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# Boundary integral equations for the computational modeling of three-dimensional groundwater flow problems

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**Abstract.** Boundary integral equations for the computational modeling of three-dimensional groundwater flow problems are derived. They follow from appropriate volume and surface source-type integral representations for the pressure and the flow velocity. The numerical handling of the integral equations is discussed in some detail, especially as far as the evaluation of singular integrals is concerned. Arbitrary anisotropy in the resistivity of the fluid-saturated soil is taken into account.

## 1 Introduction

In this paper we discuss the computational modeling of three-dimensional, steady, groundwater flow problems in piecewise homogeneous, and arbitrarily anisotropic fluid-saturated subsoils with the aid of the boundary-integral-equation method. To locate position in the configuration, we employ the coordinates $\{x_1, x_2, x_3\}$ with respect to an orthogonal Cartesian reference frame with origin $O$ and three mutually perpendicular base vectors $\{\boldsymbol{i}_1, \boldsymbol{i}_2, \boldsymbol{i}_3\}$ of unit length each. Partial differentiation is denoted by $\partial$. The subscript notation for vectors and tensors is used and the summation convention applies. Occasionally, a direct notation will be used to denote vectors; for example, $\boldsymbol{x} = x_k \boldsymbol{i}_k$ denotes the position vector.

The flow state of groundwater is characterized by the pressure $p$ and the flow velocity $v_i$. These quantities satisfy the continuity equation (e.g., Bear 1972)

$$\partial_i v_i = q, \tag{1}$$

and Darcy's law (e.g., Bear 1972)

$$\partial_i p + R_{ij} v_j = \varrho g_i + f_i, \tag{2}$$

where $q$ is the volume source density of volume injection rate, $f_i$ the volume source density of external force other than gravity, $R_{ij}$ the tensorial (symmetric and positive definite) resistivity of the fluid-saturated porous medium, $\varrho$ the volume density of fluid mass, and $g_i$ the local acceleration of free fall (assumed to be constant). Equations (1) and (2) can be derived from the creeping motion equations which describe the flow under the condition of a low Reynolds number (e.g., Slattery 1969; Whitaker 1969). Across an interface of discontinuity in resistivity and/or volume density of fluid mass, the pressure and the normal component of the flow velocity are to be continuous, while on each part of the outer surface bounding the flow configuration of interest either the pressure (e.g., at a freatic plane where it equals the atmospheric pressure), the normal component of the flow velocity (e.g., at an impervious base where it equals zero), or a linear combination of these quantities (e.g., at a relatively thin permeable layer at which the normal flow across the layer is related to the pressure difference across it) is prescribed. It is noted that upon successively integrating (1) over a bounded domain $\mathscr{D}$, occupied by the flow configuration at hand, and upon applying Gauss' theorem, (1) entails the corresponding compatibility relation:

$$\int_{\partial\mathscr{D}} v_i \nu_i \,\mathrm{d}A = \int_{\mathscr{D}} q \,\mathrm{d}V, \tag{3}$$

in which $\partial\mathscr{D}$ denotes the closed boundary surface of $\mathscr{D}$ and $v_i$ the unit vector along the direction of the outward normal to $\partial\mathscr{D}$. In (3), contributions from possible interfaces present in $\mathscr{D}$ have cancelled in view of the continuity requirements for the normal component of the flow velocity.

## 2 The reciprocity theorem for steady groundwater flow

Our derivation of the desired volume and surface source representations that hold in some bounded domain $\mathscr{D}$ is based on a reciprocity theorem that interrelates, in a specific way, the flow quantities of two admissible, but non-identical, ground-water flow states $\{p^A, v_i^A\}$ and $\{p^B, v_i^B\}$ that can occur in one and the same domain $\mathscr{D}$. To this end, we consider the following interaction quantity between the two states: $\partial_i(p^A v_i^B - p^B v_i^A)$. Taking into account that the basic equations pertaining to both states are of the form (1)–(2) and working out the interaction quantity, we are led to

$$\partial_i(p^A v_i^B - p^B v_i^A) = (R_{ij}^B - R_{ji}^A) v_i^A v_j^B + (\varrho^A v_i^B - \varrho^B v_i^A) g_i + f_i^A v_i^B - f_i^B v_i^A - q^A p^B + q^B p^A, \tag{4}$$

which is the local form of the reciprocity theorem. Integration of (4) over a bounded domain $\mathscr{D}$, the boundary of which is the closed surface $\partial\mathscr{D}$, and utilization of Gauss' theorem lead to the global form, for the domain $\mathscr{D}$, of the reciprocity theorem:

$$\int_{\partial\mathscr{D}} (p^A v_i^B - p^B v_i^A) \nu_i \,\mathrm{d}A = \int_{\mathscr{D}} (R_{ij}^B - R_{ji}^A) v_i^A v_j^B \,\mathrm{d}V + \int_{\mathscr{D}} [(\varrho^A v_i^B - \varrho^B v_i^A) g_i + f_i^A v_i^B - f_i^B v_i^A - q^A p^B + q^B p^A] \,\mathrm{d}V, \tag{5}$$

where $\nu_i$ is the unit vector in the direction of the outward normal to $\partial\mathscr{D}$. Note that on account of the continuity requirements for the pressure and the normal component of the velocity, in State $A$ as well as in State $B$, we can extend the validity of (5) to regions in which the field quantities, together with their first-order derivatives, are only piecewise continuous. The first term on the right-hand sides of (4) and (5) is characteristic for the difference in resistivity of the media present in the States $A$ and $B$, and vanishes at those points where $R_{ij}^A = R_{ji}^B$. The remaining part represents the interaction between the sources and the accompanying fluid-flow states. The reciprocity theorem (5) is now utilized to construct source-type integral representations for $p$ and $v_i$.

## 3 Source-type integral representations for the pressure and the flow velocity

To arrive at the source-type integral representations for the pressure we take in (5): $\{p^A, v_i^A\} = \{p, v_i\}$, where $p$ and $v_i$ apply to the actual flow state. Further, we take $\{p^B, v_i^B\} = \{p^{Gq}, v_i^{Gq}\}$, where $p^{Gq}$ and $v_i^{Gq}$ apply to a volume injection Green's state, i.e., they satisfy

$$\partial_i v_i^{Gq} = a\,\delta(\boldsymbol{x} - \boldsymbol{x}'), \tag{6}$$

$$\partial_i p^{Gq} + R_{ji} v_j^{Gq} = 0, \tag{7}$$

where $a$ is an arbitrary constant, $\delta(\boldsymbol{x} - \boldsymbol{x}')$ the three-dimensional spatial unit pulse (Dirac function) operative at $\boldsymbol{x} = \boldsymbol{x}'$, and $R_{ji}$ is the transpose of the resistivity $R_{ij}$ of the actual configuration (in our case, we have $R_{ij} = R_{ji}$). In (6) – (7) no explicit boundary conditions are imposed on the Green's flow state. The quantities $p^{Gq}$ and $v_i^{Gq}$ are linearly related to the constant $a$; we express this by writing $\{p^{Gq}, v_i^{Gq}\}(\boldsymbol{x}, \boldsymbol{x}') = a\{G^q, -\Gamma_i^q\}(\boldsymbol{x}', \boldsymbol{x})$, where $G^q$ and $\Gamma_i^q$ are the injection-source Green's functions. Using (1), (2), (6), (7) and the properties of the Dirac function, (5) leads to

$$-\int_{\partial\mathscr{D}} (G^q \nu_i v_i + \Gamma_i^q \nu_i p) \,\mathrm{d}A + \int_{\mathscr{D}} [G^q q + \Gamma_i^q (\varrho g_i + f_i)] \,\mathrm{d}V = \chi_{\mathscr{D}}(\boldsymbol{x}') p(\boldsymbol{x}'), \tag{8}$$

where $\chi_{\mathscr{D}}$ is the characteristic function of the set $\mathscr{D}$, defined as $\chi_{\mathscr{D}}(\boldsymbol{x}) = \{1, 1/2, 0\}$ when $\boldsymbol{x} \in \{\mathscr{D}, \partial\mathscr{D}, \mathscr{D}'\}$, in which $\mathscr{D}'$ denotes the complement of $\mathscr{D} \cup \partial\mathscr{D}$ in $\mathscr{R}^3$. For $\boldsymbol{x}' \in \partial\mathscr{D}$, (8) holds at points where $\partial\mathscr{D}$ has a unique tangent plane, provided that the surface integral is interpreted as its Cauchy principal value. Equation (8) is the desired source-type integral relation for the pressure field; when $x' \in \mathscr{D}$ it expresses the value of the pressure at the point $x = x'$ as the sum of contributions from the volume sources present in $\mathscr{D}$ and equivalent surface sources present on $\partial\mathscr{D}$.

To arrive at the source-type integral representations for the flow velocity, we take State $A$ as before, while now: $\{p^B, v_i^B\} = \{p^{Gf}, v_i^{Gf}\}$, where $p^{Gf}$ and $v_i^{Gf}$ apply to a force source (compensating gravity) Green's state and satisfy

$$\partial_i v_i^{Gf} = 0\,, \tag{9}$$

$$\partial_i p^{Gf} + R_{ji} v_j^{Gf} = b_i \delta\,(x - x')\,, \tag{10}$$

where $b_i$ is an arbitrary constant vector and where no explicit boundary conditions are imposed on this Green's flow state either. The quantities $p^{Gf}$ and $v_i^{Gf}$ are linearly related to $b_i$; we express this by writing $\{p^{Gf}, v_i^{Gf}\}\,(x, x') = b_j\{-\Gamma_j^f, G_{ji}^f\}\,(x', x)$, where $\Gamma_i^f$ and $G_{ij}^f$ are the force-source Green's functions. Using (1) and (2), the properties of the Dirac function, and (9) and (10), (5) yields:

$$-\int_{\partial\mathscr{D}} (\Gamma_i^f v_j v_j + G_{ij}^f v_j p)\,\mathrm{d}A + \int_{\mathscr{D}} [\Gamma_i^f q + G_{ij}^f(\varrho g_j + f_j)]\,\mathrm{d}V = \chi_{\mathscr{D}}(x')\,v_i(x')\,. \tag{11}$$

Equation (11) is the desired source-type integral relation for the velocity field; when $x' \in \mathscr{D}$ it expresses the value of the velocity at the point $x = x'$ as the sum of contributions from the volume sources present in $\mathscr{D}$ and equivalent surface sources present on $\partial\mathscr{D}$.

At this stage in the analysis it is emphasized that the construction of the different Green's tensor functions is, in general, complicated for inhomogeneous media, but is fairly straightforward for homogeneous media. In Sect. 5, $G^q$, $\Gamma_i^q$, $\Gamma_i^f$ and $G_{ij}^f$, are evaluated for a homogeneous and anisotropic, but reciprocal, medium of infinite extent.

## 4 The boundary-integral-equation method

To formulate the flow problem of groundwater in a piecewise homogeneous configuration, occupying the domain $\mathscr{D}$, in terms of boundary-integral equations, we assume that $\mathscr{D}$ is the union of $N$ homogeneous subdomains $\{\mathscr{D}_n;\, n = 1, \ldots, N\}$; the boundary surface of $\mathscr{D}_n$ is denoted by $\partial\mathscr{D}_n$. We now apply (8) and (11) to each homogeneous subdomain $\mathscr{D}_n$. In this, the Green's functions pertaining to each subdomain are taken to be the "infinite medium" ones (Sect. 5). Then, by taking successively $x' \in \partial\mathscr{D}_n$ for each $n = 1, \ldots, N$, (8) leads to a number of boundary-integral relations that are of the first kind in $v_i v_i$ and of the second kind in $p$, while (11) leads to boundary-integral relations that are of the first kind in $p$ and of the second kind in $v_i v_i$. At the interfaces between adjacent subdomains, the continuity of the pressure and the normal component of the velocity is used to introduce these quantities as unique unknowns in the resulting integral equations. At the outer boundary of $\mathscr{D}$ either the pressure, the normal component of the flow velocity, and/or a linear combinations of these are prescribed. The non-prescribed values at this outer boundary then are left as unknowns in the integral equations. In this way, we end up with a system of boundary-integral relations. Since the resulting number of equations equals at least twice the number of unknowns, there is a freedom in choice of equations to be employed in the actual calculations. In the literature (e.g., Liggett and Liu 1983), the boundary-integral-equation formulation is usually based on (8); this leads to integral equations of the first kind in $v_i v_i$ and of the second kind in $p$. However, since we here use (11) as well, complete systems of the second kind as well as of the first kind in both $p$ and $v_i v_i$ can be constructed.

## 5 The Green's flow states in an unbounded homogeneous domain

To evaluate the injection-source Green's flow states pertaining to a homogeneous medium of infinite extent we first multiply (7) on both sides by the, symmetric and positive definite, inverse $K_{ij}$ of $R_{ij}$. We then have

$$K_{ij}\,\partial_j p^{Gq} + v_i^{Gq} = 0\,. \tag{12}$$

Now, upon applying to both sides of (12) the operator $\partial_i$ and using (6), if follows that

$$K_{ij}\,\partial_i\,\partial_j\,p^{Gq} = -\,a\,\delta\,(\boldsymbol{x} - \mathrm{x}'). \tag{13}$$

To determine the solution of (13) we subject $x_i - x_i'$ to an orthogonal transformation such that the first term on the left-hand side is transformed on to its principal axes. Let

$$y_p = \alpha_{pq}(x_q - x_q') \tag{14}$$

be the relevant transformation, then the columns of the matrix $(\alpha_{pq})$ are the normalized right eigenvectors of $(K_{ij})$ corresponding to the $p$-th eigenvalue $t^{(p)}$ of $(K_{ij})$. We then have [cf. (13)]

$$K_{ij}\,\partial_i\,\partial_j\,p^{Gq} = t^{(p)}\partial_{y_p}\partial_{y_p}p^{Gq}, \tag{15}$$

where $\partial_{y_p}$ denotes differentiation with respect to $y_p$. Since $(\alpha_{pq})$ is orthogonal we have $\det(\alpha_{pq}) = 1$ and, hence [cf. (13)]

$$\delta\,(\boldsymbol{x} - \boldsymbol{x}') = \delta\,(\boldsymbol{y}). \tag{16}$$

Next, we introduce the variables $z_p$ through

$$z_p = (t^{(p)})^{-1/2}y_p, \tag{17}$$

then [cf. (15)]

$$t^{(p)}\partial_{y_p}\partial_{y_p}p^{Gq} = \partial_{z_p}\partial_{z_p}p^{Gq}, \tag{18}$$

and [cf. (16)]

$$\delta\,(\boldsymbol{y}) = [t^{(1)}t^{(2)}t^{(3)}]^{-1/2}\,\delta\,(\boldsymbol{z}) = [\det(R_{ij})]^{1/2}\,\delta\,(\boldsymbol{z}). \tag{19}$$

With the aid of (14)–(19), (13) transforms into

$$\partial_{z_p}\partial_{z_p}p^{Gq} = -\,a\,[\det(R_{ij})]^{1/2}\,\delta\,(\boldsymbol{z}). \tag{20}$$

Equation (20) is nothing but Poisson's equation for a point source with strength $a[\det R_{ij})]^{1/2}$ (e.g., Kellogg 1954) and its solution that is regular at infinity, i.e., vanishes as $|\boldsymbol{z}| \to \infty$, uniformly in all directions, is given by

$$p^{Gq} = a\,G, \tag{21}$$

where $G$ is given by

$$G = [\det(R_{ij})]^{1/2}/(4\pi\,|\boldsymbol{z}|). \tag{22}$$

However, $p^{Gq}$ is needed in terms of the original coordinates. Now, using (17) and (14), we obtain

$$|\boldsymbol{z}| = \{\alpha_{pi}\alpha_{pj}(t^{(p)})^{-1}(x_i - x_i')\,(x_j - x_j')\}^{1/2}. \tag{23}$$

Taking into account that $(t^{(p)})^{-1}$ are the eigenvalues of $(R_{ij})$, we have $\alpha_{pr}R_{rs}\alpha_{qs} = (t^{(p)})^{-1}\delta_{pq}$, and hence [cf. (23)]

$$\alpha_{pi}\alpha_{pj}(t^{(p)})^{-1} = \alpha_{pi}\alpha_{qj}(t^{(p)})^{-1}\delta_{pq} = \alpha_{pi}\alpha_{pr}R_{rs}\alpha_{qj}\alpha_{qs}. \tag{24}$$

Using in the right-hand side of (24) the orthogonality of $(\alpha_{pq})$ and employing the result in (23), it readily follows that [cf. (21) and (22)]

$$p^{Gq} = a\,G\,(\boldsymbol{x} - \boldsymbol{x}') = a\,[\det(R_{ij})]^{1/2}/(4\pi\,D) \tag{25}$$

in which $D$ is defined as

$$D = [R_{ij}(x_i - x_i')\,(x_j - x_j')]^{1/2}, \tag{26}$$

and can be regarded as the geodetical distance from $\boldsymbol{x}$ to $\boldsymbol{x}'$ with the resistivity as metric tensor. From (12) it further follows that

$$v_i^{Gq} = -\,a\,K_{ij}\,\partial_j\,G\,(\boldsymbol{x} - \boldsymbol{x}'). \tag{27}$$

The Green's functions $G^q$ and $\Gamma_i^q$ immediately follow from (25) and (27) as

$$G^q = G(\boldsymbol{x} - \boldsymbol{x}') \tag{28}$$

and

$$\Gamma_i^q = K_{ij}\,\partial_j\,G(\boldsymbol{x} - \boldsymbol{x}'). \tag{29}$$

To arrive at the force-source Green's flow state pertaining to a homogeneous medium of infinite extent, we apply $K_{ij}$ to both sides of (10) and obtain

$$K_{ij}\,\partial_j\,p^{Gf} + v_i^{Gf} = K_{ij}\,b_j\,\delta(\boldsymbol{x} - \boldsymbol{x}'). \tag{30}$$

Next, we apply the operator $\partial_i$ to both sides of this equation. Taking (9) into account, it then follows that

$$K_{ij}\,\partial_i\,\partial_j\,p^{Gf} = \partial_i\,K_{ij}\,b_j\,\delta(\boldsymbol{x} - \boldsymbol{x}'). \tag{31}$$

In view of the fact that $K_{ij}\partial_i\partial_j G = -\delta(\boldsymbol{x} - \boldsymbol{x}')$ [cf. (13) and (25)], $p^{Gf}$ can be expressed in terms of $G$ through

$$p^{Gf} = -K_{ij}\,b_j\,\partial_i\,G(\boldsymbol{x} - \boldsymbol{x}'). \tag{32}$$

Finally, from (30) and (32) the expression for $v_i^{Gf}$ follows as

$$v_i^{Gf} = K_{iq}\,b_j\,K_{pj}\,\partial_q\,\partial_p\,G(\boldsymbol{x} - \boldsymbol{x}') + K_{ij}\,b_j\delta(\boldsymbol{x} - \boldsymbol{x}'). \tag{33}$$

From (32) and (33) the Green's functions $\Gamma_i^f$ and $G_{ij}^f$ directly result as

$$\Gamma_i^f = K_{ji}\,\partial_j\,G(\boldsymbol{x} - \boldsymbol{x}') \tag{34}$$

and

$$G_{ij}^f = K_{jp}\,K_{qi}\,\partial_p\,\partial_q\,G(\boldsymbol{x} - \boldsymbol{x}') + K_{ji}\,\delta(\boldsymbol{x} - \boldsymbol{x}'). \tag{35}$$

## 6 Numerical aspects in solving the boundary-integral equations

To discretize any of the systems of boundary-integral equations, we first subdivide each of the boundary surfaces into planar, triangular surface elements. Let $\{S_T(n);\ n = 1, \ldots, NT\}$ denote this collection. The vertices of $S_T(n)$ have the position vectors $\{x_i(n,q),\ q = 1, 2, 3\}$ for later simplicity we take $x_i(n, q+3) = x_i(n,q)$. Each two adjacent triangles have an edge in common; their orientation is such that the direction of circulation forms a right-handed system with the (constant) normal $\nu_i(n)$ to $S_T(n)$. Next, in each triangle, the surface source distributions are linearly interpolated between their values at the vertices. Let $L_i(n,q)$ denote the vector along the normal to the $q$-th edge $C_T(n,q)$ in the plane of $S_T(n)$, having the length of this edge as its magnitude. Then, the linear function $\mathrm{K}(\boldsymbol{x}, n, q)$ that equals unity when $\boldsymbol{x} = \boldsymbol{x}(n,q)$ and is zero in the remaining two vertices can be written as

$$\mathrm{K}(\boldsymbol{x}, n, q) = 1/3 - [x_i - b_i(n)]\,L_i(n,q)/2A(n) \qquad \text{when } \boldsymbol{x} \in S_T(n), \tag{36}$$

where $b_i(n)$ is the position vector of the barycenter of $S_T(n)$ and $A(n)$ is the area of $S_T(n)$. The local expansions of the pressure and the normal component of the flow velocity are then

$$\{p, \nu_i v_i\}(\boldsymbol{x}) = \sum_{q=1}^{3} \{P(n,q),\ V(n,q)\}\,\mathrm{K}(\boldsymbol{x}, n, q) \qquad \text{when } \boldsymbol{x} \in S_T(n), \tag{37}$$

where $P(n,q)$ and $V(n,q)$ denote the values of the pressure and the normal component of the flow velocity at the $q$-th vertex of triangle $S_T(n)$. These expansion coefficients are now taken as the global unknowns over the discretized interfaces and the outer boundary surface. In correspondence to these global unknowns we now apply at the nodal points, i.e., the points where the vertices of different triangles meet, the method of collocation (point matching) to the integral expressions for the pressure and the normal component of the flow velocity. In this procedure we shall always encounter nodal points at which the unit normal vectors are not uniquely defined. This happens at nodal points where vertices of triangles in different planes meet. The relevant nodal points are considered as multiple vertices each with its own unit normal. This has the important advantage that all unit normals are uniquely defined and, hence, no ambiguities, with corresponding differences in numerical results, occur in defining normal vectors at the above "cumbersome" nodal points. Finally, we select from the resulting systems of linear, algebraic equations a proper square system from which the unknowns are solved.

In the matrix of coefficients and in the known right-hand sides of these systems of equations, surface integrals of the following types occur:

$$\{IG^q, I\Gamma^q, I\Gamma_i^f, IG_i^f\}(n,q,\boldsymbol{x}') = \int_{\boldsymbol{x}\in S_T(n)} \phi(\boldsymbol{x},n,q)\{G^q, \nu_i\Gamma_i^q, \Gamma_i^f, \nu_j G_{ij}^f\}(\boldsymbol{x}',\boldsymbol{x})\,\mathrm{d}A = \{(38\,\text{a, b, c, d})\},$$

where $\boldsymbol{x}'$ is a collocation point. The integrals (38 a, b, c, d) are evaluated analytically in the appendix. The contributions resulting from $q$ and $f_i$ in (8) and (11) can be evaluated once the sources have been specified. The remaining integrals associated with the gravity term $\varrho g_i$ are evaluated upon successively taking into account that $\varrho g_i$ has a constant value in each homogeneous subdomain, using the relations [cf. (28)–(29)] $\Gamma_i^q = K_{ij}\partial_j G^q$ and [cf. (34)–(35)] $G_{ij}^f = K_{jp}\partial_p \Gamma_i^f + K_{ji}\delta(\boldsymbol{x}-\boldsymbol{x}')$, and employing Gauss' theorem. This leads to integrals of the types $IG^q$ and $I\Gamma_i^f$, in which $\phi$ is replaced by unity; these can be evaluated analytically as well.

## 7 Numerical results

A Fortran 77 program has been written that handles the computations associated with our formulation. In order to test it we have first applied it to the given test flow $p = -3^{-1/2}(x_1 + x_2 + x_3) + x_3 + 3^{1/2} - 1$ and $\boldsymbol{v} = 3^{-1/2}(\boldsymbol{i}_1 + \boldsymbol{i}_2 + \boldsymbol{i}_3)$ in the source-free unit cube $\mathscr{D}$: $0 < x_1 < 1$, $0 < x_2 < 1$ and $0 < x_3 < 1$, where $\boldsymbol{g} = -10\boldsymbol{i}_3$, and with the homogeneous and isotropic medium $\varrho = 1$ and $R = 1$. The boundary surface of $\mathscr{D}$ is denoted by $\partial\mathscr{D} = \partial\mathscr{D}_1 \, U \partial\mathscr{D}_2$, where $p$ is prescribed on $\partial\mathscr{D}_1$ and $\nu_i v_i$ on $\partial\mathscr{D}_2$. Each face of the unit cube is divided into sixteen isosceles rectangular triangles, four triangles occupying a square region of dimension 0.5 × 0.5. Three cases were considered: (i) $\partial\mathscr{D}_1 = \{x_1 = 0, 0 < x_2 < 1, \; 0 < x_3 < 1\}$, (ii) $\partial\mathscr{D}_1 = \{x_1 = 0, 0 < x_2 < 1, \; 0 < x_3 < 1\} U \{0 < x_1 < 1, \; x_2 = 0, 0 < x_3 < 1\} U \{0 < x_1 < 1, 0 < x_2 < 1, x_3 = 1\}$, and (iii) $\partial\mathscr{D}_2 = \{0.5 < x_1 < 1, 0.5 < x_2 < 1, x_3 = 0\}$. Each nodal point was treated as a multiple vertex. Collocation in the discretized versions of the integral relations resulting from both (8) and (11) was applied in interior points located in the immediate vicinity of the vertices. The values of the relevant flow field quantities at these points have been taken to be ones that follow from the linear interpolation scheme (37). The resulting systems of linear, algebraic equations were solved by a direct method. For all three cases, the absolute errors in the computed values of the quantities in the collocation points are of the order of $10^{-11}$, i.e., within the computational accuracy employed. Obviously, this is due to the fact that the employed expansion functions exactly comply with the structure of the test flow field.

Furthermore, we have tested the code on the given flow field $p = -3^{-1/2}(x_i R_{i1} + x_i R_{i2} + x_i R_{i3}) + x_3 + 3^{-1/2}\sum_i^3\sum_j^3 R_{ij} - 1$ and $\boldsymbol{v} = 3^{-1/2}(\boldsymbol{i}_1 + \boldsymbol{i}_2 + \boldsymbol{i}_3)$ in the source-free domain $\mathscr{D}$, where $\boldsymbol{g} = -10\boldsymbol{i}_3$, and with the homogeneous and anisotropic medium $\varrho = 1$ and $R_{11} = 4$, $R_{22} = 5$, $R_{33} = 6$, $R_{12} = R_{21} = 1$, $R_{13} = R_{31} = 2$ and $R_{23} = R_{32} = 3$. Again, the linear interpolation scheme (37) was used in the discretization of the integral equations resulting from both (8) and (11), and collocation was applied in a similar manner as in the isotropic case. The three cases (i), (ii) and (iii) were considered and again results were obtained that were exact within the computational accuracy employed.

The performance of our computer code applied to more complicated (isotropic and anisotropic) test flows is still under development.

All computations have been performed on an IBM PC/AT. The CPU time for each test case was about 35 min.

In an earlier paper (Van der Weiden and De Hoop 1988), we have investigated the performance of the method for the isotropic test flow given above when taking piecewise constant values of $p$

and $\nu_i v_i$ at each triangle and applying collocation at the barycenters of the triangles. Naturally, the errors in the results are of the same order as the geometrical discretization error.

## Appendix

*Evaluation of surface integrals occurring in the discretized integral equations (isotropic case)*

In this appendix, we show how (38) is evaluated analytically for the case of an isotropic medium, i.e., $R_{ij} = R\delta_{ij}$ [cf. (2)]. From (36), (38a) and the assumed isotropy it follows that $IG^q$ has the shape:

$$IG^q(n,q,\boldsymbol{x}') = (R/4\pi)\,[S1\,(n,\boldsymbol{x}')/3 - S1Q\,(n,q,\boldsymbol{x}')/2A\,(n)], \tag{A 1}$$

where

$$S1\,(n,\boldsymbol{x}') = \int_{\boldsymbol{x}\in S_T(n)} |\boldsymbol{x}-\boldsymbol{x}'|^{-1}\mathrm{d}A, \tag{A2}$$

$$S1Q\,(n,q,\boldsymbol{x}') = \int_{\boldsymbol{x}\in S_T(n)} [x_i - b_i(n)]\,L_i(n,q)\,|\boldsymbol{x}-\boldsymbol{x}'|^{-1}\mathrm{d}A. \tag{A3}$$

To calculate $S1$, we first decompose $x_i - x_i'$ into a part normal to $S_T(n)$ and a part parallel to $S_T(n)$, i.e.,

$$x_i - x_i' = \zeta\,\nu_i(n) + y_i \qquad \text{when } \boldsymbol{x}\in S_T(n), \tag{A4}$$

where $\zeta$ is a constant given by

$$\zeta = \nu_i(n)\,(x_i - x_i'). \tag{A5}$$

Since $\boldsymbol{y}$ is a vector in the plane of $S_T(n)$, we can represent this vector with respect to some local two-dimensional orthogonal Cartesian reference frame in this plane. Let $y_\alpha$ with $\alpha = 1,2$ denote the Cartesian coordinates in this reference frame, then [cf. (A2)]

$$S1\,(\zeta) = \int_{\boldsymbol{y}\in S_T(n)} (\zeta^2 + y_\alpha y_\alpha)^{-1/2}\mathrm{d}A, \tag{A6}$$

where the summation convention to Greek subscripts applies to the range $\alpha = 1,2$. Assume $\zeta$ to be unequal to zero, i.e., $\boldsymbol{x}'$ is not in the plane of $S_T(n)$. We now differentiate (A6) on both sides twice with respect to $\zeta$ and apply in the resulting right-hand side the relation:

$$-(\zeta^2 + y_\alpha y_\alpha)^{-3/2} + 3\zeta^2(\zeta^2 + y_\alpha y_\alpha)^{-5/2} = \partial_\alpha[y_\alpha(\zeta^2 + y_\beta y_\beta)^{-3/2}]. \tag{A7}$$

Then, upon successively using the two-dimensional form of Gauss' theorem and rewriting the result with respect to the original reference frame, we end up with

$$\partial^2 S1\,(\zeta) = \sum_{q=1}^{3} \nu_i^C(n,q) \int_{\boldsymbol{y}\in C_T(n,q)} y_i(\zeta^2 + y_j y_j)^{-3/2}\mathrm{d}s, \tag{A8}$$

where $\nu_i^C(n,q)$ is the outwardly directed unit vector along the normal to the edge $C_T(n,q)$ lying in the plane of $S_T(n)$. To solve $S1\,(\zeta)$ from (A8) we simply integrate (A8) on both sides twice with respect to $\zeta$ and evaluate the remaining line integrals afterwards. After some tedious but elementary calculations the final result is obtained as

$$\begin{aligned} S1\,(n,\boldsymbol{x}') = {} & \zeta\,\mathrm{sgn}(\zeta) \sum_{q=1}^{3} \mathrm{sgn}\,[\nu_i^C(n,q)\,\varrho_i(n,q+1,\boldsymbol{x}')]\{\arctan(\theta 1\,(n,q,\boldsymbol{x}')) \\ & + (\mathrm{sgn}\,(\zeta))^{-1}\arctan(\theta 2\,(n,q,\boldsymbol{x}'))\} + \sum_{q=1}^{3} \nu_i^C(n,q)\,\varrho_i(n,q+1,\boldsymbol{x}')\,A\,(n,q,\boldsymbol{x}'), \end{aligned} \tag{A9}$$

where

$$\zeta = \nu_i(n)\,\varrho_i(n,1,\boldsymbol{x}'), \tag{A10}$$

$$\varrho_i(n,q,\boldsymbol{x}') = x_i(n,q) - x_i', \tag{A11}$$

$$1\,(n,q,\boldsymbol{x}') = \frac{|\zeta|\,|v_i^C(n,q)\,\varrho_i(n,q+1)|\,[\hat{a}_j(n,q)\,\hat{\varrho}_j(n,q+2) - \hat{a}_j(n,q)\,\hat{\varrho}_j(n,q+1)]}{|v_i^C(n,q)\,\varrho_i(n,q+1)|^2 + |\zeta|^2\,\hat{a}_i(n,q)\,\hat{\varrho}_i(n,q+1)\,\hat{a}_j(n,q)\,\hat{\varrho}_j(n,q+2)}, \tag{A12}$$

$$2\,(n,q,\boldsymbol{x}') = \frac{|v_i^C(n,q)\,\varrho_i(n,q+1)|\,[\hat{a}_j(n,q)\,\varrho_j(n,q+1) - \hat{a}_j(n,q)\,\varrho_j(n,q+2)]}{|v_i^C(n,q)\,\varrho_i(n,q+1)|^2 + \hat{a}_i(n,q)\,\varrho_i(n,q+1)\,\hat{a}_j(n,q)\,\varrho_j(n,q+2)}, \tag{A13}$$

$$\Lambda(n,q,\boldsymbol{x}') = ln\left[\frac{\hat{a}_i(n,q)\,\varrho_i(n,q+2) + \varrho\,(n,q+2)}{\hat{a}_i(n,q)\,\varrho_i(n,q+1) + \varrho\,(n,q+1)}\right], \tag{A14}$$

in which $a_i(n,q)$ denotes the $q$-th vectorial edge of $S_T(n)$, i.e.,

$$a_i(n,q) = x_i(n,q+2) - x_i(n,q+1) \qquad \text{with } q \in \{1,2,3\}, \tag{A15}$$

$\hat{a}_i(n,q)$ and $\hat{\varrho}_i(n,q+1)$ are normalized vectorial quantities defined as

$$\hat{a}_i(n,q) = a_i(n,q)/a(n,q), \tag{A16}$$

$$\hat{\varrho}_i(n,q+1) = \varrho_i(n,q+1)/\varrho\,(n,q+1), \tag{A17}$$

and $a(n,q)$ and $\varrho\,(n,q+1)$ are the lengths of $a_i(n,q)$ and $\varrho_i(n,q+1)$, respectively. For simplicity in writing we have omitted in $\varrho_i$ and $\varrho$ in the right-hand sides of (A12) – (A14) and (A17) the position vector $\boldsymbol{x}'$ of the collocation point [cf. (A11)]. Next, to evaluate $S1Q$, we first observe that [cf. (A4)]

$$x_i - b_i(n) = x_i' - b_i(n) + y_i + \zeta\,v_i(n) \qquad \text{when } \boldsymbol{x} \in S_T(n), \tag{A18}$$

and, hence, $S1Q$ leads directly to [cf. (A2) and (A3)]

$$S1Q\,(n,q,\boldsymbol{x}') = S1\,(n,\boldsymbol{x}')\,[x_i' - b_i(n)]\,L_i(n,q) + \int_{y \in S_T(n)} y_i L_i(n,q)(\zeta^2 + y_j y_j)^{-1/2}\,\mathrm{d}A, \tag{A19}$$

where we have taken into account that $v_i(n)$ and $L_i(n,q)$ are mutually perpendicular. To evaluate the surface integral on the right-hand side of (A19), we first rewrite it with respect to the local, two-dimensional reference frame in the plane of $S_T(n)$. In this, we take into account that

$$y_\alpha L_\alpha(n,q)\,(\zeta^2 + y_\beta y_\beta)^{-1/2} = \partial_\alpha\,[L_\alpha(n,q)\,(\zeta^2 + y_\beta y_\beta)^{1/2}], \tag{A20}$$

and subsequently use in the resulting integral the two-dimensional form of Gauss' theorem. Upon rewriting the result with respect to the original reference system, we then thave

$$\int_{y \in S_T(n)} y_i L_i(n,q)(\zeta^2 + y_j y_j)^{-1/2}\,\mathrm{d}A = \sum_{r=1}^{3} L_i(n,q)\,v_i^C(n,r) \int_{y \in C_T(n,r)} (\zeta^2 + y_j y_j)^{1/2}\,\mathrm{d}s. \tag{A21}$$

The remaining line integrals can be easily reduced to elementary scalar integrals. This completes the evaluation of $S1Q$, and, hence, of $IG^q$ [cf. (A1)].

The surface integrals $I\Gamma^q$, $I\Gamma_i^f$, and $IG_i^f$ follow from the expressions for $IG^q$ by carrying out the necessary differentiations after these have been written as acting on the point of observation. With this, the Green's functions integrals for the isotropic case have been covered.

To handle the corresponding integrals for the case of an anisotropic medium, we first subject the relevant expressions to the coordinate transformations discussed in Sect. 5 [cf. (14) and (17)], use the results for the isotropic case in the $\{z_1, z_2, z_3\}$ coordinate system, and transform the results back to the original $\{x_1, x_2, x_3\}$ coordinate system. This procedure has been followed in the computer program.

Integrals of the type $IG^q$ applying to the isotropic case, have also been evaluated analytically, in slightly different manners, by Waldvogel (1979) and Wilton et al. (1984).

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## References


Bear, J. (1972): Dynamics of fluids in porous media, pp. 106–192. New York: Elsevier

Kellogg, O. D. (1954): Foundations of potential theory, p. 156. New York: Dover

Liggett, J. A.; Liu, P. L.-F. (1983) The boundary integral equation method for porous media flow. London: Allen & Unwin

Slattery, J. C. (1969): Single-phase flow through porous media. Am. Inst. Chem. Eng. J. 15, 866–872

Waldvogel, J. (1979): The newtonian potential of homogeneous polyhedra. J. Appl. Math. Phys. 30, 388–398

Weiden, R. M. van der; de Hoop, A. T. (1988): The boundary-integral-equation method for computing the three-dimensional flow of groundwater. In: Cruse, Th. A. (Ed.): Advanced boundary element methods, pp. 451–458. IUTAM Symp. San Antonio TX, 1987. Berlin, Heidelberg, New York: Springer

Wilton, D. R.; Rao, S. M.: Glisson, A. W.; Schaubert, D. H.; Al-Bundak, O. M.; Butler, C. M. (1984): Potential integrals for uniform and linear source distributions on polygonal and polyhedral domains. IEEE Trans. Antennas Propag. AP-32, 276–281

Whitaker, S. (1969): Advances in the theory of fluid motion in porous media. Ind. Chem. Eng. J. 61, 14–28