ELSEVIER

Comput. Methods Appl. Mech. Engrg. 1868 (1999) 449–473

Computer methods in applied mechanics and engineering

Analysis of hypersingular residual error estimates in boundary element methods for potential problems

Govind Menon[a,1], Glaucio H. Paulino[b,*], Subrata Mukherjee[c]

[a]*Division of Applied Mathematics, Brown University, P.O. Box F, Providence, RI 02912, USA*

[b]*Department of Civil and Environmental Engineering, University of California, Davis, CA 95616, USA*

[c]*Department of Theoretical and Applied Mechanics, Cornell University, Ithaca, NY 14853, USA*

Received 30 December 1997; revised 14 July 1998

Abstract

A novel iteration scheme, using boundary integral equations, is developed for error estimation in the boundary element method. The iteration scheme consists of using the boundary integral equation for solving the boundary value problem and iterating this solution with the hypersingular boundary integral equation to obtain a new solution. The hypersingular residual r is consistently defined as the difference in the derivative quantities on the boundary, i.e.

$$r = \frac{\partial \phi^{(1)}}{\partial n} - \frac{\partial \phi^{(2)}}{\partial n}$$

where ϕ is the potential and $(\partial \phi / \partial n)^{(i)}$, $i = 1, 2$, is the flux obtained by solution (i). Here, $i = 1$ refers to the boundary integral equation, and $i = 2$ refers to the hypersingular boundary integral equation. The hypersingular residual is interpreted in the sense of the iteration scheme defined above and it is shown to provide an error estimate for the boundary value problem. Error-hypersingular residual relations are developed for Dirichlet and Neumann problems, which are shown to be limiting cases of the more general relation for the mixed boundary value problem. These relations lead to global bounds on the error. Four numerical examples, involving Galerkin boundary elements, are given, and one of them involves a physical singularity on the boundary and preliminary adaptive calculations. These examples illustrate important features of the hypersingular residual error estimate proposed in this paper. © 1999 Elsevier Science S.A. All rights reserved.

1. Introduction

An intriguing feature of the theory of singular integral equations is that the problem for the boundary unknowns can be formulated in different ways, either by *direct* or *indirect methods* [1]. In engineering applications, one usually uses the *direct method*, which has its origin in Green's theorem. Thus, one may formulate *two distinct boundary integral equations*—the standard boundary integral equation (BIE), and the hypersingular boundary integral equation (HBIE)—to represent the same boundary value problem (BVP). A unified derivation of both integral equations has been presented by Wendland [2]. Hypersingular boundary integrals have proven advantageous in a variety of applications (e.g. fracture mechanics and wave scattering), and these equations have opened possibilities of new solutions of various problems by the BEM (see the review articles by Krishnasamy et al. [3] and Tanaka et al. [4]).

In particular, the use of HBIEs for error estimation is the focus of this work. A natural measure of the error in a boundary integral method, first proposed by Paulino [5] and Paulino et al. [6], rests on the use of both the

* Corresponding author.

[1] Formerly a Graduate Research Assistant at the Department of Theoretical and Applied Mechanics, Cornell University.

0045-7825/99/$ – see front matter © 1999 Elsevier Science S.A. All rights reserved.
PII: S0045-7825(98)00297-7

standard BIE and the HBIE. Suppose that an approximate solution, using one of the BIEs, has been obtained. Then, one might expect that the *residual*, obtained when this approximate solution is substituted in the other BIE, is related to the error. Numerical experiments have suggested that this is indeed the case [5–7]. In this work, our aim is to formalize and extend the error estimates obtained by the combined use of the BIE and the HBIE for solving a BVP and estimating discretization errors.

The remainder of this paper is organized as follows. Initially, a brief literature survey and comments on previous related work are presented. Afterwards, the paper is developed in the context of two-dimensional potential theory. The error estimation method using two distinct BIEs is formally developed, the *hypersingular residual* is defined, and related to the actual error in the approximation. Interior Dirichlet and Neumann problems are considered first because a rigorous analysis is easier for these problems, and they illustrate well the central idea of the paper. The methodology is then extended to mixed BVPs. Four numerical examples using a Galerkin BEM are provided, and one of them involves a physical singularity on the boundary and adaptive calculations. It is worth mentioning that the ideas presented here are not tied down to potential problems. In fact, they extend very naturally to other linear elliptic problems, e.g. linear elasticity [5,7].

2. Related work

In recent years, the boundary element method (BEM) has become established as a powerful numerical technique for solving certain elliptic BVPs that admit integral equation formulations. Yet, there are several aspects of the theory that are not as well established as in the finite element method (FEM). A particular strength of the FEM is the well developed theory of error estimation, and its use in adaptive methods [8,9]. In comparison, error estimation in boundary element methods is a subject that has attracted attention mainly over the past ten years, and much remains to be done. For recent surveys on error estimation and adaptivity in the BEM, see [10–13].

Many error estimates in BEM are essentially heuristic and, unlike the FEM, theoretical work in the field has been quite limited. Rank [14] proposed error indicators and an adaptive algorithm for the BEM using techniques similar to those in the FEM. Most notable are Yu and Wendland [15–18], who have presented local error estimates based on a linear error-residual relation that is very effective in the FEM. Their initial arguments required the restrictive assumption of uniform meshes [15,17,18], but this was relaxed later for Galerkin methods [16]. More recently, Carstensen et al. [19–22] have presented error estimates for the BEM in a mould similar to that outlined by Eriksson et al. [9] for the FEM. There are numerous stumbling blocks in the development of a satisfactory theoretical analysis of a generic BVP. First, the theoretical analyses are easiest for Galerkin schemes, but (at the time of this writing) most engineering BEM codes use collocation-based methods [1]. Though one may view collocation schemes as variants of Petrov–Galerkin methods, and in fact numerous theoretical analyses exist for collocation methods (see the references in [10]), the mathematical analysis is difficult. Theoretical analyses for mixed boundary conditions—which is the type of the most practical importance—are limited and involved [23]. Finally, the presence of corners and cracks has been a source of challenging problems for many years [10,24,25].

In the past few years, there has been a marked interest in extending analyses of BEM for singular integrals to hypersingular integrals among mathematicians in the field, e.g. [20,21,26,27]. For instance, Feistauer et al. [27] have studied the solution of the exterior Neumann problem for the Helmholtz equation formulated as an HBIE.[2] Their paper is valuable for a rigorous analysis of hypersingular integral equations and for addressing the problem of non-computability of the residual norm, where additional hypothesis is needed to design a practical error estimate. Their work differs from ours in the sense that they use usual residuals to estimate the error, and they do not use the BIE and HBIE simultaneously, as we do.

Recently, Golberg and Bowman [28] have used the superconvergence of the Sloan iterate [29,30] to show the asymptotic equivalence of the error and the residual. They have used Galerkin methods, an iteration scheme using the same integral equation for a first approximation and for the iterates, and usual residuals in their work.

[2] There is a mistake in Eq. (2.19) of the paper by Feistauer et al. [27], which should have v in the denominator instead of ϕ.

In this paper we present a novel iteration scheme for integral equations and we use the hypersingular residuals for error estimation.

In summary, the definition and analysis of hypersingular residuals (and singular residuals), and the use of a different integral equation for the iteration step is not present in any of the papers mentioned in this section. Theoretical analysis of hypersingular residual error estimates by means of an iteration scheme using both the BIE and the HBIE is the main focus of the present work.

3. Boundary integral equations

The basic notation and boundary integral formulation for two-dimensional potential problems are introduced. Linear operators are defined, and the BIEs are rewritten as linear equations. The properties of these linear operators are elucidated using elementary Fourier analysis. The particular case for the equations on a circular region is provided, and pseudodifferential operators are introduced.

3.1. Governing equations

Various approaches exist for the formulation of problems in potential theory as integral equations [31,32]. In engineering practice, BVPs typically have mixed boundary conditions. Consequently, the approach most suited to the derivation of integral equations for these problems is the use of Green's theorem. Using Green's theorem, one obtains the *first* BIE of potential theory (which is used here for the solution of Laplace equation)[3]

$$\phi(p) = \int_{\partial B} \left[G(p,Q) \frac{\partial}{\partial \boldsymbol{n}} \phi(Q) - \frac{\partial}{\partial \boldsymbol{n}} G(p,Q) \phi(Q) \right] \mathrm{d}s_Q \tag{1}$$

where ϕ is the potential; p is a point in the interior of the domain B (source point), i.e. $p \in B$; Q is a point on the boundary ∂B (field point), i.e. $Q \in \partial B$; the domain of the body is $\Omega \equiv B \cup \partial B$ (lower case letters denote points in B, and upper case letters denote points on ∂B); $\boldsymbol{n}$ is the unit outward normal at Q; $\mathrm{d}s_Q$ is a differential length element in two-dimensional problems;

$$\rho = \|\boldsymbol{\rho}\| = \|Q - p\| ;$$

and $G(p,Q)$ is the free space Green's function or fundamental solution:

$$G(p,Q) = \frac{1}{2\pi} \log\left(\frac{1}{\rho}\right) \tag{2}$$

$$\frac{\partial}{\partial \boldsymbol{n}} G(p,Q) = -\frac{1}{2\pi} \frac{\boldsymbol{\rho} \bullet \boldsymbol{n}}{\rho^2} \tag{3}$$

It is clear that the kernels are singular as $\rho \to 0$. Thus, as $p \to P$, a singular integral equation results

$$\phi(P) = \lim_{p \to P} \int_{\partial B} \left[G(p,Q) \frac{\partial}{\partial \boldsymbol{n}} \phi(Q) - \frac{\partial}{\partial \boldsymbol{n}} G(p,Q) \phi(Q) \right] \mathrm{d}s_Q \tag{4}$$

It may be shown that the resulting integral is well-defined under suitable assumptions on the smoothness of the boundary and the potential [32,33]. In the present analysis, domains with corners are not considered.

One can obtain the gradient of the potential, for points $p \in B$, by differentiation under the integral sign. In this case, the kernels are clearly differentiable, in fact they are C^∞. Using Eq. (1), one obtains

$$\nabla_p \phi(p) = \int_{\partial B} \left[\nabla_p G(p,Q) \frac{\partial}{\partial \boldsymbol{n}} \phi(Q) - \frac{\partial}{\partial \boldsymbol{n}} \nabla_p G(p,Q) \phi(Q) \right] \mathrm{d}s_Q \tag{5}$$

where $\nabla_p(\cdot)$ denotes the gradient with respect to the source point p. Here, the kernels are

[3] For the sake of clarity of notation, note that $\partial(\cdot)/\partial \boldsymbol{d}$ refers to the 'directional derivative' of $(\cdot)$ in the direction $\boldsymbol{d}$, i.e. $\partial(\cdot)/\partial \boldsymbol{d} = \nabla(\cdot) \bullet \boldsymbol{d}$.

$$\nabla_p G(p, Q) = \frac{1}{2\pi} \frac{\boldsymbol{\rho}}{\rho^2} \tag{6}$$

$$\frac{\partial}{\partial \boldsymbol{n}} \nabla_p G(p, Q) = \frac{1}{2\pi} \left[\frac{\boldsymbol{n}}{\rho^2} - 2 \frac{(\boldsymbol{\rho} \bullet \boldsymbol{n}) \boldsymbol{\rho}}{\rho^4} \right] \tag{7}$$

Again, a singular integral equation results by taking the limit to the boundary

$$\nabla_P \phi(P) = \lim_{p \to P} \int_{\partial B} \left[\nabla_p G(p, Q) \frac{\partial}{\partial \boldsymbol{n}} \phi(Q) - \frac{\partial}{\partial \boldsymbol{n}} \nabla_p G(p, Q) \phi(Q) \right] \mathrm{d}s_Q \tag{8}$$

In this equation, the first integral is strongly singular, and the second one is hypersingular. This terminology is standard in the BEM literature [3]. One may view these integrals in the sense of suitable limits to the boundary [5,34,35]. Again, for these integrals to be well-defined, it is necessary that the potential, normal flux and boundary satisfy certain smoothness requirements. These are detailed by Krishnasamy et al. [36] and Martin and Rizzo [37]. A discussion of the self-regularized form of Laplace's equation, based on a 'limit from the interior' interpretation (as in Eq. (8) above) has been recently presented by Cruse and Richardson [38].

The boundary unknowns, or Cauchy data, in a potential problem are the potential ϕ and the normal flux $\partial \phi / \partial \boldsymbol{n}$. Equation (8) may be used to obtain a *second* description of the problem as a boundary integral equation. By taking the directional derivative in the particular direction $\boldsymbol{D}(P) = (D_1, D_2)$ at $P \in \partial B$, and taking the limit, one obtains

$$\frac{\partial}{\partial \boldsymbol{D}} \phi(P) = \lim_{p \to P} \int_{\partial B} \left[\frac{\partial}{\partial \boldsymbol{D}} G(p, Q) \frac{\partial}{\partial \boldsymbol{n}} \phi(Q) - \frac{\partial}{\partial \boldsymbol{n}} \frac{\partial}{\partial \boldsymbol{D}} G(p, Q) \phi(Q) \right] \mathrm{d}s_Q \tag{9}$$

This is an *equivalent* BIE, which is sufficient to solve the BVP. We shall refer to Eq. (4) as the boundary integral equation (BIE) and Eq. (9) as the hypersingular boundary integral equation (HBIE). Equations (4) and (9) result in well defined integral equations on the boundary, $P \in \partial B$, by defining the singular integrals in a *limit to the boundary sense* (i.e. as $p \to P$) [5,34,35].

3.2. Linear operators

A suitable analysis of the BIEs can be developed by viewing them as linear equations in a Hilbert space. The utility of this approach will become clear in the next section. A very readable account is given in the book by Kress [33]. Following Sloan [10], we shall assume that the boundary ∂B is a C^1 continuous closed Jordan curve given by the mapping

$$z : [0, 1] \to \partial B, \quad z \in C^1, \quad |z'| \neq 0$$

where $z \in \boldsymbol{C}$, the space of complex numbers. This analysis excludes domains with corners. Any integrable function v, on ∂B, may be represented in a Fourier series

$$v \sim \sum_{k=-\infty}^{\infty} \hat{v}(k) \, \mathrm{e}^{2\pi \mathrm{i} k x} = a_0 + \sum_{k=1}^{\infty} (a_k \cos 2\pi k x + b_k \sin 2\pi k x) \tag{10}$$

where $\mathrm{i} \equiv \sqrt{-1}$ and

$$\hat{v}(k) = \int_0^1 \mathrm{e}^{-2\pi \mathrm{i} k x} \, v(x) \, \mathrm{d}x, \quad k \in \boldsymbol{Z} \tag{11}$$

in which $\boldsymbol{Z}$ denotes the space of integer numbers. To establish bounds on the error, it is necessary to ensure that the functions under study satisfy certain smoothness requirements. We shall use Sobolev spaces for this purpose. For any real number ν, we define the Sobolev norm $\|v\|_\nu$ as

$$\|v\|_\nu = \left(|\hat{v}(0)|^2 + \sum_{k \neq 0} |k|^{2\nu} |\hat{v}(k)|^2 \right)^{1/2} \tag{12}$$

Correspondingly, we define the Sobolev space $H^\nu(\partial B)$ as the closure with respect to the norm $\| \cdot \|_\nu$ of the space

of 1-periodic C^∞ functions. Specifying a higher value of ν corresponds to requiring higher smoothness of the function.

LEMMA 1. If $\mathscr{A}: B_1 \to B_2$ is a continuous, linear operator between Banach spaces B_1 and B_2 that has a continuous inverse and $\mathscr{A}x = y$, then there exist real positive constants C_1 and C_2, such that

$$C_1\|y\|_{B_2} \leq \|x\|_{B_1} \leq C_2\|y\|_{B_2}$$

where $\|\cdot\|_{B_i}$ denotes the norm in the Banach space B_i.

PROOF. The linearity and continuity of $\mathscr{A}$ and $\mathscr{A}^{-1}$ imply that $\|\mathscr{A}\|$ and $\|\mathscr{A}^{-1}\|$ are finite. We have

$$\|y\| = \|\mathscr{A}x\| \leq \|\mathscr{A}\|\,\|x\|$$
$$\|x\| = \|\mathscr{A}^{-1}y\| \leq \|\mathscr{A}^{-1}\|\,\|y\|$$

The result follows by choosing $C_1 = 1/\|\mathscr{A}\|$ and $C_2 = \|\mathscr{A}^{-1}\|$. □

Returning to the problem at hand, we formally define the following linear operators associated with Eq. (4)

$$(\mathscr{V}u)(p) := \int_{\partial B} G(p, Q)u(Q)\,\mathrm{d}s_Q \tag{13}$$

$$(\mathscr{K}u)(p) := -\int_{\partial B} \frac{\partial}{\partial \boldsymbol{n}} G(p, Q)u(Q)\,\mathrm{d}s_Q \tag{14}$$

with the understanding that the operators are defined when the integrals exist. In the mathematical literature $\mathscr{V}$ is referred to as the single-layer operator, and $\mathscr{K}$ is termed the double-layer operator. Similarly, the directional components of Eq. (8) are defined as

$$(\mathscr{M}_D u)(p) := \int_{\partial B} \frac{\partial}{\partial \boldsymbol{D}} G(p, Q)u(Q)\,\mathrm{d}s_Q \tag{15}$$

$$(\mathscr{L}_D u)(p) := -\int_{\partial B} \frac{\partial}{\partial \boldsymbol{D}} \frac{\partial}{\partial \boldsymbol{n}} G(p, Q)u(Q)\,\mathrm{d}s_Q \tag{16}$$

In this work, $\boldsymbol{D} \equiv \boldsymbol{N}$, where $\boldsymbol{N}$ is the normal unit vector[4] on ∂B at P. Theoretical and numerical work on error estimation involving the above operators with $\boldsymbol{D} \equiv \boldsymbol{S}$, where $\boldsymbol{S}$ is the tangent unit vector on ∂B at P, can be found in references [5,7]. Note that $\mathscr{M}_N$ is the negative of the adjoint of $\mathscr{K}$.

The one-to-one correspondence between the linear operators and the integrals is clear. The limit to the boundary of the integral equations has been used to obtain singular BIEs, and now the limiting value of the associated operators are considered. $\mathscr{V}$ is continuous onto the boundary, whereas $\mathscr{K}$ and $\mathscr{M}_N$ are not continuous [10], and give rise to additional bounded boundary terms in the limit. The hypersingular operator $\mathscr{L}_N$ gives rise to unbounded terms that vanish when the integral is considered, for example, in the *limit to the boundary sense*. These terms depend on the smoothness of the boundary at P. In this work, we consider only C^1 boundaries. Corners present difficulties, and for a discussion of this matter one may refer to [24]. Taking the limit to the boundary, and using the linear operators defined above, one may rewrite Eqs. (4) and (9) in compact notation as

$$\phi = \mathscr{K}\phi + \mathscr{V}\frac{\partial \phi}{\partial \boldsymbol{n}} \tag{17}$$

$$\frac{\partial \phi}{\partial \boldsymbol{N}} = \mathscr{L}_N\phi + \mathscr{M}_N\frac{\partial \phi}{\partial \boldsymbol{n}} \tag{18}$$

respectively. Note that if $\boldsymbol{D} \equiv \boldsymbol{N} \equiv \boldsymbol{n}(P)$, then $\partial\phi/\partial\boldsymbol{N} \equiv \partial\phi/\partial\boldsymbol{n}$. This notation is used later in the paper.

[4] For a proper interpretation of the direction vectors, recall that the integrals are defined in a *limit to the boundary sense* [5,34,35].

3.3. Equations on a circle

As one may expect, the linear operators associated with singular integral equations are of a special nature. The singular kernels cause the operators to have some properties similar to differential operators, and they are thus known as *pseudodifferential operators*. One may refer to Friedrichs [39] for an introduction to the theory of pseudodifferential operators, and to Sloan [10] for an excellent introduction to their use in error analysis of BIEs. Potential problems in a circle are considered here. The investigation of these problems allows one to gain an intuitive understanding of pseudodifferential operators, and to identify the essential character of the operators.

Consider a disk of radius α. Denote the source point P by θ and the field point Q by $\tilde{\theta}$. Let v be an integrable function on the boundary of the disk. The kernels take on a particularly simple form because of the geometry, and one may calculate

$$(\mathscr{V}v)(\theta) := -\frac{1}{\pi}\int_{-\pi}^{\pi} \alpha \log\left|2\alpha \sin\left(\frac{\tilde{\theta}-\theta}{2}\right)\right| v(\tilde{\theta})\,\mathrm{d}\tilde{\theta} \tag{19}$$

$$(\mathscr{K}v)(\theta) = -(\mathscr{M}_N v)(\theta) := \frac{1}{2\pi}\int_{-\pi}^{\pi} v(\tilde{\theta})\,\mathrm{d}\tilde{\theta} \tag{20}$$

$$(\mathscr{L}_N v)(\theta) := -\frac{1}{4\pi\alpha}\int_{-\pi}^{\pi} \frac{1}{\sin^2\left(\frac{\tilde{\theta}-\theta}{2}\right)} v(\tilde{\theta})\,\mathrm{d}\tilde{\theta} \tag{21}$$

Let us consider the operators in more detail. First consider the logarithmic kernel in Eq. (19). It may be represented by the Fourier series:

$$-\log\left|2\alpha \sin\left(\frac{\tilde{\theta}-\theta}{2}\right)\right| \sim \sum_{k=1}^{\infty} \frac{1}{k}\cos k(\tilde{\theta}-\theta) - \log\alpha \tag{22}$$

Using the convolution theorem, and the inverse discrete Fourier transform, one obtains

$$(\mathscr{V}v)(\theta) = \alpha\left\{-a_0 \log\alpha + \sum_{k=1}^{\infty}\frac{1}{k}\left[\alpha_k \cos(k\theta) + b_k \sin(k\theta)\right]\right\} \tag{23}$$

The effect of $\mathscr{V}$ is to *attenuate the higher harmonics*, and hence smooth the function. That is, one may now show that

$$\mathscr{V} : H^{\nu} \to H^{\nu+1}, \quad \forall\, \nu \in \boldsymbol{R}$$

where $\boldsymbol{R}$ is the space of real numbers. Next, consider $\mathscr{K}$ and $\mathscr{M}_N$. From Eq. (20), note that these kernels are not singular. This is not what one would expect at first sight. These kernels arise from differentiation of the logarithmic kernel, and it is perhaps more natural that they be singular. Instead, for the circle, $\mathscr{K}$ and $\mathscr{M}_N$ act as averaging operators. They are of rank one because every trigonometric monomial other than the constant function is in their nullspace (all sines and cosines with integer frequency have average zero). For a C^{∞} boundary we have [10]

$$\mathscr{K} : H^{\mu} \to H^{\nu}, \quad \forall\, \mu, \nu \in \boldsymbol{R}$$

and similarly for $\mathscr{M}_N$. Smoothness of the boundary is critical here, and the operators are certainly not so well behaved if corners are present.

Finally, consider the hypersingular operator in Eq. (21). We use the Fourier representation [40]

$$-\frac{1}{4\sin^2\left(\frac{\theta-\theta}{2}\right)} \sim \sum_{k=1}^{\infty} k\cos k(\tilde{\theta}-\theta) \tag{24}$$

Hence,

$$(\mathscr{L}_N v)(\theta) = \frac{1}{\alpha}\sum_{k=1}^{\infty}\left\{k\left[a_k \cos(k\theta) + b_k \sin(k\theta)\right]\right\} \tag{25}$$

The hypersingular operator amplifies higher frequencies, which makes a function less smooth. This may be restated as

$$\mathscr{L}_N : H^{\nu} \to H^{\nu-1}, \quad \forall\, \nu \in \boldsymbol{R}$$

Note also, that it has a non-trivial nullspace—the constant function. This can be viewed as a manifestation of the non-uniqueness in the Neumann problem. It will be helpful to keep this simplified picture of the operators in mind when considering what follows.

3.4. Pseudodifferential operators

After having described the linear operators in the simplest setting, the main conclusions can now be generalized. For our purposes, a *pseudodifferential operator* $\mathscr{A}$ is a linear operator

$$\mathscr{A} : H^{\nu+\beta/2} \to H^{\nu-\beta/2}, \quad \forall\, \nu \in \boldsymbol{R}$$

The number β is a characteristic of the operator and is termed its order. The special case $\nu = 0$ is most natural. Then, $\mathscr{A} : H^{\beta/2} \to H^{-\beta/2}$. Typically, the operators encountered in applications have orders $-1, 0$ and $+1$ [2]. In potential theory, the log-singular operator $\mathscr{V}$ is of order -1, and is a once-smoothing operator. For smooth domains, $\mathscr{K}$ and $\mathscr{M}_N$ are compact, and $(\mathscr{I} - \mathscr{K})$ and $(\mathscr{I} - \mathscr{M}_N)$ are of order 0. The hypersingular operator, $\mathscr{L}_N$ is of order $+1$. Using pseudodifferential operators, one can restate the BVP as follows:

Given a pseudodifferential operator $\mathscr{A} : H^{\beta/2} \to H^{-\beta/2}$ and boundary data $f \in H^{-\beta/2}$ on ∂B, find $w \in H^{\beta/2}$ that is a solution of

$$\mathscr{A}w = f$$

REMARK 1. One should note, however, that key properties of the operators, such as continuity and invertibility, assume a certain regularity of the boundary, for instance, no corners or cusps [10]. These assumptions are too restrictive for the solution of a practical engineering problem, but we have made them, nevertheless, in order to obtain some mathematical understanding of our error estimation process.

4. Iterated HBIE and error estimation

The heuristic idea that is at the heart of our error estimation procedure is simple [5,6]: *the amount by which an approximate solution to the BIE fails to satisfy the HBIE is a measure of the error in the approximation.* The main result of our work is that this heuristic idea, when stated formally, immediately leads to a simple characterization of the error. In essence, the method reduces to finding a second approximation to the solution by iterating the first approximation with the HBIE. An interesting sidelight is a non-rigorous argument on accelerated convergence of the hypersingular iterate in the Dirichlet problem. We first illustrate our idea in the two basic cases of the interior Dirichlet and Neumann problems.

4.1. Problem 1: Interior Dirichlet

The interior Dirichlet problem is stated as follows: Find $\partial\phi/\partial\boldsymbol{n}$ on ∂B such that

$$\begin{aligned} \Delta\phi &= 0 \quad \text{in } \Omega \\ \phi &= g \quad \text{on } \partial B \end{aligned} \tag{26}$$

The interior Dirichlet problem can be reformulated as an integral equation using the BIE (17), i.e.

$$\mathscr{V}\frac{\partial\phi}{\partial\boldsymbol{n}} = g - \mathscr{K}g =: f_1 \tag{27}$$

Similarly, using the HBIE (18), one obtains

$$(\mathscr{I} - \mathscr{M}_N)\frac{\partial\phi}{\partial\boldsymbol{n}} = \mathscr{L}_N g =: f_2 \tag{28}$$

The notation f_1 and f_2 on the right-hand side of Eqs. (27) and (28) is arbitrary at this point, however, this will become clear in the section on the mixed BVP. Either Eqs. (27) or (28) may be used to solve the boundary problem. There is a question about existence and uniqueness though, which is discussed later, in Remark 2.

It may be shown that the operators $\mathscr{V}$ and $(\mathscr{I} - \mathscr{M}_N)$ have the following properties [2,10]:

- $\mathscr{V} : H^{\nu} \to H^{\nu+1}, \quad \forall\, \nu \in \boldsymbol{R}$
  $(\mathscr{I} - \mathscr{M}_N) : H^{\nu} \to H^{\nu}, \quad \forall\, \nu \in \boldsymbol{R}$
- $\mathscr{V}$ and $(\mathscr{I} - \mathscr{M}_N)$ are continuous (see Theorem 2 of Wendland [2]).
- In particular, if we choose ν for each problem such that
  $\mathscr{V} : H^{-1/2} \to H^{1/2}$
  $(\mathscr{I} - \mathscr{M}_N) : H^{0} \to H^{0}$
  and if we *assume a unique solution for each problem*, then it may be shown (see Lemma 3.1 of Wendland and Yu [15]) that the operators $\mathscr{V}$ and $(\mathscr{I} - \mathscr{M}_N)$ have continuous inverses.

REMARK 2. Eq. (27) is Symm's equation. The solution to Symm's equation is non-unique if the geometric scale of the body is inappropriate, i.e. the *capacity* or *transfinite diameter* is 1 [10]. By assuming the existence of a unique solution, we do not consider such degenerate geometries. It is worth noting that the HBIE (28) has no such existence-uniqueness problems.

The above formulations of the problem lead us to look for weak solutions [8,41] in distinct spaces, i.e. $H^{-1/2}$ for the BIE, and H^0 for the HBIE. That is, the use of the hypersingular approach demands that we utilize a more restricted, smoother space. In what follows, we shall assume that the true solution is smooth enough to fit in both spaces, i.e. $\partial\phi/\partial\boldsymbol{n} \in H^{\mu}$ with $\mu > 0$. Since both the formulations represent the same BVP, it is expected that they will have the same weak solution under this smoothness assumption.

4.1.1. Error estimate for the primary problem

Our method of error estimation proceeds by first finding an approximate solution $(\partial\phi/\partial\boldsymbol{n})^{(1)} \in H^0$ to the BIE, and then constructing a second approximation, $(\partial\phi/\partial\boldsymbol{n})^{(2)}$, by iterating $(\partial\phi/\partial\boldsymbol{n})^{(1)}$ using the HBIE. As mentioned before, the difference between the iterate and the initial approximation is expected to be a measure of the error. The *iterate* is defined by

$$\frac{\partial\phi^{(2)}}{\partial\boldsymbol{n}} = \mathscr{M}_N \frac{\partial\phi^{(1)}}{\partial\boldsymbol{n}} + \mathscr{L}_N g \tag{29}$$

The error in the approximation $(\partial\phi/\partial\boldsymbol{n})^{(1)}$ is

$$e_q^{(1)} = \frac{\partial\phi^{(1)}}{\partial\boldsymbol{n}} - \frac{\partial\phi}{\partial\boldsymbol{n}} \tag{30}$$

Note that by our assumptions, $e_q^{(1)} \in H^0$. Now, the *hypersingular residual* is defined as

$$r = \frac{\partial\phi^{(1)}}{\partial\boldsymbol{n}} - \frac{\partial\phi^{(2)}}{\partial\boldsymbol{n}} \tag{31}$$

Then, starting with Eq. (31) and using Eqs. (28)–(30), one obtains

$$\begin{aligned} r &= \frac{\partial\phi^{(1)}}{\partial\boldsymbol{n}} - \left(\mathscr{M}_N \frac{\partial\phi^{(1)}}{\partial\boldsymbol{n}} + \mathscr{L}_N g \right) \\ &= \frac{\partial\phi}{\partial\boldsymbol{n}} - \left(\mathscr{M}_N \frac{\partial\phi}{\partial\boldsymbol{n}} + \mathscr{L}_N g \right) + e_q^{(1)} - \mathscr{M}_N e_q^{(1)} \\ &= (\mathscr{I} - \mathscr{M}_N) e_q^{(1)} \end{aligned} \tag{32}$$

We now present one of the central new results in this paper.

THEOREM 1. There are two real positive constants, such that

$$C_1 \|r\|_0 \leq \|e_q^{(1)}\|_0 \leq C_2 \|r\|_0$$

PROOF. The operators $(\mathcal{I} - \mathcal{M}_N)$ and $(\mathcal{I} - \mathcal{M}_N)^{-1}$ are linear and continuous. The result now follows from Lemma 1 and Eq. (32). □

REMARK 3. Theorem 1 provides a global result. It does not say anything about local errors. Similar considerations, in a different context, can be found in [27].

4.1.2. Error estimate for the iterate and 'superconvergence'

It is natural to question whether the iterate $(\partial\phi/\partial\boldsymbol{n})^{(2)}$ is more accurate than the primary approximation $(\partial\phi/\partial\boldsymbol{n})^{(1)}$. The use of iteration to improve convergence rates in integral equations of the second kind has been studied extensively and it is known that iteration for compact operators may often lead to 'superconvergence' [30]. *Previous iteration schemes in the literature use the same integral equation both for a first approximation and for the iterate. Note that the present iteration scheme uses the BIE for a first approximation and the HBIE for the iterate.* We now present a non-rigorous argument, which suggests that the iterate will indeed be superconvergent. By superconvergence, we mean that the iterate has a higher order of convergence than the primary solution. The error in the primary solution is defined by Eq. (30), and the error in the iterate is defined as

$$e_q^{(2)} = \frac{\partial\phi^{(2)}}{\partial\boldsymbol{n}} - \frac{\partial\phi}{\partial\boldsymbol{n}} \tag{33}$$

Then, starting with Eq. (33) and using Eqs. (28)–(30), one obtains

$$\begin{aligned} e_q^{(2)} &= \mathcal{M}_N \frac{\partial\phi^{(1)}}{\partial\boldsymbol{n}} + \mathcal{L}_N g - \frac{\partial\phi}{\partial\boldsymbol{n}} \\ &= \mathcal{M}_N\left(e_q^{(1)} + \frac{\partial\phi}{\partial\boldsymbol{n}}\right) + \mathcal{L}_N g - \frac{\partial\phi}{\partial\boldsymbol{n}} \\ &= \mathcal{M}_N e_q^{(1)} \end{aligned} \tag{34}$$

In the special case of the circle, $\mathcal{M}_N$ is a rank one operator, and all the Fourier basis functions, except the constant function, lie in its nullspace. Thus, $\mathcal{M}_N$ filters out all the oscillatory components in $e_q^{(1)}$. Assume that the error $e_q^{(1)}$ is of the form

$$e_q^{(1)}(\theta) \sim \epsilon_0 h^{s+\delta} + h^s \sum_{k=-\infty}^{\infty} \epsilon_k \, \mathrm{e}^{(\mathrm{i}k\theta)}$$

where h is the maximum element size in the mesh, s is the order of the approximation, and $\delta > 0$ (e.g. $\delta = 1$). Note that the constant term in the solution converges faster than the oscillatory terms. Then, it is clear that

$$\|e_q^{(2)}\| = \mathcal{O}(h^{s+\delta})$$

and it is globally superconvergent. We should also mention that our numerical experiments suggest that it is reasonable to suppose that the oscillatory part of the error is of a lower order than the constant component. The averaging nature of $\mathcal{M}_N$ depends on the smoothness of the boundary. For instance, if the boundary is C^∞, then the kernel of the integral operator $\mathcal{M}_N$ is C^∞. For a domain that is sufficiently smooth (C^r), we expect $\mathcal{M}_N$ to retain its averaging behaviour, and reduce the error, though not as dramatically. Further, this shows that the hypersingular residual, which is related to the error by Eq. (32), will track the error faithfully since the oscillatory components are lower than the constant component by $\mathcal{O}(h^\delta)$.

4.2. Problem 2: Interior Neumann

Another special case is now considered, the interior Neumann problem, which is stated as follows: Find ϕ on ∂B such that

$$\begin{aligned} &\Delta\phi = 0 \quad \text{in } \Omega \\ &\frac{\partial\phi}{\partial\boldsymbol{n}} = q \quad \text{on } \partial B \end{aligned} \tag{35}$$

Additionally, we assume that the boundary conditions satisfy the consistency condition

$$\int_{\partial B} q \, \mathrm{d}s = 0 \tag{36}$$

The BVP can be reformulated as an integral equation using the BIE (17), i.e.

$$(\mathcal{I} - \mathcal{K})\phi = \mathcal{V}q =: f_1 \tag{37}$$

The identity operator $\mathcal{I}$ is a pseudo-differential operator of order 0 and the operator $\mathcal{K}$ is compact (for C^1 boundaries). In particular, for the case of a circle, $\mathcal{K}$ is given by the definite integral in Eq. (20), and it smoothes the function. It can be shown that [10]

$$(\mathcal{I} - \mathcal{K}) : H^{\nu} \to H^{\nu}, \quad \forall\, \nu \in \boldsymbol{R} \tag{38}$$

The solution to the Neumann problem is arbitrary up to a constant, and to curtail this arbitrariness we work in the *restricted Sobolev space*

$$\mathring{H}^{\nu} := \left\{ v \in H^{\nu} \,|\, \int_{\partial B} \mathrm{d}s = 0 \right\} \tag{39}$$

The operator $(\mathcal{I} - \mathcal{K})$ is invertible in the space $\mathring{H}^0$ [10], and its inverse is continuous.

The HBIE for the Neumann problem is

$$-\mathcal{L}_N \phi = (\mathcal{M}_N - \mathcal{I})q =: f_2 \tag{40}$$

$\mathcal{L}_N$ is a hypersingular operator of order $+1$ and

$$\mathcal{L}_N : H^{\nu} \to H^{\nu-1}, \quad \forall\, \nu \in \boldsymbol{R}$$

$\mathcal{L}_N$ has a non-trivial nullspace, and to make it invertible we need to restrict the space as above. It is most natural to consider $\nu = 1/2$, and thus $\mathcal{L}_N : \mathring{H}^{1/2} \to \mathring{H}^{-1/2}$ continuously, with a continuous inverse. The notation f_1 and f_2 on the right hand side of Eqs. (37) and (40) is arbitrary at this point, however, this will become clear in the next Section on the mixed BVP.

Assume that the solution is smooth enough to lie in the space $\mathring{H}^{1/2}$, and that an approximate solution $\phi^{(1)} \in \mathring{H}^{1/2}$ to the BIE (37) has been found. The error in the primary approximation to the unknown ϕ is denoted by

$$e_{\phi}^{(1)} = \phi^{(1)} - \phi \tag{41}$$

An iteration scheme, similar to the one in the previous section, is employed here. Using the HBIE (18), one obtains

$$\frac{\partial \phi^{(2)}}{\partial \boldsymbol{n}} = \mathcal{M}_N q + \mathcal{L}_N \phi^{(1)} \tag{42}$$

The *hypersingular residual* is again defined as in Eq. (31), and thus

$$r = \frac{\partial \phi^{(1)}}{\partial \boldsymbol{n}} - \frac{\partial \phi^{(2)}}{\partial \boldsymbol{n}} = q - \frac{\partial \phi^{(2)}}{\partial \boldsymbol{n}} \tag{43}$$

i.e. in the Neumann problem, the hypersingular residual is the error in the iterate. Starting with Eq. (43), and using Eqs. (40)–(42), one obtains

$$\begin{aligned} r &= q - (\mathcal{M}_N q + \mathcal{L}_N \phi^{(1)}) \\ &= ((\mathcal{I} - \mathcal{M}_N)q - \mathcal{L}_N \phi) - \mathcal{L}_N e_{\phi}^{(1)} \\ &= -\mathcal{L}_N e_{\phi}^{(1)} \end{aligned} \tag{44}$$

An interesting alternative derivation of this equation is given in Appendix A.

THEOREM 2. There are two real positive constants, C_1 and C_2, such that

$$C_1\|r\|_{-1/2} \leq \|e_\phi^{(1)}\|_{1/2} \leq C_2\|r\|_{-1/2}$$

PROOF. Clearly, the error lies in $\mathring{H}^{1/2}$. Also, $\mathscr{L}_N : \mathring{H}^{1/2} \to \mathring{H}^{-1/2}$ is linear and continuous, with a continuous inverse. Use Lemma 1 with Eq. (44). □

REMARK 4. It is necessary to point out that in the Neumann problem the unknown is the potential but the error estimator is a difference in flux. In a computer code one would need to scale the potential and flux appropriately lest the difference in scale between these two quantities dominate the error estimate. Moreover, one should not expect a phenomenon of accelerated convergence. This does not occur because the flux is known a priori as the given Cauchy data. The role of the iterate here is just error estimation. As we have seen, $\mathscr{L}_N$ has the effect of amplifying the high frequencies. Thus, we anticipate that it will indeed be a good error estimator.

4.3. Problem 3: Mixed boundary value

The previous analyses for the particular problems, namely the interior Dirichlet and Neumann problems, can be extended to a mixed BVP. This is stated as follows: Find $\partial\phi/\partial\boldsymbol{n}$ on ∂B_1 and ϕ on ∂B_2 where $\partial B \equiv \partial B_1 + \partial B_2$ and

$$\begin{aligned} \Delta\phi &= 0 \quad && \text{in } \Omega \\ \phi &= g_1 && \text{on } \partial B_1 \\ \frac{\partial\phi}{\partial\boldsymbol{n}} &= g_2 && \text{on } \partial B_2 \end{aligned} \tag{45}$$

There is a genuine difficulty in the mixed boundary value problem, even for a smooth domain with C^∞ Cauchy data. This difficulty arises because of the change in boundary conditions from Dirichlet type to Neumann type for at least one point on the boundary, say z_0 with $z \in \boldsymbol{C}$. This gives rise to a singularity of the form $\mathscr{T}(z - z_0)^{1/2}$, where $\mathscr{T}$ denotes the imaginary part of the function. This could necessitate the inclusion of singular functions in the approximating space (see [42] and the references cited therein), but this is not common in engineering practice. The mixed BVP has been studied by, among others, Wendland et al. [23] for smooth domains, and Costabel and Stephan [24] for domains with corners. A *hard analysis* of this problem is quite imposing. Our goal here is to show that a simple error-hypersingular residual relation still results. That is, Eqs. (32) and (44) are special cases of a more general relation.

In the mixed BVP, the integral equations for the boundary unknowns are coupled because of the mixed boundary conditions. To rewrite the BIEs concisely, define the operators $\mathscr{V}_{ij}$ and $\mathscr{K}_{ij}$ as

$$\left(\mathscr{V}_{ij}\frac{\partial\phi}{\partial\boldsymbol{n}}\right)(P) := \int_{\partial B_j} G(P,Q)\frac{\partial\phi}{\partial\boldsymbol{n}}(Q)\,\mathrm{d}s_Q\,, \quad P \in \partial B_i \tag{46}$$

$$(\mathscr{K}_{ij}\phi)(P) := -\int_{\partial B_j} \frac{\partial G}{\partial\boldsymbol{n}}(P,Q)\phi(Q)\,\mathrm{d}s_Q\,, \quad P \in \partial B_i \tag{47}$$

Let $(\partial\phi/\partial\boldsymbol{n})_1$ and ϕ_2 denote the boundary unknowns $\partial\phi/\partial\boldsymbol{n}$ on ∂B_1 and ϕ on ∂B_2, respectively. Using the BIE (17) together with the operators defined in Eqs. (46) and (47), and imposing the boundary conditions on Eq. (45), one obtains

$$\begin{bmatrix} \mathscr{V}_{11} & \mathscr{K}_{12} \\ -\mathscr{V}_{21} & (\mathscr{I} - \mathscr{K}_{22}) \end{bmatrix} \begin{Bmatrix} \dfrac{\partial\phi}{\partial\boldsymbol{n}_1} \\ \phi_2 \end{Bmatrix} = \begin{bmatrix} (\mathscr{I} - \mathscr{K}_{11}) & -\mathscr{V}_{12} \\ \mathscr{K}_{21} & \mathscr{V}_{22} \end{bmatrix} \begin{Bmatrix} g_1 \\ g_2 \end{Bmatrix} \tag{48}$$

The mixed BVP consists of determining w such that (see [23])

$$\mathscr{A}w = f_1 \tag{49}$$

Note that $\mathscr{A}$ is the system matrix on the left-hand side, and f_1 is the known right-hand side of Eq. (48).

Moreover,

$$w = [w_1, w_2]^{\mathrm{T}}$$

where $w_1 \equiv (\partial\phi/\partial n)_1$, $w_2 \equiv \phi_2$, and T denotes the transpose of a matrix.

Similarly, to rewrite the HBIEs appropriately, define the operators $\mathcal{M}_{N_{ij}}$ and $\mathcal{L}_{N_{ij}}$ as

$$\left(\mathcal{M}_{N_{ij}} \frac{\partial\phi}{\partial n}\right)(P) := \int_{\partial B_j} \frac{\partial G}{\partial N}(P, Q) \frac{\partial\phi}{\partial n}(Q)\, \mathrm{d}s_Q\,, \quad P \in \partial B_i \tag{50}$$

$$(\mathcal{L}_{N_{ij}}\phi)(P) := -\int_{\partial B_j} \frac{\partial^2 G}{\partial N\, \partial n}(P, Q)\phi(Q)\, \mathrm{d}s_Q\,, \quad P \in \partial B_i \tag{51}$$

Using the HBIE (18) together with the operators defined in Eqs. (50) and (51), and imposing the boundary conditions on Eq. (45), one obtains

$$\begin{bmatrix} (\mathcal{I} - \mathcal{M}_{N_{11}}) & -\mathcal{L}_{N_{12}} \\ -\mathcal{M}_{N_{21}} & -\mathcal{L}_{N_{22}} \end{bmatrix} \begin{Bmatrix} \dfrac{\partial\phi}{\partial n_1} \\ \phi_2 \end{Bmatrix} = \begin{bmatrix} \mathcal{L}_{N_{11}} & \mathcal{M}_{N_{12}} \\ \mathcal{L}_{N_{21}} & -(\mathcal{I} - \mathcal{M}_{N_{22}}) \end{bmatrix} \begin{Bmatrix} g_1 \\ g_2 \end{Bmatrix} \tag{52}$$

A brief specification of the problem, analogous to the BIE case, consists of determining w such that (see [2])

$$\mathcal{B}w = f_2 \tag{53}$$

where $\mathcal{B}$ is the system matrix on the left-hand side, and f_2 is the known right-hand side of Eq. (52).

The linear systems obtained using the BIE and the HBIE for the mixed BVP are given by Eqs. (49) and (53), respectively. With both problems in the setting of linear operators, we note that $\mathcal{A}$ and $\mathcal{B}$ are continuous pseudodifferential operators of orders 0 and 1, respectively.

Now, the a posteriori error estimate for the mixed BVP can be defined. The derivations proceed in two basic steps. The first step consists of finding an approximate solution $w^{(1)}$ to the BIE,

$$w^{(1)} = [w_1^{(1)}, w_2^{(1)}]^{\mathrm{T}}$$

where $w_1^{(1)}$ denotes the calculated flux on ∂B_1, and $w_2^{(1)}$ denotes the calculated potential on ∂B_2.

The next step consists of *iterating* $w^{(1)}$ with the HBIE to find the corresponding approximation for the flux $(\partial\phi/\partial n)^{(2)}$

$$\begin{Bmatrix} \dfrac{\partial\phi^{(2)}}{\partial n_1} \\ \dfrac{\partial\phi^{(2)}}{\partial n_2} \end{Bmatrix} = \begin{bmatrix} \mathcal{L}_{N_{11}} & \mathcal{L}_{N_{12}} \\ \mathcal{L}_{N_{21}} & \mathcal{L}_{N_{22}} \end{bmatrix} \begin{Bmatrix} g_1 \\ w_2^{(1)} \end{Bmatrix} + \begin{bmatrix} \mathcal{M}_{N_{11}} & \mathcal{M}_{N_{12}} \\ \mathcal{M}_{N_{21}} & \mathcal{M}_{N_{22}} \end{bmatrix} \begin{Bmatrix} w_1^{(1)} \\ g_2 \end{Bmatrix} \tag{54}$$

The error in the approximation $w^{(1)}$ is given by

$$e^{(1)} := [e_1^{(1)}, e_2^{(1)}]^{\mathrm{T}} = w^{(1)} - w \tag{55}$$

Once again, the *hypersingular residual* is defined by Eq. (31), which is consistent with the previous problems (i.e. interior Dirichlet and interior Neumann). Then, starting with Eq. (31) and using Eqs. (54)–(55), one obtains

$$r = \begin{Bmatrix} r_1 \\ r_2 \end{Bmatrix} = \begin{Bmatrix} w_1 + e_1^{(1)} \\ g_2 \end{Bmatrix} - \begin{bmatrix} \mathcal{L}_{N_{11}} & \mathcal{L}_{N_{12}} \\ \mathcal{L}_{N_{21}} & \mathcal{L}_{N_{22}} \end{bmatrix} \begin{Bmatrix} g_1 \\ w_2 + e_2^{(1)} \end{Bmatrix} - \begin{bmatrix} \mathcal{M}_{N_{11}} & \mathcal{M}_{N_{12}} \\ \mathcal{M}_{N_{21}} & \mathcal{M}_{N_{22}} \end{bmatrix} \begin{Bmatrix} w_1 + e_1^{(1)} \\ g_2 \end{Bmatrix} \tag{56}$$

Assuming that the solution w is smooth enough, we expect that the BIE and HBIE will have the same solution. Again, using the HBIE relations and substituting them in Eq. (56), one obtains

$$r = \begin{Bmatrix} r_1 \\ r_2 \end{Bmatrix} = \begin{bmatrix} (\mathcal{I} - \mathcal{M}_{N_{11}}) & -\mathcal{L}_{N_{12}} \\ -\mathcal{M}_{N_{21}} & -\mathcal{L}_{N_{22}} \end{bmatrix} \begin{Bmatrix} e_1^{(1)} \\ e_2^{(1)} \end{Bmatrix} \tag{57}$$

which can be rewritten using Eqs. (52) and (53) as

$$r = \mathcal{B}e^{(1)} \tag{58}$$

where

$$\mathcal{B} = \begin{bmatrix} \mathcal{B}_{11} & \mathcal{B}_{12} \\ \mathcal{B}_{21} & \mathcal{B}_{22} \end{bmatrix} = \begin{bmatrix} (\mathcal{I} - \mathcal{M}_{N_{11}}) & -\mathcal{L}_{N_{12}} \\ -\mathcal{M}_{N_{21}} & -\mathcal{L}_{N_{22}} \end{bmatrix} \tag{59}$$

As expected, the term $\mathcal{B}_{11}$ is the same as obtained with the Dirichlet problem (see Eq. (32)), and the term $\mathcal{B}_{22}$ is the same as obtained with the Neumann problem (see Eq. (44)). The off-diagonal block terms $\mathcal{B}_{12}$ and $\mathcal{B}_{21}$ are the usual coupling terms which are present in a mixed BVP.

Equation (58) is the error-hypersingular residual relation for the mixed BVP. The operator $\mathcal{B}$ in this equation is the same system operator as in the HBIE (52). Although it has been demonstrated to be invertible in numerous numerical applications (e.g. [6,36,43,44]), a rigorous proof of its invertibility is difficult [10]. If we *assume* invertibility of $\mathcal{B}$, then it is clear that the error is globally bounded by the hypersingular residual (see Lemma 1). Thus, Eqs. (32) and (44) are now seen to be the limiting cases of Eq. (58).

5. Global bounds in a Galerkin scheme

The purpose of this section is to demonstrate the use of a standard argument in the FEM to find a tighter global bound on the error. The present argument follows Eriksson et al. [9], and it will demonstrate the utility of the error-residual relation, $r = \mathcal{B}e^{(1)}$, obtained in Eq. (58).

For the sake of simplicity, consider the Dirichlet problem reformulated as Symm's equation. The continuous problem consists of finding $w \in H^{-1/2}$ such that

$$\mathcal{V}w = (\mathcal{I} - \mathcal{K})g =: f_1$$

We shall assume that there is in fact a smoother solution than this, so that $w \in H^0$. The continuous hypersingular problem consists of finding $w \in H^0$ such that

$$(\mathcal{I} - \mathcal{M}_N)w = \mathcal{L}_N g =: f_2$$

From the smoothness assumption on w, both formulations have the same solution. Let us solve the BIE using a Galerkin rather than a collocation scheme. Denote the test space by $S_h^p \subset H^0$. Then, the discretized problem is formulated as follows: Find $w^{(1)} \in S_h^p$ such that

$$(\mathcal{V}w^{(1)}, v_h) = (f_1, v_h), \quad \forall v_h \in S_h^p$$

where $(\cdot, \cdot)$ denotes the L_2 inner product on ∂B. It can be easily shown that this implies

$$(\mathcal{V}e^{(1)}, v_h) = 0, \quad \forall v_h \in S_h^p$$

which is the *Galerkin orthogonality* relation. It is also common to represent the error in the solution using the solution to the dual problem, i.e. ψ such that $\mathcal{V}^*\psi = e^{(1)}$ [8,45].

THEOREM 3. Assume that the test space S_h^p satisfies an interpolation error estimate of the form

$$\|h^{-p}(\psi - \pi_h\psi)\|_0 \leq C_i\|D^p\psi\|_0 \tag{60}$$

where h is a parameter that measures the level of discretization, $\pi_h\psi$ is the interpolant of ψ in S_h^p, and D^p denotes derivatives of order p. Also, assume that we have a strong stability[5] estimate for the dual problem of the form

$$\|D^p\psi\|_0 \leq S_c\|e^{(1)}\|_0 \tag{61}$$

[5] One may refer to Eriksson et al. [9] for a definition of strong stability.

Then, the solution to the Galerkin approximation satisfies

$$\|w - w_h\|_0 \leq C\|h^p r\|_0$$

PROOF. The error is given by

$$\|e^{(1)}\|_0^2 = (e^{(1)}, e^{(1)}) = (e^{(1)}, \mathcal{V}^*\psi) = (\mathcal{V}e^{(1)}, \psi) \tag{62}$$

The use of the Galerkin orthogonality relation leads to

$$(\mathcal{V}e^{(1)}, \psi) = (\mathcal{V}e^{(1)}, \psi - \pi_h\psi) \tag{63}$$

Now, using the interpolation error estimate (60), and the strong stability estimate (61), one obtains

$$\|e^{(1)}\|_0^2 \leq S_c C_i \|h^p \mathcal{V}e^{(1)}\|_0 \|e^{(1)}\|_0 \tag{64}$$

The only new idea consists of using Eq. (32) and introducing the error-hypersingular residual relation $e^{(1)} = (\mathcal{I} - \mathcal{M}_N)^{-1} r$ at this step. Now, using the Cauchy–Schwarz inequality a couple of times and discounting the trivial case when the error is zero, one obtains the inequality

$$\|e^{(1)}\|_0 \leq C\|h^p r\|_0 \tag{65}$$

with $C = S_c C_i \|\mathcal{V}\| \|(\mathcal{I} - \mathcal{M}_N)^{-1}\|$. □

REMARK 5. The above proof shows that certain arguments used in earlier error-residual analyses may be extended with no difficulty to error-hypersingular residual relations. Ideally, we would have preferred to use the solution of the dual problem to the HBIE, to find a bound, but this is not possible since the Galerkin orthogonality that holds for the residual $\mathcal{V}e^{(1)}$, does not hold for the hypersingular residual $(\mathcal{I} - \mathcal{M}_N)e^{(1)}$.

6. Properties of the error estimates

Three properties of the present error estimation method are discussed below. These properties involve pseudolocality of pseudodifferential operators, symmetry of the basic error estimation process, and the use of iteration as a postprocessing technique in boundary integral methods. Moreover, the last two properties are inter-related, and indicate possible extensions of the present iteration scheme.

6.1. Pseudolocality

At this stage, global bounds on the error have been provided, but not local error indicators. However, numerical experiments on potential problems [5,6] suggest that the residual is, in fact, an excellent measure of the local error. This is a result of the pseudolocal property of the pseudodifferential operators. This property has been rigorously used by Yu and Wendland [15–18] to develop adaptive boundary elements for Galerkin, and some collocation schemes. Because of the singular nature of their kernels, the operators $\mathcal{A}$ and $\mathcal{B}$ have the property that when applied to a function peaked at a point P (think of a sharp Gaussian distribution around P), they cause it to decay sufficiently fast. The pseudolocal property is stronger for kernels of higher order of singularity, as shown by Wendland and Yu [15,16]. *This provides one of the principal justifications for preferring hypersingular residuals over the usual residuals.* As a visual illustration of the pseudolocal property, Fig. 1 shows the effect of a (hyper-)singular kernel on a peaked function with compact support.[6] The output is also seen to be predominantly local. However, it does not have local support, contrary to what is suggested in Fig. 1. On a log-scale plot, the entire boundary is seen to belong to the support of the output, as illustrated by Fig. 2.

In our context, the pseudolocal property is invoked in the sense that if the error has a local peak, then so does the residual. Nevertheless, what is truly important is the pseudolocality of the inverse operators. *Does a local*

[6] The action of the hypersingular kernel on this function is obtained by computing the Fourier series of the function, and then using the Fourier representation of the kernel.

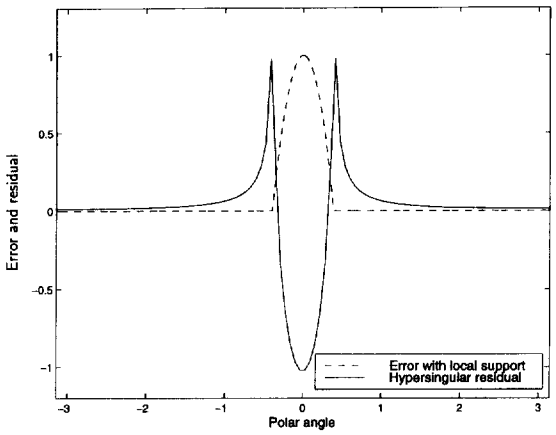

Fig. 1. Demonstration of *pseudolocality*—action of the hypersingular kernel on a function with compact support. Here, the initial function ('error') is $f(x) = 1 - (x/\delta)^2$, where $\delta = \pi/8$; and $f(x) = 0$ if $|x| > \delta$.

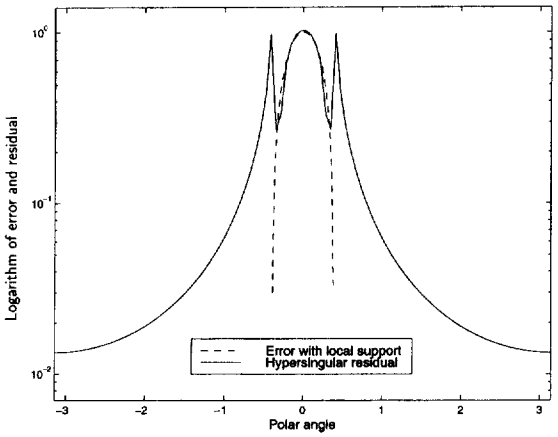

Fig. 2. Demonstration of *pseudolocality*—the operators are not local because the support of the output function is not contained in the support of the input function.

peak in the residual mean that the error is local? As stated above, a local error implies a local residual, but the converse is not clear. In a discretized setting, one could point out this difficulty by noting that the inverse of a tridiagonal matrix is not necessarily tridiagonal. At present, we do not have analytical justification for the converse argument, which is the most important result, but rely instead on numerical evidence. Several computational experiments [5,7] do suggest that the hypersingular residual is in fact a good local measure of the error as well.

6.2. Symmetry of the formulation and iterated BIE

The symmetry of the error estimation method was first realized by Paulino et al. [5,6]. In fact, as noted there, this is a very natural and appealing feature of the method. The method rests on the fact that the amount by which the approximate solution to the BIE fails to satisfy the HBIE is related to the discretization error in the primary approximate solution. Next, it is shown that the formulation is indeed symmetric, i.e. *if the primary approximation is found by solving the HBIE, and if this approximation is iterated with the BIE, then the residual*

$$\tilde{r} = \phi^{(1)} - \phi^{(2)} = \phi|_{\mathrm{HBIE}} - \phi|_{\mathrm{BIE}} \tag{66}$$

is an error indicator for the HBIE solution. Consider the mixed BVP given by Eq. (45), and the formulation given by Eq. (53). Let $w^{(1)}$ be an approximation to this solution. The following iterated approximation can be formed

$$\begin{Bmatrix} \phi_1^{(2)} \\ \phi_2^{(2)} \end{Bmatrix} = \begin{bmatrix} \mathscr{K}_{11} & \mathscr{K}_{12} \\ \mathscr{K}_{21} & \mathscr{K}_{22} \end{bmatrix} \begin{Bmatrix} g_1 \\ w_2^{(1)} \end{Bmatrix} + \begin{bmatrix} \mathscr{V}_{11} & \mathscr{V}_{12} \\ \mathscr{V}_{21} & \mathscr{V}_{22} \end{bmatrix} \begin{Bmatrix} w_1^{(1)} \\ g_2 \end{Bmatrix} \tag{67}$$

and it may be verified that

$$\tilde{r} \overset{\text{defn}}{=} \phi^{(1)} - \phi^{(2)} = \mathscr{A} e^{(1)} \tag{68}$$

where $\mathscr{A}$ is given in Eq. (49). If invertibility of $\mathscr{A}$ is assumed, then the error is globally bounded by the residual (see Lemma 1).

While the symmetry property of the present error estimation method provides an alternative definition for the residuals as given by Eq. (66), it is essential for error estimation in the symmetric-Galerkin BEM. In this method, both the BIE (17) and the HBIE (18) are used in the solution of the BVP, the choice being dictated by the prescribed boundary condition [46,47]. Therefore, in the error estimation process, the use of either Eq. (31) or Eq. (66) is also dictated by the type of boundary condition. Error estimation and adaptive calculations using the symmetric-Galerkin BEM can be found in [48].

6.3. Iteration as a postprocessing step

Iterated boundary integral methods can be found, for example, in [30,49–51]. As remarked earlier, iteration in Fredholm equations of the second kind, and some singular integral equations, has been known to result in *superconvergence*. One may refer to the article by Sloan for an elegant exposition [30], where various iteration schemes are developed using the same integral equation both for a first approximation and for the iterate. In contrast, our iteration scheme is of a different nature, in the sense that it is a 'two-level' scheme, i.e. the equation used for the initial solution and the equation used for iteration are not the same. In the present work, the BIE has been used for the initial solution and the HBIE has been used for the iterate. In addition, the above property on symmetry of the formulation points out that the role of the two integral equations can be interchanged. To the authors' knowledge, our iteration scheme does not appear to have been studied theoretically earlier.

Three examples from the literature on iterated integral equations are given next.

- Golberg and Bowman [28] have used the superconvergence of the Sloan iterate [29] to show the asymptotic equivalence of the error and residual. They have used Galerkin methods, standard iteration schemes (i.e. using the same integral equation for a first approximation and for the iterates) and usual residuals in their work.
- Tran [52] has used the K-operator and has shown how it can lead to superconvergence. Perhaps our present approach to the Dirichlet problem can also be viewed in this context.
- Numerical results due to Guiggiani [44] show that for two-dimensional elasticity problems, one can obtain high pointwise convergence using the HBIE as a postprocessing step to calculate traction. This is surprising since the kernels in the elasticity HBIE are Cauchy singular and hypersingular. There is no obvious reason to expect that they would smooth out the error when used for postprocessing.

7. Numerical examples

Four numerical examples are presented which demonstrate that the hypersingular residual tracks the local error effectively, and thus it can be used as a basis for an adaptive scheme. A Galerkin boundary element method on a circular domain has been implemented using the computer software MATLAB.[7] For this simple geometry, the discretized kernels can be computed with arbitrarily high accuracy from their representations as infinite series, i.e. there are no errors in quadrature. Also, since the geometry is represented exactly, essentially all errors are due to discretization of the function space. The calculation of the hypersingular kernels follows a method due to Yu [40], and the implementation for the BIE can be considered a straightforward extension of this method. The partition of the boundary is uniform for most experiments, except in the last example where an h-adaptive scheme is considered.

For the circular boundary, a uniform partition of the interval $[0, 2\pi]$ in N elements is considered. Note that this partition also identifies the endpoints of the elements. The basis function employed here are the 'hat functions' H_i defined by

$$\begin{aligned} H_i(\theta) &= \frac{1}{\Delta}(\theta - \theta_{i-1}), \quad \theta_{i-1} \leqslant \theta \leqslant \theta_i \\ &= \frac{1}{\Delta}(\theta_{i+1} - \theta), \quad \theta_i \leqslant \theta \leqslant \theta_{i+1} \end{aligned} \tag{69}$$

where

$$\Delta = 2\pi/N \tag{70}$$

The approximations for the potential and flux are

[7] MATLAB is a registered trademark of The MathWorks Inc.

$$\phi^{(1)} = \sum_{i=1}^{N} \phi|_i H_i \quad \text{and} \quad \frac{\partial \phi^{(1)}}{\partial \boldsymbol{n}} = \sum_{i=1}^{N} \frac{\partial \phi}{\partial \boldsymbol{n}}\bigg|_i H_i \tag{71}$$

respectively.

REMARK 6. The iterate is not constrained to lie in the approximating subspace. In the present computations, the iterate has been calculated at numerous internal points. This has the advantage of revealing the oscillatory nature of the error and hypersingular residual.

7.1. Dirichlet problems

The Galerkin approximation for the Dirichlet problem, in discretized form, is

$$\sum_{i=1}^{N} (\mathscr{V} H_i, H_j) \frac{\partial \phi}{\partial \boldsymbol{n}}\bigg|_i = \sum_{i=1}^{N} ((\mathscr{J} - \mathscr{K}) H_i, H_j) \phi|_i, \quad j = 1, \ldots, N \tag{72}$$

As before, $(\cdot, \cdot)$ refers to the L_2 inner product. The above can be rewritten as

$$\mathscr{A} w^{(1)} = f_1$$

where $\mathscr{A} \in \boldsymbol{R}^{N \times N}$ and $f_1 \in \boldsymbol{R}^N$.

Owing to the circular symmetry, the matrices have a very special structure; they are Toeplitz and circulant, and can be represented using a single vector, i.e.

$$(\mathscr{V} H_i, H_j) = A_{ij} = A_{ji} = A_{|i-j|} := a_k, \quad \text{where } k = |i - j| \tag{73}$$

Using the Fourier representations of the kernels and the integrals in Appendix B, one may show that

$$a_k = \frac{\alpha}{\pi}\left[\frac{16}{\Delta^2} \sum_{n=1}^{\infty} \frac{1}{n^5} \sin^4\left(\frac{n\Delta}{2}\right) \cos nk\Delta - \Delta^2 \log \alpha\right] \tag{74}$$

where $\Delta = 2\pi/N$ is the mesh width. One could use the 'fast Fourier transform' (FFT) to solve this system, but this is unnecessary for the simple examples we consider.

REMARK 7. The above discretization procedure illustrates two difficulties inherent in the direct BEM for the Dirichlet problem. One may write $\mathscr{A}$ in matrix form as

$$A = S - \frac{\Delta^2 \alpha \log \alpha}{\pi} \begin{bmatrix} 1 & \cdots & 1 \\ \vdots & \vdots & \vdots \\ 1 & \cdots & 1 \end{bmatrix} \tag{75}$$

where S has components S_{ij} and it refers to the summation term in Eq. (74). The first difficulty arises when $\alpha = 1$, in which case $A \equiv S$ is singular. This follows from Remark 2 on the transfinite diameter. This problem can be avoided by scaling the dimensions of the body suitably. The second difficulty is the fact that $\mathscr{A}$ becomes nearly singular as the mesh is refined, i.e. as $\Delta = 2\pi/N \to 0$. Thus, the linear system becomes ill-conditioned. This is often a problem with equations of the first kind.

7.1.1. Example 1

Consider a circular domain and the harmonic function $\phi = Cr^2 \sin 2\theta$, where (r, θ) denotes polar coordinates and C is a constant. The flux is given by $\partial\phi/\partial\boldsymbol{n} = 2Cr \sin 2\theta$. Here, $r = 5$ so that $\phi = 25C \sin 2\theta$ and $\partial\phi/\partial\boldsymbol{n} = 10C \sin 2\theta$. Choosing $C = 1/5$, one readily obtains $\phi = 5 \sin 2\theta$ and $\partial\phi/\partial\boldsymbol{n} = 2 \sin 2\theta$. Thus, $\phi_{\max} = 5$, and $\partial\phi/\partial\boldsymbol{n}|_{\max} = 2$, where $\phi_{\max}$ denotes the actual maximum potential, and $\partial\phi/\partial\boldsymbol{n}|_{\max}$ denotes the actual maximum flux (on the boundary). Consistent units are used. This is the reference solution which will be used in the first three examples.

As described above, a circle of radius 5 is considered with the analytic boundary conditions $g = 5 \sin 2\theta$. The exact solution for the boundary flux is $\partial\phi/\partial\boldsymbol{n} = 2 \sin 2\theta$. In this case, the iterate is easily computed. Using the Fourier representation of $\mathscr{L}_N$, one may show that $\mathscr{L}_N g = 2 \sin 2\theta$. Fig. 3 shows the computed solution and the

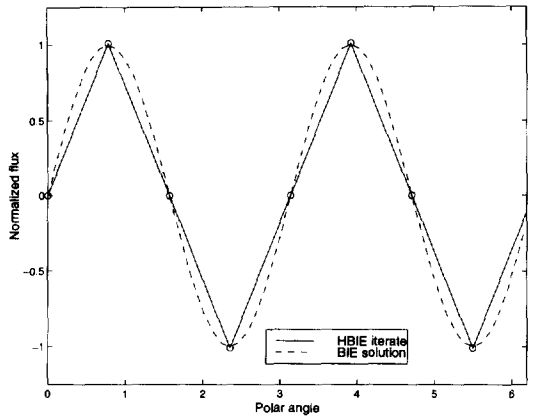

Fig. 3. Comparison of primary and iterated solutions (8 nodes). The flux is normalized with respect to $\partial\phi/\partial n|_{\max} = 2$ units.

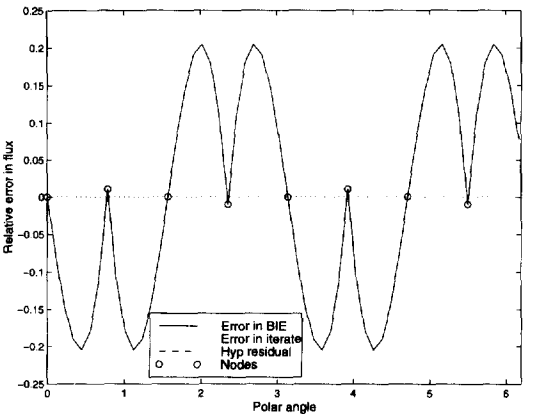

Fig. 4. Error in the primary solution (Eq. (30)), error in the iterate (Eq. (33)), and hypersingular residual (Eq. (31)) considering 8 nodes on the boundary. The 'relative error in flux' is the dimensionless quantity obtained by dividing the error (or residual) by the actual maximum value of the flux (here, $\partial\phi/\partial n|_{\max} = 2$ units). Note that the 'Error in BIE' and 'Hyp residual' curves agree within plotting accuracy.

iterate. Fig. 4 shows the comparison between the errors (in the BIE and in the iterate) and the hypersingular residual. The error in the iterate is near machine precision, indicating superconvergence. Consequently, the error and the hypersingular residual are practically identical, and therefore are indistinguishable on the plot. It is worth mentioning that the accuracy of the iterate is mainly due to the fact that the computation of $\mathscr{L}_N g = 2\sin 2\theta$ is exact. If there are interpolation errors in the boundary conditions, then the operator $\mathscr{L}_N$ increases them, counteracting the smoothing effect of $\mathscr{M}_N$, as shown in the next example.

7.1.2. Example 2

It is rare that one knows the boundary conditions exactly, as in the previous example. Consider now the discretized boundary conditions of the form $g = \Sigma_{i=1}^{N} H_i\phi|_i$ where $\phi|_i = 5\sin 2\theta_i$. The term $\mathscr{L}_N g$ is computed using the Fourier representation. This is not a fast computation since one has to sum a series that behaves as $1/n$. Figs. 5 and 6 show the exact solution, the primary approximation, and the iterate for different discretizations. It is clear from these figures that there is no superconvergence of the iterate. The smoothing effect of $\mathscr{M}_N$ is counteracted by $\mathscr{L}_N$, which amplifies the discretization errors in the boundary conditions. Nevertheless, because of the circular geometry and the uniform mesh, the errors in ϕ and $\partial\phi/\partial n$ have the same

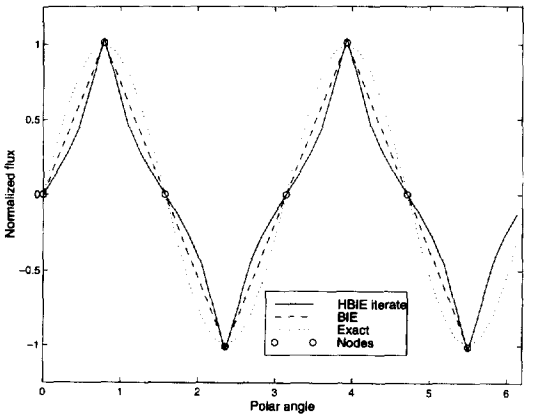

Fig. 5. Comparison of primary and iterated solution (8 nodes). The flux is normalized with respect to $\partial\phi/\partial n|_{\max} = 2$ units.

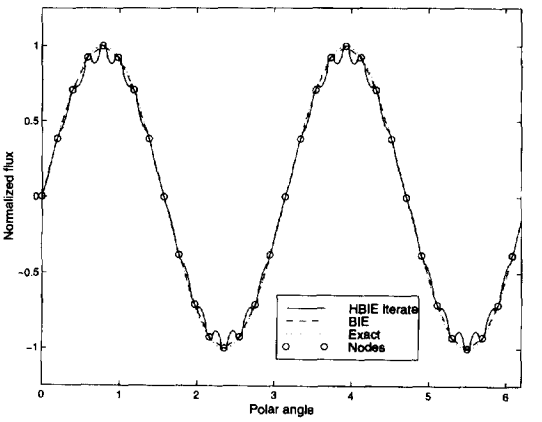

Fig. 6. Comparison of primary and iterated solution (32 nodes). The flux is normalized with respect to $\partial\phi/\partial n|_{\max} = 2$ units.

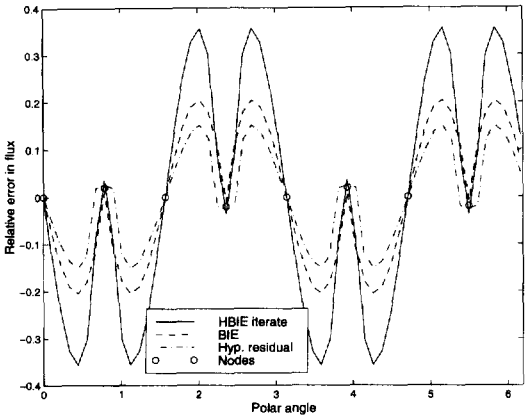

Fig. 7. Error in the primary solution (Eq. (30)), error in the iterate (Eq. (33)), and hypersingular residual (Eq. (31)) considering 8 nodes on the boundary. The error (or residual) is normalized with respect to $\partial\phi/\partial n|_{\max} = 2$ units.

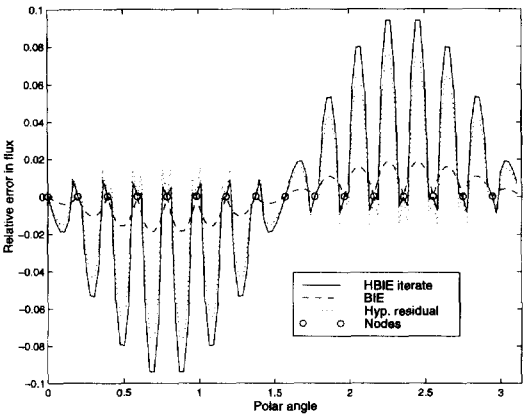

Fig. 8. Error in the primary solution (Eq. (30)), error in the iterate (Eq. (33)), and hypersingular residual (Eq. (31)) considering 32 nodes on the boundary. The error (or residual) is normalized with respect to $\partial\phi/\partial n|_{\max} = 2$ units.

harmonics, and hence the hypersingular residual tracks the primary error faithfully as shown by Figs. 7 and 8. Fig. 9 presents the information of Fig. 8 on a log-scale and, because of symmetry, both of these plots only show part of the boundary. It is apparent that there is still superconvergence at the nodes.

7.2. Neumann problems

For a Neumann problem, the approximating space $S_h^p \subset \mathring{H}^{1/2}$. In the discretized setting, this leads to

$$\int_{-\pi}^{\pi} \sum_{i=1}^{N} v_i H_i \, d\theta = 0 \tag{76}$$

i.e. $\Sigma_{i=1}^{N} v_i = 0$. This means that the constant term in the Fourier expansion of any function $v \in \mathring{H}^{1/2}$ is zero. Also, recall that the boundary condition must satisfy the consistency condition given by Eq. (36). Hence,

$$\int_{-\pi}^{\pi} \phi \, d\theta = \int_{-\pi}^{\pi} q(\theta) \, d\theta = 0 \tag{77}$$

Noting these restrictions, one obtains the Galerkin approximation for the Neumann problem,

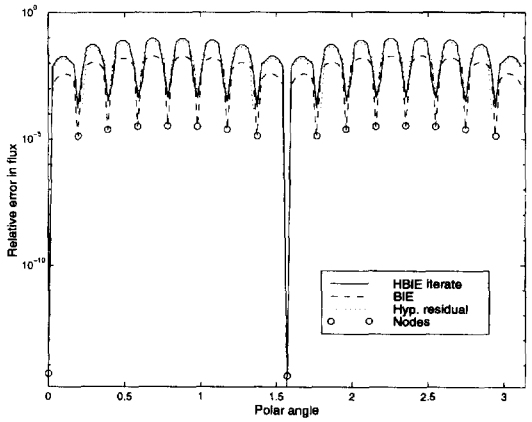

Fig. 9. Error in the primary solution, error in the iterate, and hypersingular residual on a logarithmic scale (32 nodes).

$$\sum_{i=1}^{N} ((\mathscr{I} - \mathscr{K})H_i, H_j)\phi|_i = \sum_{i=1}^{N} (\mathscr{V}H_i, H_j)\frac{\partial \phi}{\partial \boldsymbol{n}}\Big|_i \quad j = 1, \ldots, N \tag{78}$$

As before, $(\cdot, \cdot)$ refers to the L_2 inner product. Since $\mathscr{K}$ is simply the averaging operator, the use of the constraint on ϕ (see Eq. (77)) leads to $\mathscr{K}\phi = 0$. Thus, the Galerkin approximation of the BIE reduces to

$$\sum_{i=1}^{N} (H_i, H_j)\phi|_i = \sum_{i=1}^{N} (\mathscr{V}H_i, H_j)\frac{\partial \phi}{\partial \boldsymbol{n}}\Big|_i, \quad j = 1, \ldots, N \tag{79}$$

which can be written as

$$\mathscr{A}w^{(1)} = f_1$$

Note that the boundary conditions have been discretized. Moreover, the matrix A is circulant, and for linear shape functions it is given by

$$A = \frac{\Delta}{6}\begin{bmatrix} 4 & 1 & \cdots & 1 \\ 1 & 4 & 1 & \cdots \\ \vdots & & & \vdots \\ 1 & \cdots & 1 & 4 \end{bmatrix} \tag{80}$$

The hypersingular iterate given by Eq. (42) becomes

$$\frac{\partial \phi^{(2)}}{\partial \boldsymbol{n}} = \mathscr{M}_N q + \mathscr{L}_N \phi^{(1)} = \mathscr{L}_N \phi^{(1)} \tag{81}$$

Now the Fourier representation of $\mathscr{L}_N$ can be used to calculate the iterate. As discussed before, in the error-hypersingular residual relation of Eq. (44), $\mathscr{L}_N$ has the effect of amplifying the higher frequencies, and the hypersingular residual is expected to track the error effectively. Indeed, this is what the numerical experiments reveal.

7.2.1. Example 3

Consider the boundary conditions $\partial\phi/\partial\boldsymbol{n} = 2\sin 2\theta$ on a circle of radius 5. The unique solution in $\mathring{H}^{1/2}$ is $\phi = 5\sin 2\theta$. Figs. 10 and 11 show the comparison between the iterated flux and the exact flux for different discretizations. It is clear that the iterate does not converge faster than the primary approximation. $\mathscr{L}_N$ has the effect of amplifying errors instead of smoothing them, and one does not expect the iterate to converge faster. The residual does track the error as illustrated by Figs. 12 and 13. Note that in these figures, the error in *potential* for the primary solution is being compared with the *residual in flux*. However, as shown in Appendix A, the same error-hypersingular residual relation of Eq. (44) also results by using the residual in potential (see

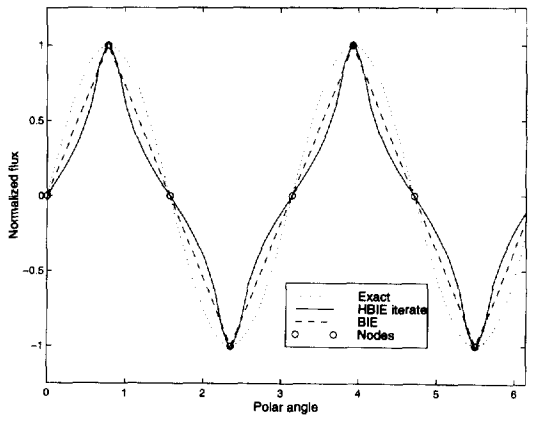

Fig. 10. Exact and iterated flux (8 nodes). The flux is normalized with respect to $\partial\phi/\partial\boldsymbol{n}|_{\max} = 2$ units.

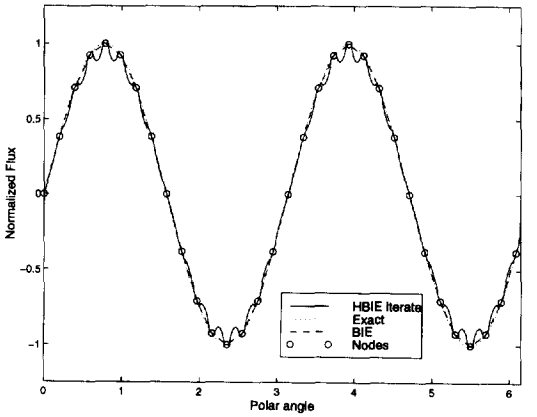

Fig. 11. Exact and iterated flux (32 nodes). The flux is normalized with respect to $\partial\phi/\partial\boldsymbol{n}|_{\max} = 2$ units.

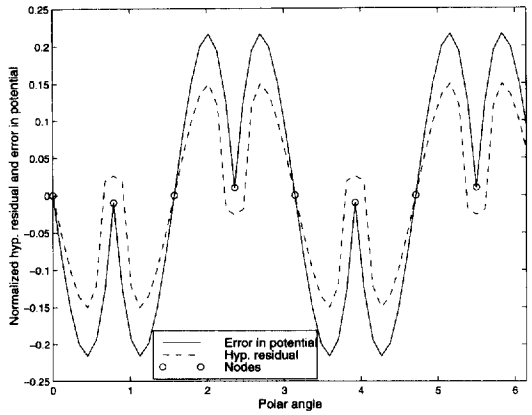

Fig. 12. Error in potential (Eq. (41)) and flux residual (Eq. (43)) considering 8 nodes on the boundary. The error in potential is normalized with respect to $\phi|_{\max} = 5$ units and the hypersingular residual is normalized with respect to $\partial\phi/\partial n|_{\max} = 2$ units.

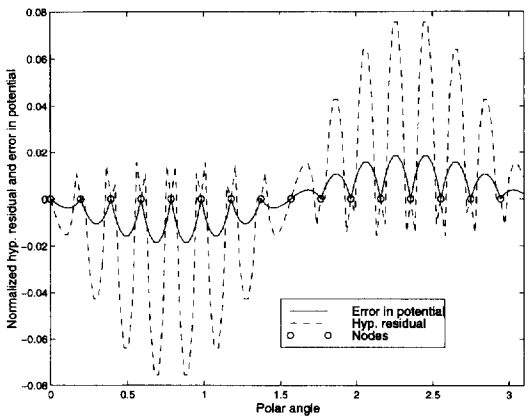

Fig. 13. Error in potential (Eq. (41)) and flux residual (Eq. (43)) considering 32 nodes on the boundary. The error in potential is normalized with respect to $\phi|_{\max} = 5$ units and the hypersingular residual is normalized with respect to $\partial\phi/\partial n|_{\max} = 2$ units.

Eq. (A.3)) to derive this relation. In summary, notice that although our analytical results provide only global bounds, the numerical experiments strongly suggest that the hypersingular residual and error are closely related locally. In the Neumann problem the hypersingular residual is related to the error through an operator of order $+1$, and hence it has 'high' pseudolocality.

7.2.2. Example 4

This example is distinct from the previous ones in the sense that it has a physical singularity on the boundary. Consider a Neumann problem on the unit disk. The exact solution is $\phi = \Re\sqrt{z-1}$, where $\Re$ denotes the real part of the function. The flux $\partial\phi/\partial n$ is singular at $z = 1 + 0i$. Fig. 14 shows a comparison between exact and computed solutions for the potential. The computed solution matches the calculated one quite well, with a slight discrepancy near the singular point. Fig. 15 shows a comparison between the hypersingular iterate and the exact flux. The flux is singular at $\theta = 0$. As expected, the iterate is unable to capture the singularity and oscillates near the singularity. Moreover, for this specific problem, the effect of the singularity seems to spread through the whole boundary and the iterated flux oscillates mildly even far from the singularity. The hypersingular residual has been observed to track the error locally, but this plot has not been included here. Instead, error indicators η_j on each boundary element ∂B_j are defined as

$$\eta_j = \|r\|_{H^0(\partial B_j)} = \|r\|_{L_2(\partial B_j)}$$

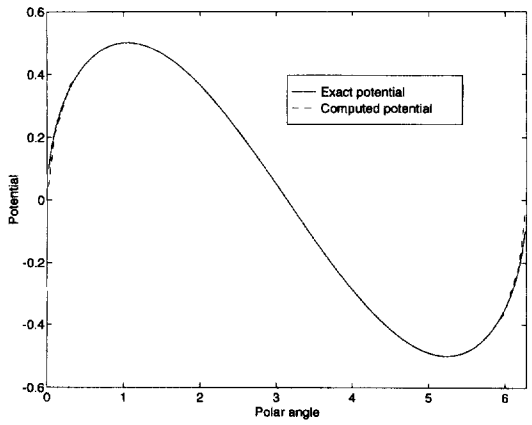

Fig. 14. Exact and computed potential (32 nodes).

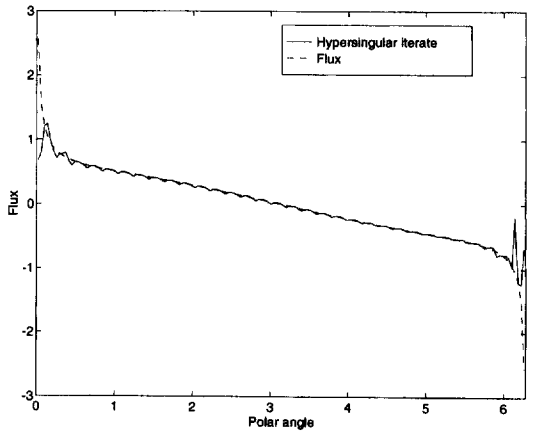

Fig. 15. Hypersingular iterate and exact flux (32 nodes).

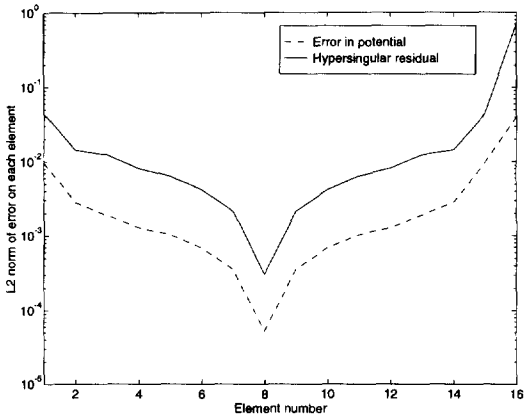

Fig. 16. Element error indicators (16 nodes and 16 elements).

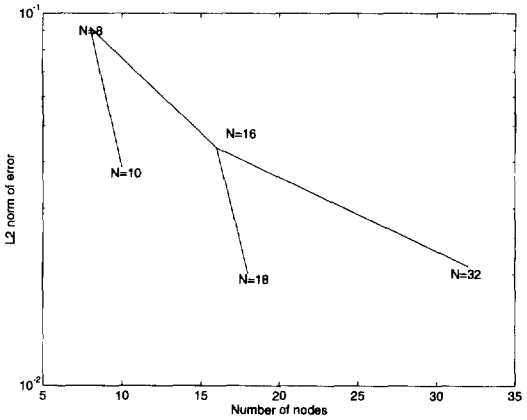

Fig. 17. Performance of adaptive and uniform meshes.

Fig. 16 shows the comparison between the element error indicators (using hypersingular residuals) and the error. These element error indicators may be used as the basis for an h-adaptive mesh refinement scheme. For instance, elements in which the error indicator is higher than some threshold value can be partitioned. In Fig. 17, the element with the highest error indicator is trisected. It is clear that the adaptive refinement leads to higher convergence rates than the uniform refinement. This simple example demonstrates that the hypersingular residual error estimates have potential applications in adaptivity.

8. Conclusions and extensions

A novel iteration scheme, using integral equations, has been used to assess discretization errors in the BEM. The basic iteration scheme consists of using the BIE for solving the BVP and iterating this solution with the HBIE. A residual is defined as the difference in the derivative quantities, and this residual is used as a BEM error estimate. Linear error-hypersingular residual relations have been developed for Dirichlet and Neumann problems, which are special cases of the general relation for the mixed boundary value problem. Four numerical examples, involving Galerkin boundary elements, have been presented. These examples illustrate important features of the error estimation method, e.g. they show that the iterate does not lie in the approximating space and that the hypersingular residual may also be used in adaptive calculations (e.g. [48]).

There are limitations in the theory presented here in the sense that non-smooth domains have not been considered, and the mixed BVP does deserve a more rigorous analysis. The mathematical analysis of these problems is quite difficult, especially for collocation methods. As remarked by Sloan [10, p. 331], 'it is fair to say that even for plane problems corners still present many theoretical challenges.' It is only recently that error estimates for Galerkin boundary integral methods on non-smooth domains have begun to appear [19–21,24,25]. However, numerical results for the two-dimensional Laplace equation on mixed BVP with corners indicate that the hypersingular residuals do provide reliable error estimates [5].

Several interesting topics associated with this work deserve further study. For example, these topics include: (a) analysis of hypersingular residual error estimates for mixed BVP in both smooth and non-smooth domains; (b) investigation of the symmetry property of Section 6.2 for error estimation in collocation methods and in the symmetric-Galerkin BEM; (c) theoretical and computational investigation of the 'two-level' iteration scheme as a general postprocessing technique in the BEM; (d) generalization of the hypersingular residual error estimates to other elliptic partial differential equations which admit formulations in terms of boundary integral equations; and (e) investigation of three-dimensional problems and use of the error estimates as driving parameters for adaptive mesh refinement algorithms. *We feel that the range of application of hypersingular residual error estimates in BEM is broad, and that these estimates, together with self-adaptive procedures, seem promising for applications to actual engineering problems. Finally, we hope that the new iteration scheme for boundary integral methods ('two-level' scheme), presented in this paper, will find further applications and use in both the mathematical and engineering fields.*

Acknowledgments

Prof. Paulino acknowledges the support from National Science Foundation under Grant No. CMS-9713008. The authors thank Prof. Lars Wahlbin, Department of Mathematics, and Prof. Steven Vavasis, Department of Computer Science, both from Cornell University, for elucidating discussions on the content of this paper. The idea behind the superconvergence argument of Section 4.1.2 is due to Prof. Wahlbin.

Appendix A. Neumann problem revisited

An alternative derivation of Eq. (44) is presented here. The derivation is carried out within the context of Section 4.2. By adding and subtracting the term $\mathcal{I}\phi$ on the left-hand side of Eq. (40), one obtains

$$\phi = (\mathcal{L}_N + \mathcal{I})\phi - (\mathcal{I} - \mathcal{M}_N)q \tag{A.1}$$

The solution $\phi^{(1)}$, obtained with the BIE (37), can be iterated with the HBIE (A.1) to obtain the approximate solution $\phi^{(2)}$, i.e.

$$\phi^{(2)} = (\mathcal{L}_N + \mathcal{I})\phi^{(1)} - (\mathcal{I} - \mathcal{M}_N)q \tag{A.2}$$

Now the *hypersingular residual* is redefined in terms of the potential as

$$r = \phi^{(1)} - \phi^{(2)} \tag{A.3}$$

which is a different definition from the one in Eq. (31). Also note that Eqs. (66) and (A.3) have different meaning. Starting with Eq. (A.3) and using Eqs. (40), (41) and (A.2), one obtains

$$\begin{aligned} r &= \phi^{(1)} - (\mathcal{L}_N + \mathcal{I})\phi^{(1)} + (\mathcal{I} - \mathcal{M}_N)q \\ &= e_\phi^{(1)} + \phi - (\mathcal{L}_N + \mathcal{I})(e_\phi^{(1)} + \phi) + (\mathcal{I} - \mathcal{M}_N)q \\ &= -\mathcal{L}_N e_\phi^{(1)} \end{aligned} \tag{A.4}$$

which is the same as Eq. (44). It is interesting to note that with two different definitions of the hypersingular residual, Eqs. (43) and (A.3), the relationship between the residual and the error remains the same.

Appendix B. Some useful integrals

The following integrals are useful in discretizing the kernels for the Galerkin BEM on a circle. The parameter Δ has been defined in Eq. (70).

$$\int_{-\pi}^{\pi} H_i(\tilde{\theta}) \cos k(\tilde{\theta} - \theta)\, \mathrm{d}\tilde{\theta} = \frac{4}{k^2\Delta} \sin^2 \frac{k\Delta}{2} \cos k(\theta_i - \theta)$$

$$\int_{-\pi}^{\pi} H_i(\tilde{\theta}) \sin k(\tilde{\theta} - \theta)\, \mathrm{d}\tilde{\theta} = -\frac{4}{k^2\Delta} \sin^2 \frac{k\Delta}{2} \sin k(\theta_i - \theta)$$

$$\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} H_i(\tilde{\theta}) H_j(\theta) \cos k(\tilde{\theta} - \theta)\, \mathrm{d}\tilde{\theta}\, \mathrm{d}\theta = \frac{16}{k^4\Delta^2} \sin^4 \frac{k\Delta}{2} \cos k(\theta_i - \theta_j)$$

$$\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} H_i(\tilde{\theta}) H_j(\theta) \sin k(\tilde{\theta} - \theta)\, \mathrm{d}\tilde{\theta}\, \mathrm{d}\theta = \frac{16}{k^4\Delta^2} \sin^4 \frac{k\Delta}{2} \sin k(\theta_i - \theta_j)$$

References

[1] P.K. Banerjee, The Boundary Element Methods in Engineering, 2nd edition (McGraw Hill, London, 1994).

[2] W.L. Wendland, Strongly elliptic boundary integral equations, in: A. Iserles and M.J.D. Powell, eds., The State of the Art in Numerical Analysis, Vol. 9 of New Series (Oxford University Press, 1987) 511–562.

[3] G. Krishnasamy, F.J. Rizzo and T.J. Rudolphi, Hypersingular boundary integral equations: Their occurrence, interpretation, regularization and computation, in: P.K. Banerjee and S. Kobayashi, eds., Developments in Boundary Element Methods, Vol. 7, Chap. 6 (Elsevier Applied Science, London and New York, 1992) 207–252.
[4] M. Tanaka, V. Sladek and J. Sladek, Regularization techniques applied to boundary element methods, Appl. Mech. Rev. 47(10) (1994) 457–499 (cites 350 references).
[5] G.H. Paulino, Novel formulations of the boundary element method for fracture mechanics and error estimation, Ph.D. Thesis, Cornell University, 1995.
[6] G.H. Paulino, L.J. Gray and V. Zarikian, Hypersingular residuals—A new approach for error estimation in the boundary element method, Int. J. Numer. Methods Engrg. 39(12) (1996) 2005–2029.
[7] G. Menon, Hypersingular error estimates in boundary element methods, Master's Thesis, Cornell University, 1996.
[8] P.G. Ciarlet, Basic error estimates for elliptic problems, in: P.G. Ciarlet and J.L. Lions, eds., Finite Element Methods (Part 1), Vol. 2 of Handbook of Numerical Analysis (Elsevier Science Publishers B.V., 1991).
[9] K. Eriksson, D. Estep, P. Hansbo and C. Johnson, Introduction to adaptive methods for differential equations, in: A. Iserles, ed., Acta Numerica 1995, Chap. 3 (Cambridge University Press, 1995) 105–158.
[10] I.H. Sloan, Error analysis in boundary integral methods, in: A. Iserles, ed., Acta Numerica 1992, Chap. 7 (Cambridge University Press, 1992) 287–339.
[11] E. Kita and N. Kamiya, Recent studies on adaptive boundary element methods, Adv. Engrg. Software 19 (1994) 21–32.
[12] S. Liapis, A review of error estimation and adaptivity in the boundary element method, Engrg. Anal. Boundary Elem. 14(4) (1995) 315–323.
[13] G.H. Paulino, F. Shi, S. Mukherjee and P. Ramesh, Nodal sensitivities as error estimates in computational mechanics, Acta Mech. 121(1–4) (1997) 191–213.
[14] E. Rank, Adaptive *h*-, *p*- and *hp*-versions for boundary integral element methods, Int. J. Numer. Methods Engrg. 28(6) (1989) 1335–1349.
[15] W.L. Wendland and D.-H. Yu, Adaptive boundary element methods for strongly elliptic integral equations, Numer. Math. 53 (1988) 539–558.
[16] W.L. Wendland and D.-H. Yu, A posteriori local error estimates of boundary element methods with some pseudo-differential equations on closed curves, J. Comput. Math. 10(3) (1992) 273–289.
[17] D.-H. Yu, A posteriori error estimates and adaptive approaches for some boundary element methods, in: C. Brebbia, W.L. Wendland and G. Kuhn, eds, Mathematical and Computational Aspects, Vol. 1 of Boundary Elements IX (Computational Mechanics Publications, Springer-Verlag, 1987) 241–256.
[18] D.-H. Yu, Self-adaptive boundary element methods, Z. Angew. Math. Mech. 68(5) (1988) T435–T437.
[19] C. Carstensen, Adaptive boundary element methods and adaptive finite element methods and boundary element coupling, in: M. Costabel, M. Dauge and S. Nicaise, eds., Boundary Value Problems and Integral Equations in Nonsmooth Domains (Marcel Dekker, Inc., 1995) 47–58.
[20] C. Carstensen, Efficiency of a posteriori BEM error estimates for first kind integral equations on quasi-uniform meshes, Math. Comput. 65(213) (1996) 69–84.
[21] C. Carstensen and E.P. Stephan, A posteriori error estimates for boundary element methods, Math. Comput. 64(210) (1995) 483–500.
[22] C. Carstensen, D. Estep and P. Stephan, *h*-adaptive boundary element schemes, Comput. Mech. 15(4) (1995) 372–383.
[23] W.L. Wendland, E.P. Stephan and G.C. Hsiao, On the integral equation method for the plane mixed boundary value problem for the Laplacian, Math. Methods Appl. Sci. 1 (1979) 265–321.
[24] M. Costabel and E. Stephan, Boundary integral equations for mixed boundary value problems in polygonal domains and Galerkin approximation, in: W. Fiszdon and K. Wilmanski, eds., Mathematical Models and Methods in Mechanics, Vol. 15 (Banach Center Publications, 1985).
[25] M. Costabel, M. Dauge and S. Nicaise, eds., Boundary Value Problems and Integral Equations in Nonsmooth Domains, number 167 in Lecture Notes in Pure and Applied Mathematics (Marcel Dekker Inc., 1995).
[26] E.P. Stephan, The *h-p* boundary element method for solving 2- and 3-dimensional problems, Comput. Methods Appl. Mech. Engrg. 133(3–4) (1996) 183–208.
[27] M. Feistauer, G.C. Hsiao and R.E. Kleinman, Asymptotic and a posteriori error estimates for boundary element solutions of hypersingular integral equations, SIAM J. Numer. Anal. 33(2) (1996) 666–685.
[28] M.A. Golberg and H. Bowman, Superconvergence and the use of the residual as an error estimator in the BEM—I: Theoretical development, Boundary Elem. Comm. 8(4) (1998) 230–238.
[29] I.H. Sloan, Improvement by iteration for compact operator equations, Math. Comput. 30 (1976) 758–764.
[30] I.H. Sloan, Superconvergence, in: M.A. Golberg, ed., Numerical Solution of Integral Equations, Chap. 2 (Plenum Press, New York, 1990) 35–70.
[31] O.D. Kellog, Potential Theory (Dover Publications, 1967).
[32] S.G. Mikhlin, Integral Equations (Pergamon Press, 1957).
[33] R. Kress, Linear Integral Equations (Springer-Verlag, 1989).
[34] L.J. Gray, Symbolic computation of hypersingular boundary integrals, in: J.H. Kane, G. Maier, N. Tosaka and S.N. Atluri, eds., Advances in Boundary Element Techniques (Springer-Verlag, 1993) 157–172.
[35] D. Rosen and D.E. Cormack, Singular and near singular integrals in the BEM: A global approach, SIAM J. Appl. Math. 53(2) (1993) 340–357.
[36] G. Krishnasamy, F.J. Rizzo and T.J. Rudolphi, Continuity requirements for density functions in the boundary element method, Comput. Mech. 9(4) (1992) 267–284.

[37] P.A. Martin and F.J. Rizzo, Hypersingular integrals: how smooth must the density be? Int. J. Numer. Methods Engrg. 39(4) (1996) 687–704.
[38] T.A. Cruse and J.D. Richardson, Self-regularized gradient potential formulation. Report 98-01, Department of Mechanical Engineering, Vanderbilt University, Nashville, TN 37235, USA, 1998.
[39] K.O. Friedrichs, Pseudo-differential Operators. Courant Institute of Mathematics, Lecture Notes, 1970.
[40] D.-H. Yu, Numerical solutions of harmonic and biharmonic canonical integral equations in interior or exterior circular domains, J. Comput. Math. 1 (1983) 52–62.
[41] G. Chen and J. Zhou, Boundary Element Methods (Academic Press, 1992).
[42] I. Babuška, T. Von Petersdorff and B. Andersson, Numerical treatment of vertex singularities and intensity factors for mixed boundary value problems for the Laplace equation in $\boldsymbol{R}^3$, SIAM J. Numer. Anal. 31(5) (1994) 1265–1288.
[43] L.F. Martha, L.J. Gray and A.R. Ingraffea, Three-dimensional fracture simulation with a single-domain direct boundary element formulation, Int. J. Numer. Methods Engrg. 35(9) (1992) 1907–1921.
[44] M. Guiggiani, Hypersingular integral equations and superaccurate stress evaluation, in: C.A. Brebbia and J.J. Rencis, eds., Fluid Flow and Computational Aspects, Vol. 1 of Boundary Elements XV (Computational Mechanics Publications, Southampton, and Elsevier Science Publishers, London, 1993) 413–428.
[45] L.B. Wahlbin, Local behavior in finite element methods, in: P.G. Ciarlet and J.L. Lions, eds., Finite Element Methods (Part 1), Vol. 2 of Handbook of Numerical Analysis (Elsevier Science Publishers B.V., 1991).
[46] F. Hartmann, C. Katz and B. Protopsaltis, Boundary elements and symmetry, Ingenieur-Archiv. 55(6) (1985) 440–449.
[47] S. Sirtori, G. Maier, G. Novati and S. Miccoli, A Galerkin symmetric boundary-element method in elasticity: formulation and implementation, Int. J. Numer. Methods Engrg. 35 (1992) 255–282.
[48] G.H. Paulino and L.J. Gray, Galerkin residuals for adaptive Galerkin-boundary element methods, ASCE J. Engrg. Mech., in press.
[49] D. Porter and D.S.G. Stirling, Integral Equations: A Practical Treatment, from Spectral Theory to Applications (Cambridge University Press, Cambridge, 1990).
[50] F. Chatelin and B. Lebbar, Superconvergence results for the iterated projection method applied to a Fredholm integral equation of the second kind and the corresponding eigenvalue problem, J. Integral Eqns. 6 (1984) 71–91.
[51] I.G. Graham, S. Joe and I.H. Sloan, Iterated Galerkin versus iterated collocation for integral equations of the second kind, IMA J. Numer. Anal. 5 (1985) 355–369.
[52] T. Tran, The K-operator and the Galerkin method for strongly elliptic equations on smooth curves: local estimates, Math. Comput. 64(210) (1995) 501–513.