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ON AN INDIRECT INTEGRAL EQUATION APPROACH FOR STATIONARY HEAT TRANSFER IN SEMI-INFINITE LAYERED DOMAINS IN $\mathbb{R}^3$ WITH CAVITIES

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Анотація. Області, які містять внутрішні границі, наприклад, композитні матеріали, виникають у багатьох застосуваннях. Ми розглядаємо випадок шаруватої частково-необмеженої області в $\mathbb{R}^3$ з скінченним числом обмежених порожнин. Моделлю є стаціонарний теплоперенос, що описується рівнянням Лапласа з кусково-постійним коефіцієнтом теплопровідності. Тепловий потік (умова Неймана) задається на нижній поверхні шаруватої області і різні граничні умови на межах порожнин. На поверхні контакту шару і півпростору з порожнинами виконуються звичайні умови спряження (неперервність розв'язку і нормальної похідної). Для ефективного обчислення стаціонарного температурного поля в частково-необмеженій області ми використовуємо техніку матриці Гріна і зводимо задачу до граничних інтегральних рівнянь з слабкими особливостями по поверхнях порожнин. Чисельне розв'язування цих інтегральних рівнянь здійснюється методом Вінерта [20]. Припускаючи, що кожна порожнина є гомеоморфна сфері, пропонується дискретний проекційний метод з супер-алгебраїчним порядком збіжності. Приведено доведення оцінки похибки методу. Здійснені чисельні експерименти підтверджують ефективність і високу точність запропонованого методу.

Abstract. Regions containing internal boundaries such as composite materials arise in many applications. We consider a situation of a layered domain in $\mathbb{R}^3$ containing a finite number of bounded cavities. The model is stationary heat transfer given by the Laplace equation with piecewise constant conductivity. The heat flux (a Neumann condition) is imposed on the bottom of the layered region and various boundary conditions are imposed on the cavities. The usual transmission (interface) conditions are satisfied at the interface layer, that is continuity of the solution and its normal derivative. To efficiently calculate the stationary temperature field in the semi-infinite region, we employ a Green's matrix technique and reduce the problem to boundary integral equations (weakly singular) over the bounded surfaces of the cavities. For the numerical solution of these integral equations, we use Wienert's approach [20]. Assuming that each cavity is homeomorphic with the unit sphere, a fully discrete projection method with super-algebraic convergence order is proposed. A proof of an error estimate for the approximation is given as well. Numerical examples are presented that further highlights the efficiency and accuracy of the proposed method.

1. Introduction

Regions having internal boundaries, that is boundaries where no boundary data is given, arise in many applications. For example, composite materials such as multilayer (sandwich) beams, pipes and rocks, see for example [14]. Other applications are Li-ion battery technologies using nanoarchitectured carbon networks [19], applied potential tomography [2], and the distribution of stress in a medium containing holes or inclusions [4].

Key words. Semi-infinite multilayer domain; Green's matrix; Boundary integral equations; Weak singularities; Galerkin method; Spherical functions, Gauss-Legandre quadratures, Sinc-quadratures.

The governing equations in these examples is the Laplace equation with piecewise constant physical parameters. Moreover, the conditions at the interfaces are usually continuity of the solution and its normal derivative.

Only in special cases and for certain domains there are explicit analytical solutions to these problems. Thus, in general, numerical methods are needed to generate an approximation to the physical quantities of interest. As is well-known, standard domain discretisation methods such as the finite element method (FEM) is not easily adjustable to problems with internal boundaries. Instead, boundary integral methods are more suitable for this class of problems since they provide a natural treatment of the interface.

An additional complication from a numerical point of view is models posed on unbounded domains. Such models include the irrotational flow of an incompressible fluid exterior to a body [9], heat flow in the oceans [16] and the distribution of stresses in an infinite medium with holes or inclusions [4]. In all these cases, the surrounding media can be treated as infinite, thus leading to unbounded domain problems. Employing for example the FEM, truncation of the solution domain is usually needed. Also, from a theoretical point of view, partial differential equations in unbounded domains are challenging and non-standard function spaces are needed to prove properties of solutions, for an overview, see the introduction in [15].

We shall consider a model having both these difficulties, that is we have a layered unbounded region. We consider a semi-infinite bi-material represented by the upper half-space in $\mathbb{R}^3$ and having an internal boundary described by a plane parallel with the xy-plane. Moreover, above this interface, the medium contains a finite number of bounded smooth cavities, see further Fig. 1. The heat flux is prescribed at the bottom of the region and various boundary conditions such as the temperature or heat flux or a combination of them are imposed on the surfaces of the cavities. The interface conditions are continuity of the solution and its normal derivative. We assume stationary heat transfer modelled by the Laplace equation with piecewise constant conductivity. The aim is to construct the temperature field throughout the region.

As mentioned above, integral equations are suitable to use for interface problems. Thus, using a Green's matrix technique, we reduce the problem to boundary integral equations on the (bounded) surfaces of the cavities. In general, we obtain equations of the second kind with kernels having a weak singularity. An explicit expression for this Green's matrix was recently derived in [18].

To numerically solve the obtained boundary integral equations, we shall employ the Wienert's approach [20]. This approach has attracted much attention recently, see for example, [5, 6, 8, 11], and advantages being that smaller linear systems are obtained as well as high accuracy. The higher accuracy is partly due to, as opposed to the boundary element method (BEM) [10], there is no need to discretize the surfaces in the boundary integral equations. To use [20], we assume that each of the cavities can be mapped one-to-one to the unit sphere. Clearly, this is a restriction of our approach, however, one can generalize and use differential geometry and assume that the cavities are parametrized by surface patches of the unit sphere or one can numerically construct an approximation to such a map. This is though deferred to future work.

Using the assumption that the cavities can be parametrized via the unit sphere, a fully discrete projection method with super-algebraic convergence order is proposed to solve the obtained boundary integral equations. The densities in the boundary integral equations are approximated in the finite-dimensional space of spherical harmonics. A proof of an error estimate for the approximation is given as well. Numerical examples are presented that further highlights the efficiency and accuracy of the proposed method.

The main novelty of this paper is the reduction of the problem using the Green's matrix and the combination and extension of [20] to obtain a numerical method with high accuracy for semi-infinite layered materials, as well as proving error estimates. Clearly, our work is timely due to the recent interest into the method [20] and the recent derivation of the Green's matrix [18]. Moreover, it is of importance due to the many practical engineering applications mentioned above that can be formulated in terms of our equations, and the problem of solving these using standard numerical techniques. Also, having an efficient solver for these direct problems opens the possibility to consider inverse problems, and, for example, generalize the work [3] to $\mathbb{R}^3$.

For the outline of this paper, in Section 2, we formulate our problem mathematically. In Section 3, we show how to reduce our problem using a Green's matrix technique, to weakly singular boundary integral equations over the surfaces of the cavities, see Theorem 3.3. Solvability of these equations are also mentioned, see Theorem 3.4. The discrete projection method to solve these singular integral equations is given in Section 4. Moreover, we prove an error estimate for our approach, see Theorem 4.2. Numerical examples are given in Section 5, both for regions with one and several cavities. These examples illustrate the efficiency and accuracy of our proposed approach.

2. Formulation of the problem

Let $D_1 := \{x = (x_1, x_2, x_3) : 0 < x_3 < h, (x_1, x_2) \in \mathbb{R}^2\}$ be a (strip) layer in $\mathbb{R}^3$ having thickness h and contained within the two parallel planes Γ_1 and Γ_2 (which constitutes the boundary parts of ∂D_1). Moreover, let $D_2 := \{x = (x_1, x_2, x_3) : x_3 > h, (x_1, x_2) \in \mathbb{R}^2\}$ be the half-space in $\mathbf{R}^3$ bounded by the plane Γ_2, and let $\mathcal{C} := \bigcup_{k=1}^{m} \mathcal{C}_k$, $m \in \mathbb{N}$, be a set of cavities (smooth bounded non-overlapping domains in $\mathbb{R}^3$) contained in the half-space D_2, i.e. $\mathcal{C}_k \subset D_2$, having boundary $S_k = \partial\mathcal{C}_k$ (see Fig. 1). Physical properties, such as conductivity or fluid viscosity, in $\mathcal{D}_1 := D_1$ and $\mathcal{D}_2 := D_2 \setminus \bar{\mathcal{C}}$ are characterized by constants $\lambda^{(1)}$ and $\lambda^{(2)}$, respectively.

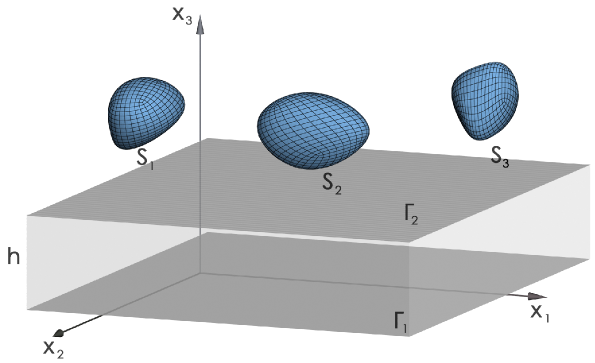


Fig. 1. A semi-infinite layer domain and cavities with surfaces S_k, $k = 1, 2, 3$

The function

$$t(x) = \begin{cases} t_1(x), & x \in \mathcal{D}_1, \\ t_2(x), & x \in \mathcal{D}_2, \end{cases}$$

defined in the piecewise-homogeneous solution domain $\mathcal{D} := \mathcal{D}_1 \cup \mathcal{D}_2$ is assumed to satisfy the Laplace equation

$$\Delta t = 0 \ \text{ in } \mathcal{D}, \tag{2.1}$$

together with the Neumann boundary condition

$$\lambda^{(1)}\frac{\partial t_1}{\partial x_3} = -\beta \quad \text{on } \Gamma_1, \tag{2.2}$$

the usual transmission conditions

$$t_1 = t_2, \qquad \lambda^{(1)}\frac{\partial t_1}{\partial x_3} = \lambda^{(2)}\frac{\partial t_2}{\partial x_3} \quad \text{on } \Gamma_2, \tag{2.3}$$

the boundary conditions

$$\ell t_2 = f_k \quad \text{on } S_k, \quad k = 1, \dots, m \tag{2.4}$$

and the regularity condition

$$t(x) = O(\,|x|^{-1}), \quad x \in \mathcal{D}, \quad |x| \to \infty. \tag{2.5}$$

Here, the boundary operator ℓ corresponds to the Dirichlet ($\ell u := u$), Neumann ($\ell u := \partial u/\partial \nu$) or Robin ($\ell u := \lambda^{(2)}\partial u/\partial \nu + \alpha_k u$) boundary condition, and β, α_k and f_k, $k = 1, \dots, m$, are given boundary functions with α_k being non-negative.

Clearly, the standard Green's formula for the Laplace equation holds in $\mathcal{D}$. Thus, following the usual steps for potential problems, one obtains the following result.

Theorem 2.1 *Every boundary value problem of the form* (2.1) – (2.5) *has at most one classical solution.*

We assume that data are given and compatible such that (2.1) – (2.5) has a classical solution (which in particular is assumed to be twice continuously differentiable in $\mathcal{D}$).

3. Indirect boundary integral equation method

To reduce the boundary value problem (2.1) – (2.5) to boundary integral equations over the surfaces of the cavities $\mathcal{C}_k$, we introduce the Green's matrix [13] for the equation (2.1) with homogeneous Neumann boundary condition (2.2) and the transmission conditions (2.3).

Definition 3.1 *The* 2×2 *function matrix* $\{G_{ij}\}_{i,j=1}^{2}$ *with elements that satisfy the conditions*

$$\Delta G_{ii}(x, y) = -\frac{1}{\lambda^{(i)}}\delta(x - y), \quad x \in D_i, \quad y \in D_i, \tag{3.1}$$

$$\Delta G_{3-i,i}(x, y) = 0, \quad x \in \ D_{3-i}, \quad y \in D_i, \tag{3.2}$$

$$\lambda^{(1)}\frac{\partial G_{1i}}{\partial x_3}(x, y) = 0, \quad x \in \Gamma_1, \quad y \in D_i, \tag{3.3}$$

$$G_{1i}(x, y) = G_{2i}(x, y), \quad \lambda^{(1)}\frac{\partial G_{1i}}{\partial x_3}(x, y) = \lambda^{(2)}\frac{\partial G_{2i}}{\partial x_3}(x, y), \quad x \in \Gamma_2, \quad y \in D_i, \tag{3.4}$$

where $i = 1, 2$, *and* δ *denotes the Dirac's function, is called the Green's matrix or influence matrix for the boundary value problem* (2.1) – (2.3).

We use the following notation $\tilde{x}_n = (x_1, x_2, 2nh + x_3)$ for $n \in \mathbf{N}$, $y^* = (y_1, y_2, -y_3)$, $v = (\lambda^{(1)} - \lambda^{(2)})/(\lambda^{(1)} + \lambda^{(2)})$ and $G_n(x, y) = |\tilde{x}_n - y|^{-1} + |\tilde{x}_n - y^*|^{-1}$.

The Green's matrix for the boundary value problem (2.1) – (2.3) has the form [18]

$$G_{11}(x,y) = \frac{1}{4\pi\lambda^{(1)}}\left[G_0(x,y) + \sum_{n=1}^{\infty} v^n (G_{-n}(x,y) + G_n(x,y))\right],$$

$$G_{12}(x,y) = \frac{1}{2\pi(\lambda^{(1)}+\lambda^{(2)})}\left[G_0(x,y) + \sum_{n=1}^{\infty} v^n (|\tilde{x}_{-n} - y|^{-1} + |\tilde{x}_n - y^*|^{-1})\right],$$

$$G_{21}(x,y) = G_{12}(y,x),$$

$$G_{22}(x,y) = \frac{1}{4\pi\lambda^{(2)}}\left[G_0(x,y) + \sum_{n=1}^{\infty} v^n (|\tilde{x}_n - y^*|^{-1} - |\tilde{x}_{n-2} - y^*|^{-1})\right].$$

With the Green's matrix we can construct an integral representation for the solution of the Neumann boundary value problem in the semi-infinite layered region consisting of D_1 and D_2.

Theorem 3.2 *For the solution of the boundary value problem*

$$\Delta\tau_i = 0 \quad \text{in } D_i,$$

$$\lambda^{(1)}\frac{\partial\tau_1}{\partial x_3} = -\beta \quad \text{on } \Gamma_1,$$

$$\tau_1 = \tau_2, \qquad \lambda^{(1)}\frac{\partial\tau_1}{\partial x_3} = \lambda^{(2)}\frac{\partial\tau_2}{\partial x_3} \quad \text{on } \Gamma_2,$$

$$\tau_i(x) = O(\,|x|^{-1}), \quad x \in D_i, \quad |x| \to \infty,$$

the following boundary integral representation formula holds

$$\tau_i(x) = \int_{\Gamma_1} G_{i1}(x,y)\beta(y)\,ds(y), \quad x \in D_i, \quad \text{for} \quad i = 1,2, \tag{3.5}$$

where $\{G_{ij}\}_{i,j=1}^2$ is the Green's matrix given above.

Proof. Taking into account the defining properties of the functions in the Green's matrix, i.e. the functions G_{ik}, and the conditions for the solutions τ_i, $i = 1,2$, we have the representations

$$\tau_i(x) := \lambda^{(1)}\int_{D_1}[G_{i1}(x,y)\Delta t_i(y) - t_i(y)\Delta G_{i1}(x,y)]\,dy$$
$$+\lambda^{(2)}\int_{D_2}[G_{i2}(x,y)\Delta t_i(y) - t_i(y)\Delta G_{i2}(x,y)]\,dy, \quad x \in D_i, \quad i = 1,2.$$

The first Green's theorem and the given interface conditions for G_{ik} (see Definition 3.1) and τ_i (see (2.3)), lead to the representation (3.5). □

We shall then construct the solution to (2.1) – (2.5) in the form of the following modified single-layer potential

$$t_i(x) = \sum_{k=1}^{m}\int_{S_k}\mu_k(y)G_{i2}(x,y)\,ds(y) + \tau_i(x), \quad x \in \mathcal{D}_i, \quad i = 1,2, \tag{3.6}$$

with densities $\mu_k \in C(S_k)$ and τ_i given by (3.5). The next result gives conditions for the densities μ_k to guarantee that t_i, $i = 1,2$, is a solution to (2.1) – (2.5).

Theorem 3.3
a) Dirichlet condition on S_k: *The solution of the mixed Neumann-Dirichlet boundary value problem* (2.1)–(2.5) *can be represented in the form* (3.6), *where the densities* μ_k *satisfy the system of integral equations of the first kind*

$$\sum_{k=1}^{m} \int_{S_k} \mu_k(y) G_{22}(x,y) ds(y) = f_i(x) - \tau_2(x), \quad x \in S_i, \quad i = 1, \dots, m. \tag{3.7}$$

b) Neumann condition on S_k: *The solution of the Neumann boundary value problem* (2.1)–(2.5) *can be represented in the form* (3.6), *where the densities* μ_k *satisfy the system of integral equations of the second kind*

$$\begin{aligned} -\frac{1}{2\lambda^{(2)}} \mu_i(x) + \sum_{k=1}^{m} \int_{S_k} \mu_k(y) \frac{\partial G_{22}(x,y)}{\partial \nu(x)} ds(y) = \\ = f_i(x) - \frac{\partial \tau_2}{\partial \nu}(x), \quad x \in S_i, \quad i = 1, \dots, m. \end{aligned} \tag{3.8}$$

c) Robin condition on S_k: *The solution of the mixed Neumann - Robin boundary value problem* (2.1)–(2.5) *can be represented in the form* (3.6), *where the densities* μ_k *satisfy the system of integral equations of the second kind*

$$\begin{aligned} -\frac{1}{2} \mu_i(x) + \sum_{k=1}^{m} \int_{S_k} \mu_k(y) \left[\lambda^{(2)} \frac{\partial G_{22}(x,y)}{\partial \nu(x)} + \alpha_i(x) G_{22}(x,y) \right] ds(y) = \\ = f_i(x) - \lambda^{(2)} \frac{\partial \tau_2}{\partial \nu}(x) - \alpha(x)_i \tau_2(x), \quad x \in S_i, \quad i = 1, \dots, m. \end{aligned} \tag{3.9}$$

Proof. From the Definition 3.1 of the Green's matrix and Theorem 3.2, it follows that the representation (3.6) satisfies the equation (2.1), the Neumann boundary condition (2.2), the transmission condition (2.3) and the regularity condition (2.5). Since the function G_{22} can be written in the form

$$G_{22}(x,y) = \frac{1}{4\pi\lambda^{(2)}} \frac{1}{|x-y|} + \tilde{G}_{22}(x,y)$$

with a smooth part $\tilde{G}_{22}$, the single-layer potentials in the representation of t_2 in (3.6) have the properties of the classical single-layer potential for the Laplace equation. Thus, the standard jump relations hold, and this then imply the corresponding integral equations for each type of boundary conditions imposed on the cavities. □

The Riesz-Schauder theory [10, 12] applied to the corresponding integral equations in Theorem 3.3 together with Theorem 2.1 lead to the following result.

Theorem 3.4
(i) Dirichlet case: *For* $\beta \in L^2(\Gamma_1)$ *and* $f_k \in C^{1,\gamma}(S_k)$, $k = 1, \dots, m$, *the system of integral equations* (3.7) *has a unique solution* $\mu_k \in C^{0,\gamma}(S_k)$, $k = 1, \dots, m$.

(ii) Neumann case: *For* $\beta \in L^2(\Gamma_1)$ *and* $f_k \in C(S_k)$, $k = 1, \dots, m$, *the system of integral equations* (3.8) *has a unique solution* $\mu_k \in C(S_k)$, $k = 1, \dots, m$.

(iii) Robin case: *For* $\beta \in L^2(\Gamma_1)$, $\alpha_k \in L^\infty(S_k)$, $\alpha_k \geq 0$ *and* $f_k \in C(S_k)$, $k = 1, \dots, m$, *the system of integral equations* (3.9) *has a unique solution* $\mu_k \in C(S_k)$, $k = 1, \dots, m$.

4. Numerical solution of the weakly singular integral equations (3.9)

We consider here in detail the system of integral equations (3.9), since this corresponds to the most general boundary condition in (2.4), and the results for the equations (3.7) and (3.8) follows as special cases. Taking into account the representation for the Green's matrix (given in the beginning of Section 3) we can rewrite the system (3.9) in the following form

$$-\frac{1}{2}\mu_i(x)+\sum_{k=1}^{m}\int_{S_k}\mu_k(y)\left[\frac{Q_1(x,y)}{|x-y|}+Q_2(x,y)\right]ds(y)= \\ = g_i(x),\quad x\in S_i,\quad i=1,\dots,m, \tag{4.1}$$

where

$$Q_1(x,y)=\frac{1}{4\pi}\left[\frac{\alpha_i(x)}{\lambda^{(2)}}+\frac{(y-x)\cdot\nu(x)}{|x-y|^2}\right],$$

$$Q_2(x,y)=\frac{\alpha_i(x)}{4\pi\lambda^{(2)}}\left[|x-y^*|^{-1}+\sum_{n=1}^{\infty}v^n(|\tilde{x}_n-y^*|^{-1}-|\tilde{x}_{n-2}-y^*|^{-1})\right]$$

$$+\frac{1}{4\pi}\left[\frac{(y^*-x)\cdot\nu(x)}{|x-y^*|^3}+\sum_{n=1}^{\infty}v^n\left\{\frac{(y^*-\tilde{x}_n)\cdot\nu(x)}{|\tilde{x}_n-y^*|^3}+\frac{(\tilde{x}_{n-2}-y^*)\cdot\nu(x)}{|\tilde{x}_{n-2}-y^*|^3}\right\}\right]$$

and

$$g_i(x)=f_i(x)-\int_{\Gamma_1}\beta(y)(\lambda^{(2)}\tilde{G}_{21}(x,y)+\alpha_i(x)G_{21}(x,y))\,ds(y) \tag{4.2}$$

with

$$\tilde{G}_{21}(x,y)=\frac{1}{2\pi(\lambda^{(1)}+\lambda^{(2)})}\left\{\frac{(y-x)\cdot\nu(x)}{|x-y|^3}+\frac{(y^*-x)\cdot\nu(x)}{|x-y^*|^3}+\right.$$

$$\left.\sum_{n=1}^{\infty}v^n\left[\frac{(y-\tilde{x}_n)\cdot\nu(x)}{|\tilde{x}_n-y|^3}+\frac{(y^*-\tilde{x}_n)\cdot\nu(x)}{|\tilde{x}_n-y^*|^3}\right]\right\}.$$

4.1. Rewriting the integral equations over the unit sphere

As mentioned in the introduction, we assume that the surfaces S_k, $k=1,\dots,m$, can be bijectively mapped onto the unit sphere Ω, i.e. there exist one-to-one mappings $q_k:\Omega\to S_k$ with the corresponding smooth Jacobian J_{q_k}.

Taking into account the parametric representation of S_k, we reduce the system of integral equations of the second kind (4.1) to the following equation over the unit sphere Ω

$$-\frac{1}{2}\boldsymbol{\psi}(\hat{x})+(\mathbf{Q}\boldsymbol{\psi})(\hat{x})=\mathbf{g}(\hat{x}),\quad \hat{x}\in\Omega. \tag{4.3}$$

Here, we used the following notation $\hat{x}=p(\theta,\varphi)=(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta)$, $\theta\in[0,\pi]$, $\varphi\in[0,2\pi]$, $\boldsymbol{\psi}(\hat{x})=(\mu_1(q_1(\hat{x})),\dots,\mu_m(q_m(\hat{x})))^\top$, the operator matrix $\mathbf{Q}=\{Q_{ik}\}_{i,k=1}^m$ with elements

$$(Q_{ik}\psi)(\hat{x})=\int_{\Omega}\psi(\hat{y})\left[\frac{Q_{ik}^{(1)}(\hat{x},\hat{y})}{|q_i(\hat{x})-q_k(\hat{y})|}+Q_{ik}^{(2)}(\hat{x},\hat{y})\right]ds(\hat{y}),\quad \hat{x}\in\Omega,$$

where $Q_{ik}^{(1)}(\hat{x},\hat{y})=Q_1(q_i(\hat{x}),q_k(\hat{y}))J_{q_k}(\hat{y})$ and $Q_{ik}^{(2)}(\hat{x},\hat{y})=Q_2(q_i(\hat{x}),q_k(\hat{y}))J_{q_k}(\hat{y})$ and the right-hand side

$$\mathbf{g}=(g_1,\dots,g_m)^\top \tag{4.4}$$

with elements $g_i(\hat{x}) = g_i(q_i(\hat{x}))$ and $g_i(x)$ is given by (4.2).

Clearly, the diagonal operators Q_{ii} have weak singularities and we can write them in the form

$$(Q_{ii}\psi)(\hat{x}) = \int_\Omega \psi(\hat{y}) \left[\frac{Q_{ii}^{(1)}(\hat{x},\hat{y})F_i(\hat{x},\hat{y})}{|\hat{x}-\hat{y}|} + Q_{ii}^{(2)}(\hat{x},\hat{y}) \right] ds(\hat{y}), \qquad \hat{x}\in\Omega, \quad i=1,\dots,m, \tag{4.5}$$

with

$$F_i(\hat{x},\hat{y}) = \frac{|\hat{x}-\hat{y}|}{|q_i(\hat{x})-q_i(\hat{y})|}.$$

Let $\hat{n} = (0,0,1)$ be the north pole of Ω. It is convenient to move the singularities in the operators Q_{ii} to the north pole [5, 8, 20]. To do this, we introduce the orthogonal transformations for $\xi \in \mathbf{R}$,

$$D_F(\xi) = \begin{pmatrix} \cos\xi & -\sin\xi & 0 \\ \sin\xi & \cos\xi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad D_T(\xi) = \begin{pmatrix} \cos\xi & 0 & -\sin\xi \\ 0 & 1 & 0 \\ \sin\xi & 0 & \cos\psi \end{pmatrix}.$$

The linear orthogonal transformation $T_{\hat{x}} = D_F(\varphi)D_T(\theta)D_F(-\varphi)$ has the property that $T_{\hat{x}}\hat{x} = \hat{n}$ for all $\hat{x}\in\Omega$. We also introduce an induced transformation $\mathcal{T}_{\hat{x}}$ on $C(\Omega)$ as

$$\mathcal{T}_{\hat{x}}\psi(\hat{y}) = \psi(T_{\hat{x}}^{-1}\hat{y}), \quad y\in\Omega, \ \ \psi\in C(\Omega)$$

and its bivariate analogue

$$\mathcal{T}_{\hat{x}}\psi(\hat{y}_1,\hat{y}_2) = \psi(T_{\hat{x}}^{-1}\hat{y}_1, T_{\hat{x}}^{-1}\hat{y}_2), \quad \psi\in C(\Omega\times\Omega).$$

Since $|\hat{x}-\hat{y}| = |T_{\hat{x}}^{-1}(\widehat{\hat{n}-\eta})| = |\hat{n}-\hat{\eta}|$ with $\hat{\eta} = T_{\hat{x}}\hat{y}$, the operators (4.5) can be transformed into

$$(Q_{ii}\psi)(\hat{x}) = \int_\Omega \mathcal{T}_{\hat{x}}\psi(\hat{\eta}) \left[\frac{\mathcal{T}_{\hat{x}}Q_{ii}^{(1)}(\hat{n},\hat{\eta})\mathcal{T}_{\hat{x}}F_i(\hat{n},\hat{\eta})}{|\hat{n}-\hat{\eta}|} + \mathcal{T}_{\hat{x}}Q_{ii}^{(2)}(\hat{n},\hat{\eta}) \right] ds(\hat{\eta}), \quad \hat{x}\in\Omega$$

for $i = 1,\dots,m$. The functions F_i are then continuous with respect to $\hat{\eta}$ for fixed $\hat{x}\in\Omega$.

4.2. A projection method on the unit sphere

For the numerical solution of the system of integral equations (4.3) we shall employ Wienert's approach [5, 8, 20] based on spherical harmonics. Let

$$\mathrm{Y}_{\ell,k}^R = \begin{cases} \operatorname{Im} Y_{\ell,|k|}, & 0 < k < \ell, \\ \operatorname{Re} Y_{\ell,|k|}, & -\ell \le k \le 0, \end{cases}$$

with the spherical harmonics $Y_{\ell,k}$ [1]. Let $\mathbb{P}_n$ denote the space of spherical polynomials of degree at most n on Ω. A basis for $\mathbb{P}_n$ is the set of orthonormal spherical harmonics $Y_{\ell,k}^R$, $0\le\ell\le n$, $|k|\le\ell$.

We introduce the orthogonal projector

$$\mathcal{L}_{n'}\psi = \sum_{\ell=0}^{n'} \sum_{|j|\le\ell} (\psi, Y_{\ell,j}^R)_{n'} Y_{\ell,j}^R, \quad \psi\in C(\Omega)$$

with the discrete inner product $(\cdot,\cdot)_{n'}$ given by

$$(v,w)_{n'} = \sum_{\rho'=0}^{2n'+1} \sum_{s'=1}^{n'+1} \tilde{\mu}_{\rho'} \tilde{a}_{s'} v(p(\theta_{s'},\varphi_{\rho'})) w(p(\theta_{s'},\varphi_{\rho'})),$$

where $\varphi_{\rho'} = \rho'\pi/(n'+1)$, $\theta_{s'} = \arccos z_{s'}$ with $z_{s'}$ being the zeros of the Legendre polynomials $P_{n'+1}$, $\tilde{a}_{s'} = 2(1-z_{s'}^2)/((n'+1)P_{n'}(z_{s'}))^2$ and $\tilde{\mu}_{\rho'} = \pi/(n'+1)$. This discrete inner product is the result of applying the rectangular Gauss quadrature rule (Gauss-Legendre rule) to the corresponding integral over the unit sphere Ω.

The following quadrature is used for the continuous integrands in (4.3):

$$\int_\Omega f(\hat{y})\, ds(\hat{y}) \approx \int_\Omega (\mathcal{L}_{n'} f)(\hat{y})\, ds(\hat{y}) = \sum_{\rho'=0}^{2n'+1} \sum_{s'=1}^{n'+1} \tilde{\mu}_{\rho'} \tilde{a}_{s'} f(p(\theta_{s'},\varphi_{\rho'})). \tag{4.6}$$

The numerical quadrature employed to obtain high accuracy for integrands having a weak singularity has the form

$$\int_\Omega \frac{f(\hat{y})}{|\hat{n}-\hat{y}|} ds(\hat{y}) \approx \int_\Omega \frac{(\mathcal{L}_{n'} f)(\hat{y})}{|\hat{n}-\hat{y}|} ds(\hat{y}) = \sum_{\rho'=0}^{2n'+1} \sum_{s'=1}^{n'+1} \tilde{\mu}_{\rho'} \tilde{b}_{s'} f(p(\theta_{s'},\varphi_{\rho'})) \tag{4.7}$$

with weights

$$\tilde{b}_{s'} = \frac{\pi \tilde{a}_{s'}}{n'+1} \sum_{i=0}^{n'} P_i(z_{s'}).$$

In [5,8] it is shown that the quadratures (4.6) and (4.7) have super-algebraic convergence order.

Thus, for the case of continuous kernels $\tilde{Q}_{ik}(\hat{x},\hat{y}) = Q_{ik}^{(1)}(\hat{x},\hat{y})/|q_i(\hat{x}) - q_k(\hat{y})| + Q_{ik}^{(2)}(\hat{x},\hat{y})$ in (4.3) we have the approximation operators

$$(Q_{ik}^{n'}\psi)(\hat{x}) = \int_\Omega (\mathcal{L}_{n'}\{\tilde{Q}_{ik}(\hat{x},\cdot)\psi(\cdot)\})(\hat{y})\, ds(\hat{y}), \quad i \neq k$$

and for the kernels with a weak singularity,

$$(Q_{ii}^{n'}\psi)(\hat{x}) = \int_\Omega \left[\frac{(\mathcal{L}_{n'}\{\mathcal{T}_{\hat{x}} Q_{ii}^{(1)}(\hat{n},\cdot)\mathcal{T}_{\hat{x}}\psi(\cdot)\})(\hat{\eta})}{|\hat{n}-\hat{\eta}|} + (\mathcal{L}_{n'}\{\mathcal{T}_{\hat{x}} Q_{ii}^{(2)}(\hat{n},\cdot)\mathcal{T}_{\hat{x}}\psi(\cdot)\})(\hat{\eta}) \right] ds(\hat{\eta}).$$

We seek the numerical solution $\boldsymbol{\psi}^{(n)} \in \mathbb{P}_n \times \ldots \times \mathbb{P}_n = \Pi_{k=1}^m \mathbb{P}_n$ of (4.3) via a projection method, which leads to the (projected) operator equation

$$-\frac{1}{2}\boldsymbol{\psi}^{(n)} + \mathcal{L}_n \mathbf{Q}^{n'} \boldsymbol{\psi}^{(n)} = \mathcal{L}_n \mathbf{g}_M, \tag{4.8}$$

where $\mathbf{Q}^{n'} = \{Q_{ik}^{n'}\}_{i,k=1}^m$ and $\mathbf{g}_M = (g_{1,M},\ldots,g_{m,M})^\top$ with

$$g_{i,M}(\hat{x}) = f_i(q_i(\hat{x})) - \int_{\Gamma_1} \mathcal{S}_M\{\beta(\cdot)\tilde{G}_{21}(q_i(\hat{x}),\cdot) + \alpha_i(q_i(\hat{x}))G_{21}(q_i(\hat{x}),\cdot)\}(y)\, ds(y). \tag{4.9}$$

Here, $\mathcal{S}_M$ is the operator corresponding to sinc-approximation [17]

$$(\mathcal{S}_M\psi)(y) = \sum_{j,k=-M}^{M} \psi(jh_\infty, kh_\infty) \frac{\sin\left[\frac{\pi}{h_\infty}(y_1 - jh_\infty)\right]}{\frac{\pi}{h_\infty}(y_1 - jh_\infty)} \frac{\sin\left[\frac{\pi}{h_\infty}(y_2 - kh_\infty)\right]}{\frac{\pi}{h_\infty}(y_2 - kh_\infty)}. \tag{4.10}$$

Throughout the rest of the paper, we assume that n' and M depend on n and satisfy $n' > n$ and $M > n^2$.

Let

$$\psi_i^{(n)} = \sum_{\ell=0}^{n} \sum_{j=-\ell}^{\ell} a_{\ell j}^i Y_{\ell,j}^R, \quad i = 1, \ldots, m, \tag{4.11}$$

with unknown coefficients $a_{\ell j}^i \in \mathbb{R}$. Then, using (4.8), we obtain the linear system

$$\left(-\frac{1}{2}\mathbf{I} + \tilde{\mathbf{Q}}\right)\mathbf{a} = \tilde{\mathbf{g}} \tag{4.12}$$

with $\mathbf{a} = (a_{\ell j}^1, \ldots, a_{\ell j}^m)^\top$, $\tilde{Q}_{\ell' j', \ell j}^{ik} = (Q_{ik}^{n'} Y_{\ell,j}^R, Y_{\ell',j'}^R)_n$ and $\tilde{g}_{\ell' j'}^i = (g_{i,M}, Y_{\ell',j'}^R)_n$ for $\ell, \ell' = 0, \ldots, n$, $|j| \le \ell$, $|j'| \le \ell'$, $i, k = 1, \ldots, m$.

We can write (4.12) in a more detailed form

$$-\frac{1}{2} a_{\ell' j'}^i + \sum_{k=1}^{m} \sum_{\ell=0}^{n} \sum_{j=-\ell}^{\ell} a_{\ell j}^k \tilde{Q}_{\ell' j', \ell j}^{ik} = \tilde{g}_{\ell' j'}^i$$

with matrix coefficients

$$\tilde{Q}_{\ell' j', \ell j}^{ik} = \sum_{\rho,s} \sum_{\rho',s'} \mu_\rho \tilde{\mu}_{\rho'} a_s \tilde{a}_{s'} \tilde{Q}_{ik}(\hat{x}_{s\rho}, \hat{y}_{s'\rho'}) Y_{\ell',j'}^R(\hat{x}_{s\rho}) Y_{\ell,j}^R(\hat{y}_{s'\rho'}), \quad i \ne k,$$

$$\tilde{Q}_{\ell' j', \ell j}^{ii} = \sum_{\rho,s} \sum_{\rho',s'} \mu_\rho \tilde{\mu}_{\rho'} a_s [\tilde{b}_{s'} Q_{ik}^{(1)}(\hat{x}_{s\rho}, \hat{y}_{s\rho}^{s'\rho'}) F_i(\hat{x}_{s\rho}, \hat{y}_{s\rho}^{s'\rho'}) +$$

$$+ \tilde{a}_{s'} Q_{ik}^{(2)}(\hat{x}_{s\rho}, \hat{y}_{s\rho}^{s'\rho'})] Y_{\ell',j'}^R(\hat{x}_{s\rho}) Y_{\ell,j}^R(\hat{y}_{s,\rho}^{s'\rho'})$$

and the coefficients in the right-hand side are given as

$$\tilde{g}_{\ell' j'}^i = \sum_{\rho,s} \mu_\rho a_s [f_i(q_i(\hat{x}_{s\rho})) - h_\infty^2 \sum_{\tilde{k},\bar{k}=-M}^{M} \{\beta(y_{\tilde{k}\bar{k}})(\tilde{G}_{21}(q_i(\hat{x}_{s\rho}), y_{\tilde{k}\bar{k}})$$
$$+ \alpha_i(q_i(\hat{x}_{s\rho})) G_{21}(q_i(\hat{x}_{s\rho}), y_{\tilde{k}\bar{k}}))\}] Y_{\ell',j'}^R(\hat{x}_{s\rho}), \tag{4.13}$$

where $\hat{x}_{s\rho} = p(\theta_s, \varphi_\rho)$, $\hat{y}_{s\rho}^{s'\rho'} = T_{p(\theta_s,\varphi_\rho)}^{-1} p(\theta_{s'}, \varphi_{\rho'})$, $y_{\tilde{k}\bar{k}} = (h_\infty \tilde{k}, h_\infty \bar{k}, 0)$, $\ell, \ell' = 0, \ldots, n$, $|j| \le \ell$, $|j'| \le \ell'$, $i, k = 1, \ldots, m$.

Note here that the direct calculation of the matrix coefficients (4.13) needs $O(n^8)$ operations. This number can be reduced to $O(n^5)$ by using the approach described in [5].

4.3. Error estimates for the numerical approximation of (4.3)

Let $H^1(SD)$ be the Hardy space consisting of all complex-valued functions w, which are analytic in the strip $SD = \{z \in \mathbb{C} : |\mathrm{Im} z| < d\}$ and which satisfy

$$\int_{\partial SD} |w(z)||dz| = \int_{\mathbb{R}} (|w(x+id)| + |w(x-id)|)\, dx < \infty.$$

For a function $v : \mathbb{R} \to \mathbb{R}$, we say that $v \in H^1(SD)$ provided that v is the restriction to $\mathbb{R}$ of an analytic function in $H^1(SD)$.

Lemma 4.1 *Let $v : \mathbb{R}^2 \to \mathbb{R}$ be such that $v \in H^1(SD)$ with respect to each variable. Assume that*

$$|v(x_1, x_2)| \le \hat{C} e^{-\sigma_1 |x_1|} e^{-\sigma_2 |x_2|}$$

with $\hat{C} > 0$, $\sigma_1 > 0$ and $\sigma_2 > 0$. Then the following estimate

$$\Big| \int_{\mathbb{R}^2} v(x)dx - \int_{\mathbb{R}^2} (\mathcal{S}_M v)(x)dx \Big| \le C e^{-\sigma\sqrt{M}} \tag{4.14}$$

holds, where $\mathcal{S}_M$ is the operator corresponding to sinc-approximation in (4.10), *$C > 0$ and $\sigma > 0$.*

Proof. The one-dimensional case of sinc-quadrature rules and corresponding estimates were considered in [17]. The more general case of the sinc-quadrature rule over a plane for operator-valued functions was analysed in [7], and the estimate (4.14) follows from Theorem 3.3 in [7]. □

By $\|\cdot\|_\infty$ we mean the standard sup-norm for continuous functions (for both scalar and vector-valued functions). We sometimes indicate over which region this norm is taken, for example, $\|\cdot\|_{\infty, S_k}$ means the norm over the surface S_k.

Theorem 4.2 *For $f_k \in C^{r+2}(S_k)$, $r > 0$, $\beta \in H^1(SD)$ with $\beta(x) = O(e^{-\sigma|x|})$ and $\sigma > 0$, the following estimate*

$$\|\boldsymbol{\psi}^{(n)} - \boldsymbol{\psi}\|_\infty \le \frac{C_1}{n^r}$$

holds with $C_1 > 0$, where $\boldsymbol{\psi}$ and $\boldsymbol{\psi}^{(n)}$ are given by (4.3) *and* (4.8), *respectively.*

Proof. Let $\hat{\boldsymbol{\psi}}^{(n)}$ be the solution to (4.8) with the right-hand side changed from $\mathbf{g}_M$ to $\mathbf{g}$, that is $\hat{\boldsymbol{\psi}}^{(n)}$ satisfies

$$-\frac{1}{2}\hat{\boldsymbol{\psi}}^{(n)} + \mathcal{L}_n \mathbf{Q}^{n'} \hat{\boldsymbol{\psi}}^{(n)} = \mathcal{L}_n \mathbf{g},$$

where $\mathbf{g}$ have elements given by (4.4). Then we have the estimate

$$\|\boldsymbol{\psi} - \boldsymbol{\psi}^{(n)}\|_\infty \le \|\boldsymbol{\psi} - \hat{\boldsymbol{\psi}}^{(n)}\|_\infty + \|\boldsymbol{\psi}^{(n)} - \hat{\boldsymbol{\psi}}^{(n)}\|_\infty. \tag{4.15}$$

Taking into account the properties of the orthogonal projector $\mathcal{L}_n$, see [8], and in particular the estimates

$$\|\mathcal{L}_n\|_{\infty,\Omega} \le C n^{1/2}, \qquad \|\mathcal{L}_n \psi - \psi\|_{\infty,\Omega} \le \frac{C_r}{n^{r-1/2}} \|\psi\|_{r,\Omega}, \ \psi \in C^r(\Omega), \tag{4.16}$$

it is straightforward to show, see [5, 8], that for sufficiently large n, the inverse operators $(-\frac{1}{2}I + \mathcal{L}_n \mathbf{Q}^{n'})^{-1}$ exist and are bounded,

$$\Big\|(-\frac{1}{2}I + \mathcal{L}_n \mathbf{Q}^{n'})^{-1}\Big\| \le C n^{1/2}. \tag{4.17}$$

Moreover, the following estimate holds,

$$\|\boldsymbol{\psi} - \hat{\boldsymbol{\psi}}^{(n)}\|_\infty \le \frac{C_1}{n^r}, \tag{4.18}$$

due to the assumed smoothness of f_k and β and the implied smoothness of the right-hand side $\mathbf{g}$.

For the second term in (4.15) using the first estimate in (4.16) together with (4.17), we have

$$\|\boldsymbol{\psi}^{(n)} - \hat{\boldsymbol{\psi}}^{(n)}\|_\infty = \Big\|(-\frac{1}{2}I + \mathcal{L}_n \mathbf{Q}^{n'})^{-1} \mathcal{L}_n (\mathbf{g} - \mathbf{g}_M)\Big\|_\infty \le C n \|\mathbf{g} - \mathbf{g}_M\|_\infty.$$

For the elements of $\mathbf{g}$, due to the assumed smoothness of β, the element

$$v(y) = \beta(y)\tilde{G}_{21}(q_i(\hat{x}), y) + \alpha_i(q_i(\hat{x}))G_{21}(q_i(\hat{x}), y)$$

in the integrand in (4.2) is such that Lemma 4.1 can be applied. Combining this with the expression (4.9) for the elements of $\mathbf{g}_M$, it follows that the integrals in the difference $\mathbf{g}-\mathbf{g}_M$ can be estimated using Lemma 4.1 and the remaining terms can be estimated using the second estimate in (4.16). This and since, by assumption from Section 4.2, $M > n^2$, it follows that $\|\mathbf{g} - \mathbf{g}_M\|_\infty$ can be bounded by a term involving $1/n^r$. Thus, using this bound and (4.18) in (4.15) imply the statement of the theorem. □

According to (3.6) we have the following representation for the numerical solution of the problem (2.1)–(2.5)

$$t_i^{(n)}(x) = \sum_{k=1}^{m}\sum_{\ell=0}^{n}\sum_{j=-\ell}^{\ell} a_{\ell j}^k \sum_{\rho',s'} \tilde{\mu}_{\rho'}\tilde{a}_{s'} G_{i2}(x, q_k(\hat{y}_{\rho' s'}))J_{q_k}(\hat{y}_{\rho' s'})Y_{\ell,j}^R(\hat{y}_{s'\rho'})$$

$$+h_\infty^2 \sum_{\tilde{k},\bar{k}=-M}^{M} \beta(y_{\tilde{k}\bar{k}})\tilde{G}_{i1}(x, y_{\tilde{k}\bar{k}}), \quad x \in \mathcal{D}_i, \quad i = 1, 2.$$

5. Numerical examples

Example 5.1 We consider the case of a layer with thickness $h = 1$ and an ellipsoidal cavity (i.e. $m = 1$, see further Fig. 2a) with boundary surface:

$$S_1 = (\sin\theta\cos\varphi, 0.5\sin\theta\sin\varphi, 0.75\cos\theta + 3)^\top,$$

where $\theta \in [0, \pi]$, and $\varphi \in [0, 2\pi]$. The boundary data functions are given as

$$\beta(x) = e^{-|x|^2},\ x \in \Gamma_1, \qquad \alpha_1(x) = 1,\ f_1(x) = 0,\ x \in S_1.$$

The numerical solution of the problem (2.1)–(2.5), obtained using the indirect integral

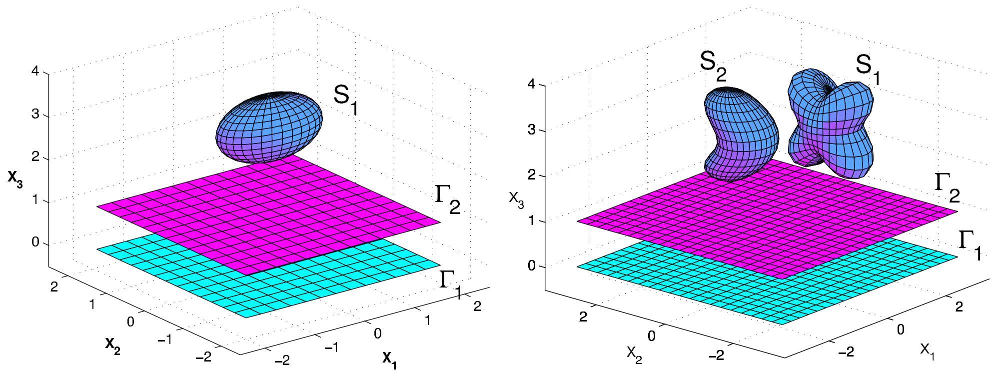
Tabl. 5.1. Numerical results for Example 5.1

	$x = (0, 0, 0.5)$		$x = (0, 0, 1.5)$	
n	Direct BIE	Indirect BIE	Direct BIE	Indirect BIE
4	0.1671504153	0.1671511644	0.0847707848	0.0848520554
8	0.1671514503	0.1671514513	0.0848589574	0.0848596942
16	0.1671514518	0.1671514518	0.0848597327	0.0848597327
32	0.1671514518	0.1671514518	0.0848597327	0.0848597327

equation approach outlined above, with $\lambda^{(1)} = 3$ and $\lambda^{(2)} = 4$, at two observation points (one inside the layer and one above) is presented in Table 1. This shows the exponential convergence of our method, and included in Table 1 is a comparison with the direct integral equation approach described in [18]. Here, we used $M = 100$ in the corresponding sinc quadratures and $\epsilon = 10^{-8}$ is the fixed precision for the series in the Green's matrix.

Example 5.2 Assume that the semi-infinite domain contains two cavities (i. e. $m = 2$) with surfaces (see Fig. 2b)

$$S_1 = (r(\theta, \varphi)p(\theta, \varphi)) + (1, -1, 3)^\top,$$



a) One ellipsoidal cavity b) Two cavities

Fig. 2. Semi-infinite layered domains with cavities

where $r(\theta, \varphi) = 0.8\sqrt{0.8 + 0.5(\cos 2\varphi - 1)(\cos 4\theta - 1)}$, $\theta \in [0, \pi]$, $\varphi \in [0, 2\pi]$ and

$$S_2 = \begin{pmatrix} 0.8\sqrt{1 - 0.1\cos(\pi\cos\theta)}\sin\theta\cos\varphi - 1 \\ 0.8\sqrt{1 - 0.1\cos(\pi\cos\theta)}\sin\theta\sin\varphi + 0.3\cos(\pi\cos\theta) \\ \cos\theta + 3 \end{pmatrix}.$$

The boundary functions are given as

$$\beta(x) = \frac{1}{(x_1^2 + x_2^2 + 1)^2}, \ x \in \Gamma_1,$$

$$\alpha_1(x) = 1, \ f_1(x) = 0, \ x \in S_1, \quad \alpha_2(x) = 1, \ f_2(x) = 1, \ x \in S_2.$$

The numerical solution with $\lambda^{(1)} = 3$ and $\lambda^{(2)} = 4$ in the two planes $x_3 = 0.5$ and $x_3 = 4.5$, respectively, are presented in Fig. 3 and in Fig. 4. Here, we used following values for the parameters needed in the method: $n = 8$, $\epsilon = 10^{-5}$ and $M = 50$. Also, note that in this case, the sinh substitution in the integral over the plane in (4.2) was employed to obtain the necessary asymptotic behaviour (see Lemma 3.1) according to the recommendation in [17].

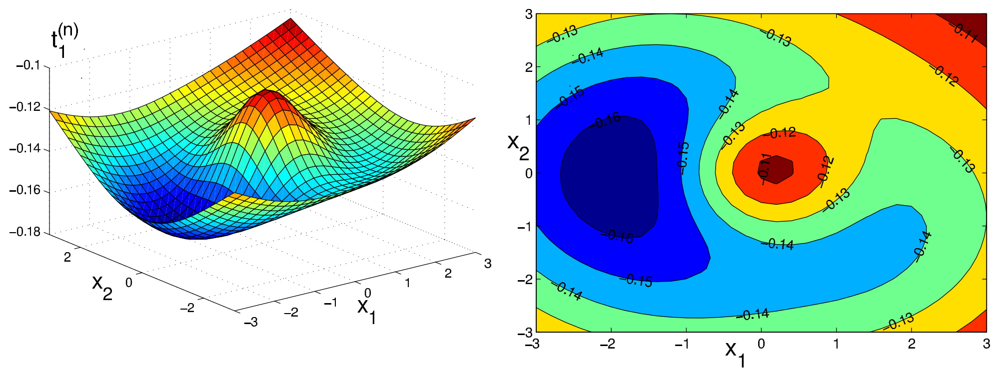


Fig. 3. The numerical solution on the plane $x_3 = 0.5$

The algorithm was implemented in MATLAB 7.1. All calculations were made on an Intel Xeon E5506 @ 2.14 Gz (4 core) processor. In Example 5.2, the CPU time for the

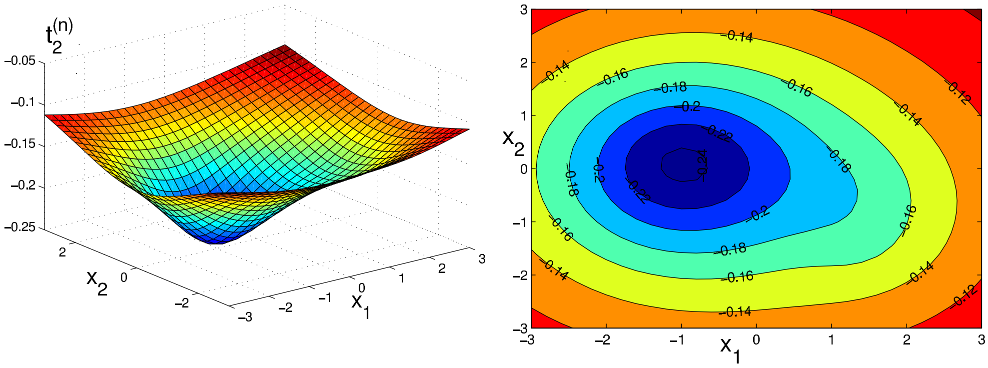


Fig. 4. The numerical solution on the plane $x_3 = 4.5$

calculation of the coefficients $a_{l,j}^k$ in (4.11) via (4.12) was 257.28 s and for the temperature field calculation at 900 spatial points on each of the two planes $x_3 = 0.5$ and $x_3 = 4.5$, the total time needed was 2027.04 s and 1296.75 s, respectively.

6. Conclusion

Using a Green's matrix technique, boundary value problems for the Laplace equation with piecewise constant conductivity in a semi-infinite layered 3-dimensional domain containing a finite number of bounded cavities, was reduced to weakly singular boundary integral equations over the surfaces of the cavities. For the surfaces, which are assumed to be homeomorphic to the unit sphere, a fully discrete projection method with super-algebraic convergence order was proposed based on Wienert's approach [20]. Our next investigations of this approach are connected with numerical construction of the bijective map q_k to the unit sphere for a given surface and with the use of the obtained direct solver for the numerical solution of some inverse problems.

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