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Corner singularities for elliptic problems: special basis functions versus "brute force"

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Abstract

A method is presented for the fast and accurate solution of elliptic boundary value problems on domains with corners. The method is based on integral equations and Nyström discretization. Close to corners two representations for the solution coexist – a pointwise representation and a representation in terms of special basis functions. Mappings and kernel evaluations are constructed on a symmetric corner panel. In a numerical example the electrostatic equation is solved for an array of square prisms. A dramatic improvement in efficiency over previous schemes is observed.

Key words: Corner, singularity, elliptic problem, integral equation of Fredholm type

1 Introduction

The determination of potential fields in domains containing geometric singularities is an important task in computational mechanics. Corners frequently occur in polycrystalline aggregates, and more generally as a result of geometric simplification in material design. V-notches, sometimes nearly atomically sharp, and kinks play a crucial role in fracture mechanics [1, 2, 3].

Domains with corners are easy to draw. It has been more difficult to resolve potential fields on them. Many standard numerical methods actually fail to give meaningful results in the vicinity of singularities such as corners [4]. Poor resolution tends to slow down the convergence rate of most iterative solvers [5].

Solving an elliptic problem on a domain with corners is seldom an ill-conditioned operation in itself. A small change in the geometry often does not change the solution much. Furthermore, asymptotically correct or exact solutions for simple geometries can be found by analytical methods [4, 6, 7, 8, 9]. Now, if simple corner problems are well conditioned and easy to solve, should it not be possible to find fast and accurate solutions also for corner problems that are more involved? As we shall soon see, this is indeed the case.

With "brute force" we mean adaptive mesh refinement for the purpose of approximating a singular function with polynomials. "Brute force" is an expensive way to achieve accuracy. One somehow needs to incorporate additional information into a numerical method in order to get efficiency for corners. Givoli and Rivkin [10] list a few possibilities: Superposition is an approximate scheme. An assumed asymptotically valid solution is subtracted from the original problem. A regular problem is left. In the context of the finite element method one can simply employ singular elements. A more refined approach is to introduce artificial boundaries. Szabó and Yosibash [11] use an approximate finite element solution as boundary condition for a complementary problem on a small subdomain around a singular point. Singular basis functions are then used to solve the complementary problem. Givoli, Rivkin, and Keller [4] use a Dirichlet to Neuman map as boundary condition between an analytic singular solution and a regular finite element solution. This last scheme is believed to be one of the more accurate [4]. Givoli, Rivkin, and Keller [4] report a relative accuracy in the solution of about $5 \cdot 10^{-4}$ for Laplace's equation in an example which has an analytical solution. Givoli and Vigdergauz have subsequently extended the method to the Helmholtz equation [12].

The leading idea of the present paper is in a sense similar to the ideas listed above. We will rely on knowledge about the asymptotic form of the solution close to the corners. However, the artificial boundary is avoided. On the mesh, close to a corner, a regular and a special representation of the solution coexist. The mapping between the two representations is made efficient by the introduction of a symmetric corner panel. The paper specializes to the electrostatic PDE in a two-component composite material. For stability reasons the PDE is reformulated as an integral equation of Fredholm's second kind. A careful strategy for the evaluation of the action of an integral operator in different topological situations is developed. In a non-trivial example the potential and effective properties of a dense suspension of square prisms is computed with a relative accuracy estimated to be about $5 \cdot 10^{-13}$.

The paper is organized as follows: A basic corner problem is solved by variable separation in Section 2. The transition to an integral equations takes place in Section 3. Basis functions for corners are constructed in Section 4. Section 5 introduces the symmetric corner panel, presents mappings, and discusses the evaluation of the integral operator. Numerical comparison between our new algorithm and "brute force" is given in Section 6.

2 A basic corner problem

A basic corner geometry is depicted in Figure 1. The computational domain D is a closed disk with a boundary S and local conductivity $\sigma(\mathbf{r})$. The disk D is divided into a dark sector D_1 with conductivity σ_1 and a light sector D_2 with conductivity σ_2 . The opening angle of D_2 is 2β . We seek the potential $U_{\mathbf{r}}$ at position \mathbf{r} in the disk subjected to a Dirichlet boundary condition $f(\mathbf{r})$. The electrostatic PDE can be written

$$(\nabla \cdot \sigma \nabla) U_{\mathbf{r}} = 0, \qquad \mathbf{r} \in D, \tag{1}$$

$$U_{\mathbf{r}} = f(\mathbf{r}), \qquad \mathbf{r} \in S.$$
⁽²⁾

Variable separation in polar coordinates ϕ and r shows that solutions to (1) can be found as functions Φ_n and Ψ_n of the form

$$\Phi_n = \begin{cases} r^{\nu_n} \cos[\nu_n \phi], & \mathbf{r} \in D_2, \\ a_n r^{\nu_n} \cos[\nu_n (\pi - \phi)], & \mathbf{r} \in D_1, \end{cases}$$
(3)



Figure 1: A disk D is divided into a dark sector D_1 with conductivity σ_1 and a light sector D_2 with conductivity σ_2 . The opening angle of D_2 is 2β .

$$\Psi_n = \begin{cases} r^{\lambda_n} \sin[\lambda_n \phi], & \mathbf{r} \in D_2, \\ b_n r^{\lambda_n} \sin[\lambda_n (\pi - \phi)], & \mathbf{r} \in D_1. \end{cases}$$
(4)

In equation (3) a_n and ν_n are given as the simultaneous solutions to the equations

$$\cos[\nu_n\beta] = a_n \cos[\nu_n(\pi - \beta)],$$

$$-\sigma_2 \sin[\nu_n\beta] = a_n \sigma_1 \sin[\nu_n(\pi - \beta)].$$
(5)

In equation (4) b_n and λ_n are given as the simultaneous solutions to the equations

$$\sin[\lambda_n \beta] = b_n \sin[\lambda_n(\pi - \beta)],$$

$$-\sigma_2 \cos[\lambda_n \beta] = b_n \sigma_1 \cos[\lambda_n(\pi - \beta)].$$
(6)

The solution to the electrostatic problem (1-2) can be written as a linear combination of the functions Φ_n and Ψ_n . The coefficients in this combination are determined from the boundary condition (2) by use of an inner product over the boundary S defined for two functions f_1 and f_2 on D as

$$\langle f_1, f_2 \rangle = \int_S f_1 f_2 \sigma \mathrm{d}t \,,$$

$$\tag{7}$$

where t is arclength. The calculation of the coefficients simplifies from the observation that all Φ_n and Ψ_n are mutually orthogonal with respect to the inner product (7).

3 Integral equation and effective properties of a suspension

Consider now a doubly periodic suspension of inclusions with conductivity σ_2 embedded in an infinite matrix filler of conductivity σ_1 . The material's geometry is defined in a unit cell taken to be the square $D_{\text{unit}} = (-1/2, 1/2] \times (-1/2, 1/2]$. The area fraction of the filler and the inclusions is p_1 and p_2 , respectively. The interfaces between all inclusions and the filler is denoted Γ . The restriction of Γ to D_{unit} is Γ_{unit} . The outward unit normal on Γ at arclength t is \mathbf{n}_t .

An average electric field \mathbf{e} of unit strength is applied to the suspension. This means that

$$\int_{D_{\text{unit}}} \nabla U_{\mathbf{r}} \mathrm{d}x \mathrm{d}y = \mathbf{e} \,. \tag{8}$$

The potential $U_{\mathbf{r}}$ in the suspension can be represented on the form [13]

$$U_{\mathbf{r}} = -\frac{1}{2\pi} \int_{\Gamma} \frac{(\mathbf{n}_t \cdot (\mathbf{r}_t - \mathbf{r}))}{|\mathbf{r}_t - \mathbf{r}|^2} U_{\mathbf{r}_t} dt - \frac{1}{2\pi} \int_{\Gamma} \log|\mathbf{r} - \mathbf{r}_t| (\nabla U_{\mathbf{r}_t} \cdot \mathbf{n}_t) dt, \qquad (9)$$

where \mathbf{r}_t denotes $\mathbf{r}(t)$. In terms of a scaled potential $u_{\mathbf{r}}$ defined by

$$u_{\mathbf{r}} = \frac{(\sigma_2 - \sigma_1)}{\sigma_1} U_{\mathbf{r}},\tag{10}$$

and with the use of Green's second identity, equations (1) and (8) can be reformulated as an integral equation of Fredholm's second kind [14]

$$(I - K)u_{\mathbf{r}} = 2\rho(\mathbf{e} \cdot \mathbf{r}), \qquad \mathbf{r} \in \Gamma.$$
 (11)

Here ρ is the material constant

$$\rho = \frac{\sigma_2 - \sigma_1}{\sigma_2 + \sigma_1},\tag{12}$$

and K is the compact integral operator defined by

$$Ku_{\mathbf{r}} = \frac{\rho}{\pi} \int_{\Gamma} \frac{(\mathbf{n}_t \cdot (\mathbf{r}_t - \mathbf{r}))}{|\mathbf{r}_t - \mathbf{r}|^2} u_{\mathbf{r}_t} \mathrm{d}t, \qquad \mathbf{r} \in \Gamma.$$
(13)

The effective conductivity in the direction \mathbf{e} can be computed from $u_{\mathbf{r}}$ via

$$\sigma_{\text{eff}} = \sigma_1 + \sigma_1 \int_{\Gamma_{\text{unit}}} (\mathbf{e} \cdot \mathbf{n}_t) u_{\mathbf{r}_t} \mathrm{d}t.$$
(14)

Remark: There are many ways to represent the electric potential $U_{\mathbf{r}}$ in a suspension. Equation (9) is just a convenient choice. For a detailed study of the computational properties of different integral equation reformulations of the electrostatic PDE, see Referece [15].

4 Representation of the potential close to a corner

We shall solve equation (11) with a Nyström scheme [16]. This means approximating integral operators with matrices and solving a system of linear equations via the following steps

- 1. The integral in (11) is discretized according to a quadrature rule. We will chiefly choose 16-point composite Gaussian quadrature.
- 2. The scaled potential $u_{\mathbf{r}}$ and the right hand side of (11) are represented with pointwise values at quadrature nodes. If we use N quadrature nodes we will have N unknown values of $u_{\mathbf{r}}$ to solve for.



Figure 2: Two panels with 16 quadrature points. The panel Γ_r to the left is intented for a part of the boundary which is smooth. The symmetric panel Γ_c to the right is intented for a part of the boundary which contains a corner.

- 3. It is required that the discretized integral equation should be satisfied pointwise at all N quadrature nodes. This gives rise to a system of N linear equations for the N unknown values of $u_{\mathbf{r}}$.
- 4. The system of N linear equations is solved with any suitable method. We choose the GMRES iterative solver [17].

Wherever the interfaces are smooth, the potential $u_{\mathbf{r}}$ will be polynomial-like and Gaussian quadrature will do fine in the Nyström scheme.

Close to a corner the the potential $u_{\mathbf{r}}$ will not be polynomial-like. Equations (3) and (4) suggest that $u_{\mathbf{r}}$ should be represented by a power series involving the positive exponents ν_n and λ_n . Let us take a corner with opening angle $2\beta = \pi/2$ as an example. Solutions ν_n and λ_n to equations (5-6) involve integral as well as non-integral numbers. Furthermore, for some integral values of ν_n and λ_n the functions Φ_n and Ψ_n will vanish on the corner interface. From now on, ν_n and λ_n will denote the solutions to equations (5-6), in ascending order, for which Φ_n and Ψ_n do not vanish on the corner interface. As an additional representation for $u_{\mathbf{r}}$ on the interface close to a corner we suggest

$$u_{\mathbf{r}} \approx \sum_{n=1}^{8} c_n s^{\nu_n} \pm c_{n+8} s^{\lambda_n},$$
 (15)

where c_n are 16 coefficients, s is the distance from the corner, and \pm indicates that different signs should be chosen depending on if **r** is on the right or on the left of the corner.

5 The action of K

Figure 2 depicts two quadrature panels $\Gamma_{\rm r}$ and $\Gamma_{\rm c}$, each containing 16 quadrature points. The panel $\Gamma_{\rm r}$ belongs to a regular part of the interfaces. The symmetric panel $\Gamma_{\rm c}$ is centered around a corner. On $\Gamma_{\rm r}$ the points are placed with a spacing determined by the nodes of the 16th Legendre polynomial. On each of the legs of $\Gamma_{\rm c}$ the points are placed with a spacing determined by the nodes of the 8th Legendre polynomial. In this section we will explain how to calculate the action of the operator K of (13) on $u_{\rm r}$ for source- and target points on panels of the types $\Gamma_{\rm r}$ and $\Gamma_{\rm c}$.

The evaluation of K is trivial when the source points are located on panels of the type $\Gamma_{\rm r}$. This holds irrespective of where the target points are. Let $K^{\rm or}$ be the part of the

operator K which describes interaction between target points on a panel of the type Γ_r and source points on some other panel. We just follow the Nyström scheme with 16-point composite Gaussian quadrature and write

$$K_{ij}^{\rm or} = K_{in}^{\rm 0or} W_{nj}^0 \,, \tag{16}$$

where $K_{in}^{0\text{or}}$ is a straight-forward discretization of the kernel of K^{or} and W_{nj}^{0} is a diagonal matrix of scaled Gaussian weights.

When the source points are on a panel of the type Γ_c we distinguish between two cases. The first case is when the target points are also on that same panel Γ_c . We call the part of the operator K which describes this self-interaction K^{cc} . The second case is when the target points are on some other segment. We call the part of the operator K which describes this interaction K^{cc} .

We now show how to calculate the 16×16 entries of the two matrices

$$K_{ij}^{\rm cc}$$
, and $K_{ij}^{\rm oc}$, $i, j = 1, ..., 16$,

where K_{ij}^{cc} is the mapping of K from target point j on a panel of type Γ_c to source point i on that same panel, and where K_{ij}^{oc} is the mapping of K from target point j on a panel of type Γ_c to source point i on some other panel.

Some auxiliary mappings are introduced. For a corner panel where each leg has length unity, let A_{ij} be the mapping from the coefficient c_j in the expansion (15) to the corresponding value of $u_{\mathbf{r}}$ at points t_i on the panel. For that same corner panel, let B_{ij} be the action of K on the *j*th basis function in the expansion of (15) evaluated at t_i on the panel. The entries B_{ij} are integrals of the type

$$\frac{\rho}{\pi} \int_0^1 \frac{t_i \sin(2\beta) s^{\nu_j} \mathrm{d}s}{s^2 + t_i^2 - 2st_i \cos(2\beta)}, \quad \text{and} \quad \frac{\rho}{\pi} \int_0^1 \frac{t_i \sin(2\beta) s^{\lambda_j} \mathrm{d}s}{s^2 + t_i^2 - 2st_i \cos(2\beta)}.$$
(17)

Let v_{ij} and w_{ij} , i, j = 1, ..., 8, be the weights at node x_i in an 8-point quadrature rule for computing the integrals

$$\int_0^1 f(x) x^{\nu_j} \mathrm{d}x \approx \sum_{i=1}^8 f(x_i) v_{ij} ,$$

$$\int_0^1 f(x) x^{\lambda_j} \mathrm{d}x \approx \sum_{i=1}^8 f(x_i) v_{ij} ,$$
 (18)

where f is a smooth function. We are now ready to write

$$K_{ij}^{\rm cc} = (BA^{-1})_{ij} \,, \tag{19}$$

and

$$K_{ij}^{\rm oc} = \frac{\gamma_{\rm c}}{2} K_{in}^{\rm 0oc} (WA^{-1})_{nj} \,, \tag{20}$$

where γ_c is the arclength of Γ_c , K_{in}^{0oc} is a straight-forward discretization of the kernel of K^{oc} and W is a full 16×16 block matrix which contains permutations of the 8×8 matrices v and w with positive or negative signs.

Note that the entries of the matrix products BA^{-1} , and WA^{-1} only depend on the opening angle of the corners involved in a particular problem. They do not depend on the orientation or on the size of the corner panel. They can therefore be computed and stored prior to solving the actual PDE.



Figure 3: A doubly periodic square array of square prisms. The darker background matrix has conductivity $\sigma_1 = 1$. The lighter prisms have conductivity $\sigma_2 = 100$ and occupy an area fraction of $p_2 = 0.49$.

6 Numerical examples and conclusion

Figure 3 depicts a periodic square array of square prisms. The conductivity of the filler is $\sigma_1 = 1$ and of the prisms $\sigma_2 = 100$. The volume fraction of the prisms is $p_2 = 0.49$. Solving equation (11) on this geometry is a non-trivial problem in the sense that there is no known analytic solution and that some prism corners are close to touching. We prefer to test our method on a non-trivial problem, rather than on one which has an analytical solution. The reason for this is that we believe that problems which have analytical solutions sometimes are rather easy to solve also with numerical methods. Especially so if, as in our algorithm, the numerical scheme makes heavy use of analytical information. As a consequence, high accuracy for an example which has an analytical solution does not necessarily prove that a numerical method is efficient. A drawback with testing on non-trivial problems is, of course, that one does not know the answer in advance. However, there are indirect ways of estimating accuracy which, when they are compounded, can become quite convincing. Such ways include test for stability of the solution under overresolution, test for consistency with analytical relations for functionals on the solution, and comparison with the predictions of other, well-tested, codes. These indirect ways will be used for error estimation in this section.

At least three studies have been performed in the past on solutions to the electrostatic PDE on the geometry of Figure 3. Milton, McPhedran, and McKenzie [18] used a variational fractional power series approach and determined the effective conductivity to $\sigma_{\text{eff}} = 5.15$. Hui and Ke-da [19] used a series expansion approach and improved this result to $\sigma_{\text{eff}} = 5.147$. Helsing [20] used a second kind Fredholm integral equation approach based on a single layer representation of $U_{\mathbf{r}}$ together with "brute force" and reported $\sigma_{\text{eff}} = 5.14729406$. The code used in [20] has been extensively tested for accuracy and consistency against analytical results [20], against Fourier series based computations [20, 21], on large scale geometries [15], and against bounds for extreme cases [22]. The typical accuracy in σ_{eff} for non-trivial but well-conditioned problems involving smooth interfaces is twelve digits [20, 21].

We use the evaluation techniques of Section 5 to solve equation (11) adaptively with a Nyström scheme. The GMRES iterative solver [17] is used for the system of linear equations.

Table 1: Effective conductivity σ_{eff} of the square array of prisms depicted in Figure 3. The background material has conductivity $\sigma_1 = 1$. The prisms have conductivity $\sigma_2 = 100$ and their area fraction is $p_2 = 0.49$. In the table 'points' denote the number of discretization points in the unit cell, 'basis' refers to the method of this paper, "brute" refers to regular adaptive mesh refinement, and 'iter' is the number of iterations required by GMRES to achieve a residual less than 10^{-14} .

points	$\sigma_{\rm eff}$ basis	iter basis	$\sigma_{\rm eff}$ "brute"	iter "brute"
64	5.1	11	5	12
320	5.14729	13	5	14
576	5.1472940563	14	5.15	15
832	5.14729405633	16	5.15	16
1088	5.147294056325	17	5.147	17
1344	5.147294056325	18	5.1473	19
1600	5.147294056325	18	5.1473	20
1856	5.147294056325	19	5.14729	20
2112	5.147294056325	20	5.14729	21
2368	5.147294056325	20	5.1472941	22
2642	5.147294056326	21	5.1472941	23
2880	5.147294056327	22	5.1472941	23
3136	5.147294056325	22	5.14729406	25

The applied average electric field \mathbf{e} of (8) is taken to be parallel to the x-axis. We start out with dividing the interface in the unit cell (and all its periodic images) into four panels of the type Γ_c , corresponding to 64 discretization points. This gives the estimate $\sigma_{\text{eff}} = 5.1$. We then proceed to refine the mesh where needed, that is, chiefly in the corners that point in the direction of the applied field \mathbf{e} , and solve again. A convergence study for σ_{eff} is given in Table 1. The converged value $\sigma_{\text{eff}} = 5.147294056325$ was reached with 1,088 discretization points and did not change upon overresolution up to over 3,000 points. We also performed calculations with the applied average electric field \mathbf{e} rotated an angle of $\pi/4$. The local electric field then becomes quite different, exhibiting equal magnitudes in all four corners of each prism. With 1,984, or more, discretization points on the interface we again reached the converged value $\sigma_{\text{eff}} = 5.147294056325$. The square array of prisms of Figure 3 has an isotropic effective conductivity tensor.

For comparison Table 1 also shows computations done with "brute force" according to my algorithm [20] but with the integral equation in [20] replaced by equation (11). As we can see, the difference in efficiency between the two approaches is substantial, particularly so in terms of economy of discretization points, but to a lesser extent also in terms of achievable accuracy. The converged results for σ_{eff} in Table 1 agree completely with the value $\sigma_{\text{eff}} = 5.14729406$ in [20]. We also observe that the convergence rate of the GMRES iterative solver does not seem sensitive to whether the corner singularity is well resolved or not.

In Figure 3 we let the prisms have area fraction $p_2 = 0.49$. If we let $p_2 \rightarrow 0.5$, some corners will lie very close to each other. The region, near a corner, where the asymptotic form for $u_{\mathbf{r}}$ of equation (15) is a good approximation will shrink due to interaction with a neighboring prism. The need for resolution grows while our ability to resolve the interface is

Table 2: Effective conductivity σ_{eff} of a square array of prisms at various area fractions p_2 . The background material has conductivity $\sigma_1 = 1$. The prisms have conductivity $\sigma_2 = 100$. The entry 'points' denotes the smallest number of discretization points in the unit cell needed for the reported accuracy of σ_{eff} . The entry 'iter' denotes the number of iterations required by the GMRES solver for that calculation.

p_2	points	$\sigma_{ m eff}$	iter
0.49	1088	5.147294056325	17
0.499	1088	6.96143566063	17
0.4999	1088	8.1830855833	16
0.49999	1344	8.944642384	17
0.499999	1600	9.39762485	17
0.4999999	1856	9.6596761	18
0.49999999	2112	9.808851	18
0.4999999999	2368	9.89299	18

limited by the IEEE double precision standard. The problem becomes more ill-conditioned. A study of the behavior of σ_{eff} under this limiting process is presented in Table 2. Note that good accuracy can be achieved also for values of p_2 that are rather extreme.

We conclude that it is certainly possible to find geometries for which elliptic problems are difficult to solve. A very dense suspension is one example. However, the presence of a geometric singularity, such as a corner, should not cause any additional loss of accuracy.

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