

## NUMERICAL CALCULATION OF THE LEADING SINGULAR COEFFICIENTS IN LAPLACIAN PROBLEMS OVER L-SHAPED DOMAINS

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**Abstract.** *We solve a Laplacian problem over an L-shaped domain using a singular function boundary integral method as well as the  $p/hp$  finite element method. In the former method, the solution is approximated by the leading terms of the local asymptotic expansion, and the unknown singular coefficients are calculated directly. In the latter method, these coefficients are computed by post-processing the finite element solution. The predictions of the two methods are discussed and compared with recent numerical results in the literature.*

### 1 INTRODUCTION

In the past few decades, many different methods have been proposed for the numerical solution of plane elliptic boundary value problems with boundary singularities, aiming at improving the accuracy and resolving the convergence difficulties that are known to appear in the neighborhood of such singular points. These methods range from special mesh-refinement schemes to sophisticated techniques that incorporate, directly or indirectly, the form of the local asymptotic expansion, which is known in many occasions. In polar coordinates  $(r, \theta)$  centered at the singular point, the local solution is of the general form

$$u(r, \theta) = \sum_{j=1}^{\infty} \alpha_j r^{\mu_j} f_j(\theta) \quad (1)$$

where  $\mu_j$  are the eigenvalues and  $f_j$  are the eigenfunctions of the problem, which are uniquely determined by the geometry and the boundary conditions along the boundaries sharing the singular point. The singular coefficients  $\alpha_j$ , also known as generalized stress intensity factors, are determined by the boundary conditions in the remaining part of the boundary. Knowledge of the singular coefficients is of importance in many engineering applications.

In the Finite Element Method (FEM), which is the most commonly used method for solving structural mechanics problems, the singular coefficients are calculated by post-processing the numerical solution. Generally speaking, the most effective versions of the FEM are the high-order  $p$  and  $hp$  versions, in which instead of simply refining the mesh, convergence is achieved by: (i) increasing the degree of the piecewise polynomials in the case of the  $p$  version, and (ii) by increasing  $p$  and decreasing  $h$  in the case of the  $hp$  version. The reason for the success of these methods is that they are able to approximate singular components of the solution to elliptic boundary value problems (that arise, for example, at corners of the domain) very efficiently. For instance, the  $hp$  version, over appropriately designed meshes, approximates these singularities at an exponential rate of convergence<sup>[1]</sup>.

In the past few years, Georgiou and co-workers<sup>[2-4]</sup> developed the Singular Function Boundary Integral Method (SFBIM), in which the unknown singular coefficients are calculated directly. The solution is approximated by the leading terms of the local asymptotic solution expansion and the Dirichlet boundary conditions are weakly enforced by means of Lagrange multipliers. The method has been tested on standard

Laplacian problems, yielding extremely accurate estimates of the leading singular coefficients, and exhibiting exponential convergence with respect to the number of singular functions.

The objective of the present paper is to compare the predictions of the SFBIM against those of the  $p/hp$  version of the FEM. We consider as a test problem the Laplacian problem over an  $L$ -shaped domain solved by Igarashi and Honma<sup>[5]</sup> with a singular boundary integral method. The accuracy of the calculated singular coefficients is restricted to five significant digits. As shown below, the predictions of both the SFBIM and the  $p/hp$  FEM are of much higher accuracy.

## 2 APPLICATION OF THE SFBIM TO A TEST PROBLEM

We consider the same Laplacian problem over an  $L$ -shaped domain as that solved by Igarashi and Honma<sup>[5]</sup>. This is shown in Figure 1. Taking into account the symmetry of the problem, we consider only half of the domain and note that even-numbered coefficients are zero. The local solution expansion around the singularity at  $O$  may be written as follows:

$$u = \sum_{j=1}^{\infty} \alpha_j W^j \quad (2)$$

where

$$W^j = r^{2(4j-3)/3} \sin\left[\frac{2}{3}(4j-1)\theta\right] \quad (3)$$

are the singular functions.

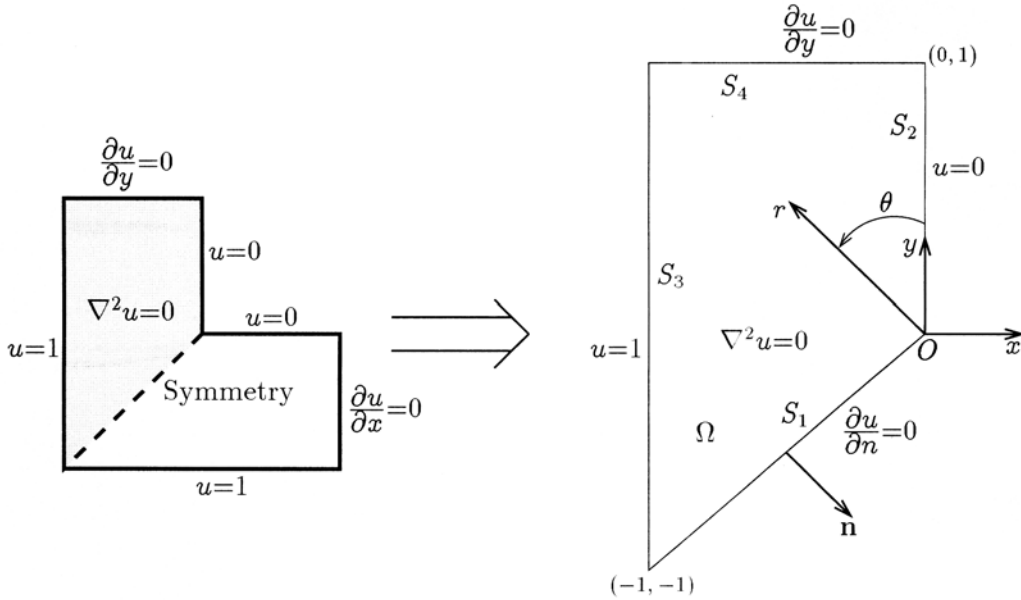


Figure 1. Geometry and boundary conditions of the test problem

The SFBIM is based on the approximation of the solution by the leading terms of the local solution expansion:

$$\bar{u} = \sum_{j=1}^{N_\alpha} \bar{\alpha}_j W^j \quad (4)$$

where  $N_\alpha$  is the number of singular functions. It should be noted that this approximation is valid only if the domain  $\Omega$  is a subset of the convergence domain of the expansion (2). Given that the singular functions  $W^j$  are harmonic, applying Galerkin's principle and the second identity of Green, we obtain the following discretized equations:

$$\int_{\partial\Omega} \left( \frac{\partial \bar{u}}{\partial n} W^i - \bar{u} \frac{\partial W^i}{\partial n} \right) dS = 0, \quad i = 1, \dots, N_\alpha \quad (5)$$

Since  $W^j$  exactly satisfy the boundary conditions along  $S_1$  and  $S_2$ , the above integral along these boundary

segments is identically zero. Along boundary  $S_4$  the normal derivative is zero. Finally, the Dirichlet condition along  $S_3$  is imposed by means of a Lagrange multiplier function  $\lambda$ , replacing the normal derivative. The function  $\lambda$  is expanded in terms of standard, polynomial functions  $M^j$ ,

$$\lambda = \frac{\partial \bar{u}}{\partial n} = \sum_{j=1}^{N_\lambda} \lambda_j M^j \quad (6)$$

where  $N_\lambda$  represents the total number of the unknown discrete Lagrange multipliers along  $S_3$ . The basis functions  $M^j$  are used to weight the Dirichlet condition along the corresponding boundary segment  $S_3$ . We thus obtain the following system of  $N_\alpha + N_\lambda$  discretized equations:

$$-\int_{S_3} \left( \lambda W^i - \bar{u} \frac{\partial W^i}{\partial x} \right) dy - \int_{S_4} \left( \bar{u} \frac{\partial W^i}{\partial y} \right) dx = 0, \quad i = 1, \dots, N_\alpha \quad (7)$$

$$\int_{S_3} \bar{u} M^i dy = \int_{S_3} M^i dy, \quad i = 1, \dots, N_\lambda \quad (8)$$

It is easily shown that the above linear system is symmetric. The integrands in Eq. (7) are non-singular and all integrations are carried out far from the boundaries causing the singularity.

In Ref. [5], the quantity

$$C = 2 \int_{S_3 \cup S_4} \frac{\partial u}{\partial n} dS = -2 \int_{-1}^1 \left[ \frac{\partial u}{\partial x} \right]_{x=-1} dy \quad (9)$$

referred to as the capacitance, was of interest; we will also consider this quantity in our computations.

### 3 NUMERICAL RESULTS WITH THE SFBIM

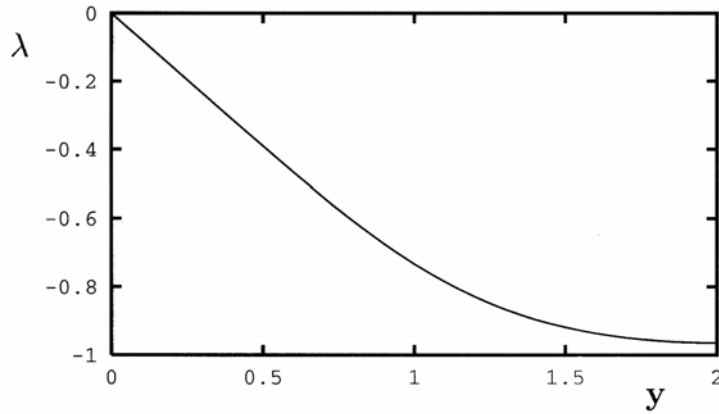
The Lagrange multiplier function  $\lambda$  used to impose the Dirichlet condition along  $S_3$  is expanded in terms of quadratic basis functions. Boundaries  $S_3$  and  $S_4$  are subdivided, respectively, into  $2N$  and  $N$  quadratic elements of equal size. Thus, the number of Lagrange multipliers is  $N_\lambda = 4N + 1$ . The integrals in Eqs. (7) and (8) are calculated numerically by subdividing each quadratic element into 10 subintervals and using a 15-point Gauss-Legendre quadrature over each subinterval. In computing the coefficient matrix, its symmetry is taken into account.

Several series of runs were performed in order to obtain the optimal values of  $N_\alpha$  and  $N_\lambda$ . Our search was guided by the fact that  $N_\lambda$  should be large enough in order to assure accurate integrations along the boundary (which is divided into smaller elements) but much smaller than  $N_\alpha$  in order to avoid ill-conditioning of the stiffness matrix. On the other hand,  $N_\alpha$  cannot be very high, given that the computer accuracy cannot handle the contributions of the higher-order singular functions which become very small for  $r < 1$  or very large for  $r > 1$ . Hence,  $N_\lambda$  was varied from 4 up to 65 and  $N_\alpha$  from a value slightly above  $N_\lambda$  up to 100.

The convergence of the solution with the number of Lagrange multipliers is shown in Table 1, where we tabulate the values of  $\alpha_1$ ,  $\alpha_2$  and  $\alpha_5$  and the capacitance  $C$  calculated with  $N_\alpha = 60$ . We observe that the values of the singular coefficients converge rapidly with  $N_\lambda$ , up to  $N_\lambda = 41$ , and that very accurate estimates are obtained. For higher values of  $N_\lambda$ , however, signs of divergence are observed, due to the ill-conditioning of the stiffness matrix. In addition to the divergence of the singular coefficients, another manifestation of ill-conditioning is the appearance of wiggles on the calculated Lagrange multiplier function<sup>[4]</sup>. The quality of the solution for  $N_\alpha = 60$  and  $N_\lambda = 41$  was checked by verifying that  $\lambda$  is smooth and free of oscillations (Figure 2).

$N_\lambda$	$\alpha_1$	$\alpha_2$	$\alpha_5$	$C$
5	1.12797118414119	0.16993982990692	0.00096430271538	2.5585187
9	1.12798030920688	0.16993376833638	0.00091656933158	2.5585226
17	1.12798039995306	0.16993386409437	0.00091515473431	2.5585229
25	1.12798040098244	0.16993386632558	0.00091515689483	2.5585231
33	1.12798040105726	0.16993386650219	0.00091515710753	2.5585226
41	1.12798040105939	0.16993386650225	0.00091515709910	2.5585231
49	1.12798038900362	0.16993384321933	0.00091522372105	2.5556215

Table 1: Convergence of the solution with  $N_\lambda$ ; SFBIM with  $N_\alpha = 60$ .

Figure 2. Calculated Lagrange multipliers with  $N_\alpha = 60$  and  $N_\lambda = 41$ 

The values of the leading singular coefficients and the capacitance  $C$  calculated for  $N_\lambda = 41$  and various values of  $N_\alpha$  are shown in Table 2. Exponential convergence with respect to  $N_\alpha$  is observed and extremely accurate estimates of the singular coefficients are obtained. Our calculations with different values of  $N_\alpha$  and  $N_\lambda$  show that the optimal values are  $N_\alpha = 60$  and  $N_\lambda = 41$ . In Table 3, the converged values of the singular coefficients calculated with these optimal choices are present. The CPU time required for the above run is 1.6 s on an IBM RS6000 (Processor type: Power PC 604e/375 MHz).

$N_\alpha$	$\alpha_1$	$\alpha_2$	$\alpha_5$	$C$
45	1.12798046929652	0.16993391450191	0.00091337482002	2.5467734
50	1.12798040111620	0.16993386693468	0.00091509465304	2.5585230
55	1.12798040105939	0.16993386650225	0.00091515709909	2.5585231
60	1.12798040105939	0.16993386650225	0.00091515709910	2.5585231
65	1.12798040105939	0.16993386650223	0.00091515709917	2.5585231
70	1.12798040105938	0.16993386650176	0.00091515710049	2.5585230
75	1.12798040105929	0.16993386650304	0.00091515709264	2.5585230
80	1.12798040105953	0.16993386650246	0.00091515710302	2.5585232

Table 2: Convergence of the solution with  $N_\alpha$ ; SFBIM with  $N_\lambda = 41$ .

In Table 3, we see that the contributions of the higher-order terms are progressively vanishing. Note that the converged value of  $\alpha_1$  (1.12798040105939) is accurate to fifteen significant digits, while the value provided by Igarashi and Honma<sup>[5]</sup> (1.1280) is accurate only to five significant digits. The improved accuracy is also reflected on the calculated value of the capacitance which is converged to eight significant digits,  $C = 2.5585231$ .

Finally, in Figure 3, we plot the errors in the calculated values of the leading singular coefficients for  $N_\alpha = 60$  versus the number of Lagrange multipliers. The errors are based on the converged values tabulated in Table 3. It is clear that the SFBIM converges exponentially with  $N_\lambda$ , and the error is reduced rapidly down to machine accuracy.

$i$	$\alpha_i$	Ref. [5]
1	1.12798040105939	1.1280
2	0.16993386650225	0.1699
3	-0.02304097399348	-0.0230
4	0.0034711966582	0.0035
5	0.0009151570991	0.0009
6	-0.0001128038345	
7	0.0000877165245	
8	0.0000277603137	
9	-0.0000044161578	
10	0.0000027539457	
11	0.0000009219619	
12	-0.0000001554459	
13	0.0000001088408	
14	0.0000000379699	
15	-0.0000000066619	
16	0.000000004711	
17	0.00000000168	
18	0.00000000030	
19	0.00000000022	
20	0.00000000008	
$C$	2.5585231	2.5585

Table 3: Converged values of the leading singular coefficients; SFBIM with  $N_\lambda = 41$  and  $N_\alpha = 60$ .

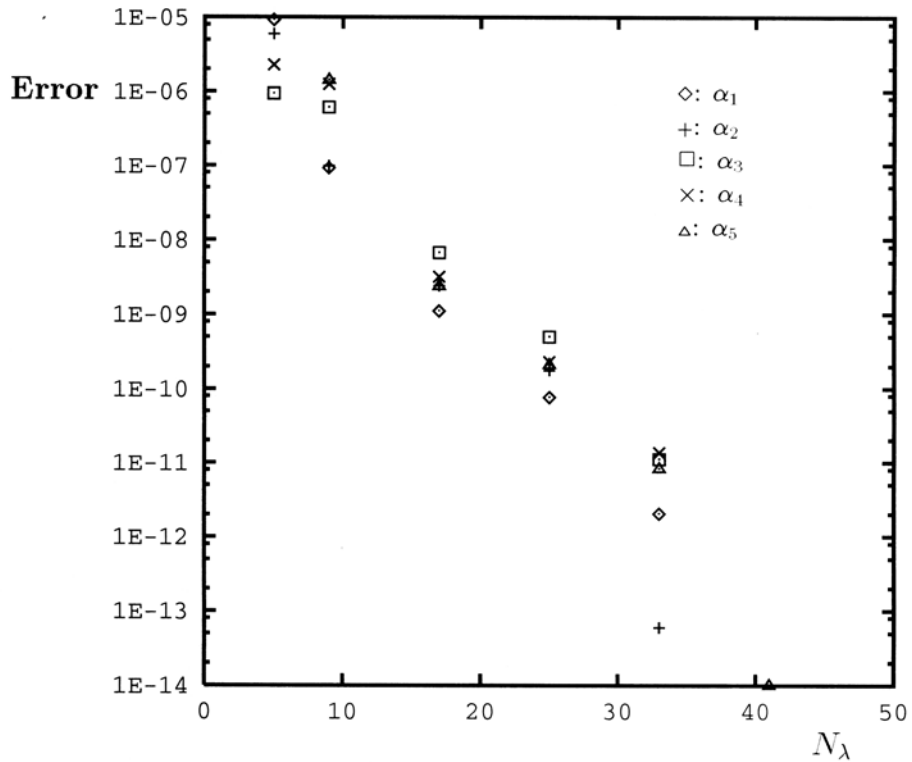


Figure 3. Convergence of the SFBIM with  $N_\lambda$ ;  $N_\alpha = 60$

#### 4 NUMERICAL RESULTS WITH THE $p/hp$ VERSION OF THE FINITE ELEMENT METHOD

In this section we present the results of solving the same test problem, using the  $p/hp$  version of the FEM a geometrically graded mesh seen in Figure 4. This is, to our knowledge, the most effective technique for approximating the solution to elliptic boundary value problems with corner singularities in the context of the FEM. We refer to the book of Szabo and Babuska<sup>[6]</sup> for more details on corner singularities and geometrically graded meshes in conjunction with the  $p$  and  $hp$  versions of the FEM. Once the solution is obtained, the singular coefficients are obtained as a post-solution operation. In particular, the algorithm for computing the  $\alpha_i$ 's is based on an  $L^2$ -projection of the finite element solution into the space of functions characterized by the asymptotic expansion in terms of the eigenpairs, which are computed using a modified Steklov method<sup>[7,8]</sup>.

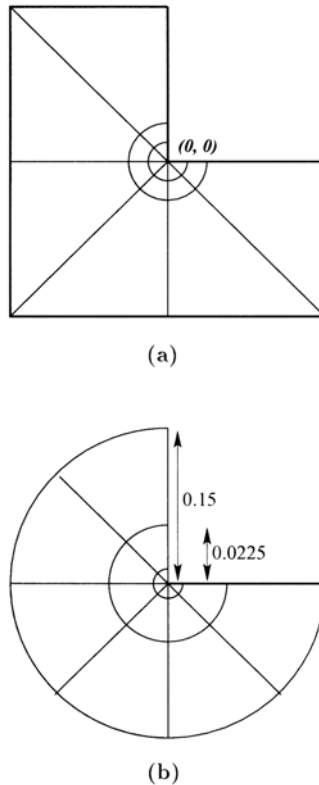


Figure 4. (a) Geometrically graded mesh over the domain  $\Omega$ ; (b) Mesh detail near the re-entrant corner

The computations were performed using the commercial FEM package STRESSCHECK (E.S.R.D. St. Louis, MO) on an IBM Pentium III machine. Since this is a  $p$  version package, the geometrically graded mesh was constructed a priori and the polynomial shape functions were taken to have degree  $p = 1, \dots, 8$ , uniformly over all elements in the (fixed) mesh. The CPU time was approximately 9 s for the calculation of the finite element solution,  $u_{FE}$ , and about 2 s for the calculation of the singular coefficients. Table 4 shows the potential energy as well as the (estimated) percentage relative error in the energy norm,

$$Error = 100 \times \frac{\|u_{EX} - u_{FE}\|_{E(\Omega)}}{\|u_{EX}\|_{E(\Omega)}} \quad (10)$$

indicating that the solution  $u_{FE}$  is computed accurately. Table 5 shows the computed singular coefficients, which were obtained using the finite element solution corresponding to  $p = 8$ . These results show that the  $p$  version of the FEM (on geometrically graded meshes) seems to perform quite well when compared with the results obtained using other methods found in the literature.

$p$	DOF	Energy	Error (%)
1	10	1.3385078	21.52
2	39	1.2819648	4.60
3	74	1.2806200	3.26
4	127	1.2793571	0.85
5	198	1.2792877	0.43
6	287	1.2792738	0.28
7	394	1.2792690	0.20
8	519	1.2792667	0.15

Table 4: Values of the potential energy and the percentage relative error in the  $p/hp$  method

The capacitance  $C$ , defined by Eq. (9), was calculated using the finite element solution  $u_{FE}$  corresponding to  $p = 8$ , by employing a 5-point Gaussian quadrature (to ensure the integral in Eq. (9) is evaluated exactly). We obtained  $C = 2.557256$ , an approximation which is not as good as that obtained using the SFBIM. We believe this is due to the pollution effects that are influencing the extraction of the data of interest (see e.g. Ref. [6]). Pollution is a phenomenon that occurs when singularities are present in the solution of an elliptic boundary value problem. These singularities cause the numerical method to yield inaccurate results away from the singularity point (as is the case here), when certain quantities of engineering interest are computed. The  $p$  version of the FEM is especially susceptible to pollution effects (in contrast to the  $h$  and  $hp$  versions). We repeated the calculation using a more refined mesh near the re-entrant corner, as seen in Figure 5. The newly computed singular coefficients are shown in Table 5 and the capacitance is recomputed as  $C = 2.558588$ , which is a much better approximation. The refined mesh required 691 degrees of freedom (for  $p = 8$ ) as opposed to 519 used before, and the CPU time increased by 1 s.

$i$	$\alpha_i$ , DOF=519	$\alpha_i$ , DOF=691
1	1.12797960	1.12798010
2	0.16993396	0.16993387
3	-0.0230434	-0.0230419
4	-0.0034780	-0.0034755
5	0.0009115	0.0009126
$C$	2.557256	2.558588

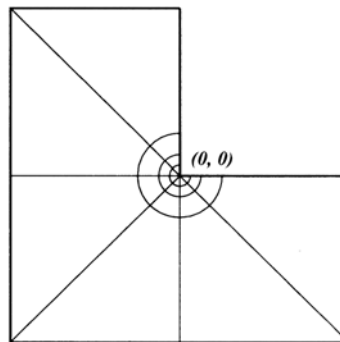
Table 5: Values of the leading singular coefficients obtained with the  $p/hp$  finite element method

Figure 5. Refined mesh

## 5 CONCLUSIONS

We have solved a Laplacian problem over an  $L$ -shaped domain using both the SFBIM and the  $p/hp$  finite element method, and studied the convergence of the solution with the numbers of singular functions and of Lagrange multipliers, and the number of degrees of freedom, respectively. With the SFBIM the leading singular coefficients of the local singularity expansion are calculated explicitly, whereas with the  $p/hp$ -FEM they are calculated by post-processing the numerical solution.

Fast convergence is achieved and highly accurate results are obtained with both methods, which perform considerably better than other techniques found in the literature (e.g. that of Igarashi and Honma<sup>[5]</sup>). Given that there are no known exact values for the singular coefficients, the very good agreement between the SFBIM and the  $p/hp$  FEM serves as validation for the computational results presented here. We should point out that, in terms of efficiency, the SFBIM is a better choice, since the singular coefficients are computed directly and no post-processing is necessary. On the other hand, the FEM can be applied to a much wider class of problems than those that can efficiently and effectively be handled by the SFBIM. We should mention that currently there is no mathematical theory that establishes the observed exponential convergence rate of the SFBIM. This is the focus of our current research efforts.

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