \text{ If } \mathsf{supp}(\Psi) \subseteq \{\boldsymbol{\xi} \cdot \boldsymbol{n}(\boldsymbol{\zeta}) > 0\}, \text{ then } \quad \left\langle \Psi, B^+u - w^+ \right\rangle_\partial = 0. \tag{34}$$

Since the set of all Ψ satisfying the premise of (34) is dense in V, we deduce $B^+u = w^+$ from (34). The identity $B^-u = w^-$ follows in analogy. Finally we have $(\mathsf{id} - D)Tu = B^+u + B^-u = w^+ + w^- \in V$, from which we readily deduce $u \in H$, thus $A_1 u = Au$. □

Identifying the operators and norms of Theorem 5 as throughout this subsection, we obtain the statements of Theorem 7. □

Remark 12. *The statements of theorem* (7) *answer the questions Q1. and Q2. in the following sense. Concerning Q1. we deduce* $\overline{u} \in H$ *is sufficient to guarantee the validity of* (7) *(naturally, provided* **A.1** - **A.6** *hold). The answer to the "geometric" question Q2. is less direct, because one has to check for a given geometry whether assumptions* **A.1** - **A.6** *hold. This is seemingly not very inspiring. On the other hand, there are quite a few "classical" sets G for which assumptions* **A.1** - **A.6** *are certainly valid: Polygons, smooth domains, cylinders, cones, to mention a few. This class of domains certainly covers real-life needs. On the other hand, it is an open problem whether* (7) *also holds for domains whose boundary contains cusps. The proof given here cannot be extended to such geometries because an extension result like* (9) *is lacking.*

7 Conclusion

A recently proposed hybrid method [5] to simulate cooling processes of high quality glass relies on a residual based error formula for RTEs. We gave a rigorous proof for this error formula by means of Hilbert space methods and trace arguments. In particular, we showed that the residual based error formula is reliable for (de facto all) real-life geometries and therefore rigorously increased the credibility of the proposed hybrid method.

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