

# Methods of fundamental solutions for harmonic and biharmonic boundary value problems

A. Poullikkas, A. Karageorghis, G. Georgiou

416

**Abstract** In this work, the use of the Method of Fundamental Solutions (MFS) for solving elliptic partial differential equations is investigated, and the performance of various least squares routines used for the solution of the resulting minimization problem is studied. Two modified versions of the MFS for harmonic and biharmonic problems with boundary singularities, which are based on the direct subtraction of the leading terms of the singular local solution from the original mathematical problem, are also examined. Both modified methods give more accurate results than the standard MFS and also yield the values of the leading singular coefficients. Moreover, one of them predicts the form of the leading singular term.

## 1 Introduction

Standard numerical methods for solving elliptic boundary value problems perform poorly in the neighbourhood of boundary singularities. The accuracy is, in general, low and the convergence with mesh refinement slow. Special methods taking into account the local form of the singularity appear to give much better results and have thus received considerable attention in the past years (Symm 1973; Kelmanson 1983; Li et al. 1987; Mason et al. 1984; Olson et al. 1991; Nagarajan and Mukherjee 1993; Guiggiani 1995). The form of the singularity for the Laplace or the biharmonic equation is obtained locally using separation of variables techniques. For the two-dimensional case, the asymptotic solution in polar coordinates  $(r, \theta)$  centered at the singular point is given by:

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

where  $u$  is the dependent variable,  $\alpha_j$  are the singular coefficients,  $\lambda_j$  are the singularity powers which in biharmonic problems might be complex,  $f_j(\theta)$  represent the  $\theta$  dependence of the eigensolution, and  $\Omega$  is the bounded domain of the problem. The values of the singular coefficients  $\alpha_j$  depend on the global problem and they are often useful in many applications. For example, in fracture mechanics, the first singular coefficient is the stress intensity factor, a measure of the stress at which fracture occurs.

Boundary methods have become popular in recent years due to their computational efficiency. This is a consequence of the fact that only the boundary of the domain needs to be discretised. The dimension of the problem is therefore reduced by one. The Method of Fundamental Solutions (MFS), which can be viewed as an indirect boundary element method, has found extensive application in computing solutions to a broad range of problems (Mathon and Johnston 1977; Karageorghis and Fairweather 1987, 1989; Karageorghis 1992a,b). The basic idea is to approximate the solution in terms of a set of fundamental solutions of the governing equation. These depend on the position of a fixed number of sources located outside the domain of solution. The coefficients in the linear combination of the fundamental solutions and the final location of the sources are calculated in order to satisfy the boundary conditions in some optimal sense. Two of the advantages of the method are its relatively easy implementation and, since it takes into account sharp changes in the geometry of the domain, its adaptivity. Like other boundary methods, the MFS, in its present form, is applicable to any elliptic boundary value problem, provided the fundamental solution of the governing equation is known.

One drawback of the MFS is its high computational cost resulting from the use of a non-linear least squares minimization routine (Mathon and Johnston 1977; Karageorghis and Fairweather 1987). In order to improve the efficiency of the method, the use of two sets of least squares routines is investigated. For the routines in the first set, the Jacobian is evaluated internally by a finite-difference scheme whereas in the second set the Jacobian must be provided by the user. The routines are tested on simple harmonic and biharmonic problems, the analytical solutions of which are known. Subsequently, two modified versions of the MFS for solving two elliptic problems with boundary singularities, namely, the Motz problem (Symm 1973) and the stick-slip problem (Richardson 1970), are examined. Both methods incorporate the singular behav-

Communicated by D. E. Beskos, 15 November

A. Poullikkas  
Electricity Authority of Cyprus, P.O. Box 113,  
CY-6301 Larnaca, Cyprus

A. Karageorghis, G. Georgiou  
Department of Mathematics and Statistics,  
University of Cyprus, Kallipoleos 75, P.O. Box 537,  
CY-1678 Nicosia, Cyprus

Correspondence to: A. Karageorghis

The authors wish to thank Professor Graeme Fairweather of the Colorado School of Mines for his useful comments and suggestions and the two referees for their constructive comments.

our of the problem under investigation and are based on the subtraction of the leading terms of the singularity. The first one was developed by Karageorghis (1992b). The second one is new and allows the prediction of the nature of the leading singular term. This is particularly useful when the analytic behaviour of the singularity is not known a priori.

In Sect. 2, the MFS formulations for harmonic and biharmonic problems are presented. In Sect. 3, the description of the two test problems and a discussion of the computational efficiency of the various minimization routines are given. In Sect. 4, results obtained with the modified MFS of Karageorghis (1992b) are presented, and a new modified MFS, that predicts not only the first singular coefficient but also the radial and angular dependence of the leading singular term in the Motz and the stick-slip problems, is developed. The conclusions are summarized in Sect. 5.

## 2 MFS formulation

### 2.1 Harmonic problems

Consider the problem

$$\nabla^2 u = 0 \quad \text{in } \Omega, \quad (2)$$

subject to the boundary condition

$$u = g(x, y) \quad \text{on } \partial\Omega, \quad (3)$$

where  $\nabla^2$  denotes the Laplace operator,  $g$  is a given function,  $\Omega$  is a bounded domain in the plane, and  $\partial\Omega$  denotes its boundary. In the MFS,  $N$  sources, the coordinates of which are to be calculated, are placed outside the domain  $\Omega$ , and  $M$  fixed points are chosen along the boundary  $\partial\Omega$ . Let  $\mathbf{t}_j = (t_{jx}, t_{jy})$  denote the coordinates of source  $j$  and  $\mathbf{p}_i = (p_{ix}, p_{iy})$  be the coordinates of boundary point  $i$ . The vector  $\mathbf{t}$  contains the unknown coordinates of all the sources,  $\mathbf{t} = [t_{1x}, t_{1y}, t_{2x}, t_{2y}, \dots, t_{Nx}, t_{Ny}]^T$ . Let  $\bar{u}$  be the approximation of the solution and  $\bar{u}_i$  be its value at the point  $\mathbf{p}_i$ :

$$\bar{u}_i \equiv \bar{u}(\mathbf{c}, \mathbf{t}, \mathbf{p}_i) = \sum_{j=1}^N c_j k(\mathbf{t}_j, \mathbf{p}_i), \quad (4)$$

where  $\mathbf{c} = [c_1, c_2, \dots, c_N]^T$  is the vector of the unknown coefficients and  $k(\mathbf{t}_j, \mathbf{p}_i) = \log r_{ij}$  is the fundamental solution of Laplace's equation with

$$r_{ij} = \sqrt{(p_{ix} - t_{jx})^2 + (p_{iy} - t_{jy})^2}.$$

Because  $\bar{u}$  satisfies the differential equation (2), the coefficients  $c_j$  and the positions of the sources  $\mathbf{t}_j$  are chosen so that the boundary conditions are satisfied in a least-squares sense, i.e. by minimizing the nonlinear functional

$$F(\mathbf{c}, \mathbf{t}) = \sum_{i=1}^M (\bar{u}_i - g(\mathbf{p}_i))^2. \quad (5)$$

### 2.2 Biharmonic problems

Consider the problem

$$\nabla^4 u = 0 \quad \text{in } \Omega, \quad (6)$$

subject to either

$$u = g_1(x, y), \quad \frac{\partial u}{\partial n} = h_1(x, y) \quad \text{on } \partial\Omega, \quad (7)$$

or

$$u = g_2(x, y), \quad \nabla^2 u = h_2(x, y) \quad \text{on } \partial\Omega, \quad (8)$$

where  $\partial u / \partial n$  denotes the outward normal derivative and  $g_1, g_2, h_1$  and  $h_2$  are prescribed functions.

As in Karageorghis and Fairweather (1987), the solution at point  $\mathbf{p}_i$  is approximated by a linear combination of fundamental solutions of both the Laplace and biharmonic equations:

$$\bar{u}(\mathbf{c}, \mathbf{d}, \mathbf{t}, \mathbf{p}_i) = \sum_{j=1}^N c_j k_1(\mathbf{t}_j, \mathbf{p}_i) + \sum_{j=1}^N d_j k_2(\mathbf{t}_j, \mathbf{p}_i), \quad (9)$$

where  $\mathbf{d} = [d_1, d_2, \dots, d_N]^T$  is another vector of unknown coefficients, and  $k_2(\mathbf{t}_j, \mathbf{p}_i) = r_{ij}^2 \log r_{ij}$  is the fundamental solution of the biharmonic equation.

As with harmonic problems, the approximation  $\bar{u}$  of the solution satisfies the differential equation (6), and the coefficients  $c_j, d_j$  and the positions of the sources  $\mathbf{t}_j$  must be chosen so that the boundary conditions are satisfied. To achieve this, the following functional is minimized

$$F(\mathbf{c}, \mathbf{d}, \mathbf{t}) = \sum_{i=1}^M \left[ (\bar{u}_i - g_1(\mathbf{p}_i))^2 + \left( \frac{\partial \bar{u}_i}{\partial n} - h_1(\mathbf{p}_i) \right)^2 \right], \quad (10)$$

or

$$F(\mathbf{c}, \mathbf{d}, \mathbf{t}) = \sum_{i=1}^M [(\bar{u}_i - g_2(\mathbf{p}_i))^2 + (\nabla^2 \bar{u}_i - h_2(\mathbf{p}_i))^2], \quad (11)$$

depending on the type of the boundary conditions.

## 3 Efficient implementation of the MFS algorithm

The minimization of the functional  $F$  for both harmonic and biharmonic problems is performed using existing least squares algorithms. The routines LMDIF and LMDER from MINPACK (Garbow et al. 1980) were first used. Both routines minimize the sum of the squares of  $M$  nonlinear functions in  $N$  variables by a modification of the Levenberg-Marquardt algorithm and require the user to provide a subroutine that calculates the values of  $\bar{u}$ . LMDIF evaluates the Jacobian internally by a forward-difference approximation, whereas LMDER requires the user to provide a subroutine that evaluates the Jacobian analytically. The subroutine E04UPF from NAG (see NAG 1991) was also used. This subroutine employs a sequential quadratic programming algorithm and minimizes a functional consisting of a sum of squares. In our case, this functional is given by Eqs. (5) and (10) or (11). The subroutine can be

used either for unconstrained or constrained optimization. The user must provide subroutines that define the function values of  $\bar{u}$  and nonlinear constraints and as many of their first partial derivatives as possible, or the exact Jacobian. Unspecified derivatives are approximated by finite-differences. The computational effort is measured in terms of the CPU time required by the routine to converge to a user-specified tolerance  $\epsilon$ , that is,  $|u - \bar{u}| \leq \epsilon$ .

The initial placement of the moving sources and the positioning of the fixed boundary points greatly affect the convergence of the least squares procedure. Customarily, the sources are distributed uniformly at a fixed distance from the boundary (Karageorghis and Fairweather 1987), and the boundary points are placed uniformly on the boundary. The number  $M$  of boundary points is chosen to be approximately three times the number of unknowns, as recommended in the literature (Mathon and Johnston 1977; Karageorghis and Fairweather 1987). The tendency of the sources to move to the interior of the domain  $\Omega$  is overcome by an internal check of the position of singularities during the iterative process. If a source is found inside  $\Omega$  it is repositioned at the exterior of the domain (Karageorghis and Fairweather 1987; Karageorghis 1992a,b).

The computational efficiency of LMDIF, LMDER and E04UPF was investigated when solving the harmonic test problem shown in Fig. 1:

$$\nabla^2 u = 0 \quad \text{in } \Omega = (-1, 1) \times (-1, 1), \quad (12)$$

subject to  $u(x, y) = x$  on  $\partial\Omega$ . The exact solution is  $u = x$ .

The sources were initially placed at (uniformly) selected points, at a fixed distance  $d$  from the boundary. The MFS converges for a wide range of values of  $d$ . In all the results of this section,  $d = 0.1$ . All computations were performed in double precision on an IBM AIX RISC 6000 computer.

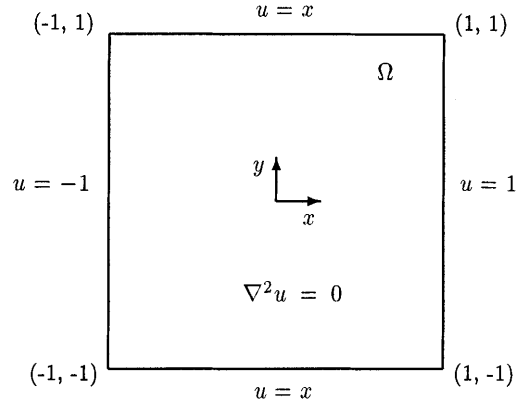


Fig. 1. Harmonic test problem

In Table 1, the computational performance of all subroutines is presented, for different values of the tolerance  $\epsilon$ . It was observed that when providing the Jacobian (i.e., with LMDER and the corresponding option in E04UPF) the CPU times needed to reach a given tolerance were very similar. When the Jacobian is evaluated internally, it was observed that LMDIF performed much better than the corresponding version of E04UPF. The CPU times required by LMDIF and LMDER versus the number of sources are plotted in Fig. 2. In general, the latter requires much less CPU time than the former to reach a given tolerance.

Similar results were obtained for the following simple biharmonic test problem:

$$\nabla^4 u = 0 \quad \text{in } \Omega = (-1, 1) \times (-1, 1), \quad (13)$$

subject to  $u(x, y) = x^2$  and  $\nabla^2 u(x, y) = 2$  on the boundary (Fig. 3). The exact solution is  $u = x^2$ .

Table 1. CPU times (in s) required by the least squares minimization routines for the harmonic test problem

$\epsilon$	$N$	$M$	LMDIF	LMDER	E04UPF Jacobian evaluated internally	E04UPF Jacobian provided by the user
$10^{-1}$	6	56	1.1	0.5	1.3	0.1
	7	64	0.6	0.3	0.8	0.1
	8	72	0.7	0.3	10.0	0.3
	9	84	0.8	0.4	61.2	1.1
	10	92	1.0	0.6	83.9	1.0
$10^{-2}$	6	56	1.1	0.6	1.4	0.2
	7	64	2.3	1.2	1.3	0.2
	8	72	3.7	2.0	93.1	0.4
	9	84	3.4	1.9	141.2	1.3
	10	92	3.5	3.3	151.8	1.1
$10^{-3}$	6	56	1.1	0.7	2.6	1.6
	7	64	20.1	1.8	4.3	0.7
	8	72	18.6	10.2	129.6	3.9
	9	84	22.4	12.6	243.4	6.1
	10	92	22.3	15.6	260.0	8.3
$10^{-4}$	6	56	3.3	0.8	3.7	1.9
	7	64	56.8	56.0	60.3	10.5
	8	72	159.7	93.4	339.9	46.7
	9	84	398.6	146.3	506.4	95.3
	10	92	463.3	178.3	617.7	110.4

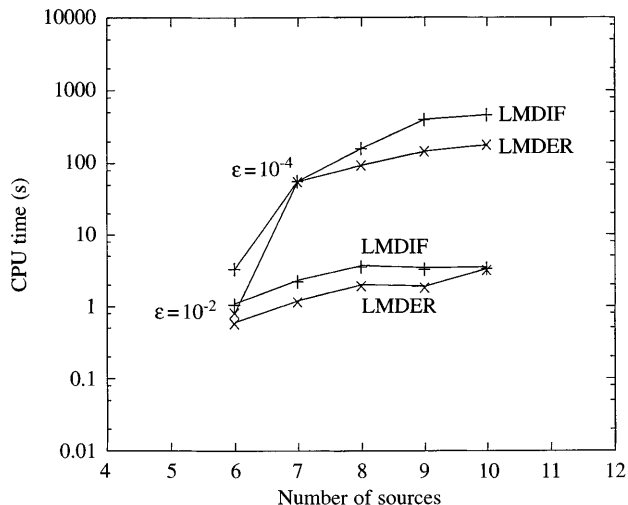


Fig. 2. CPU times required by LMDIF and LMDER for the harmonic test problem

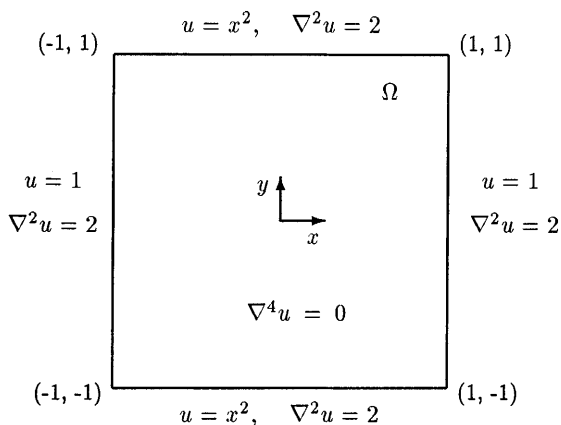


Fig. 3. Biharmonic test problem

Comparison of the performance of all subroutines of interest leads to the same observations as with the harmonic test problem. The computational performance of all subroutines is shown in Table 2, for different values of the tolerance  $\epsilon$ . In Fig. 4, the CPU times required are plotted versus the number of sources. Again, the CPU time required by LMDER to reach a specified tolerance is much less than that required by LMDIF.

**4 Modified versions of the MFS**

In Karageorghis (1992b), a modified MFS is presented which is based on the direct subtraction of the leading terms of the singularity from the solution, as suggested by Symm (1973). The method has been applied to standard

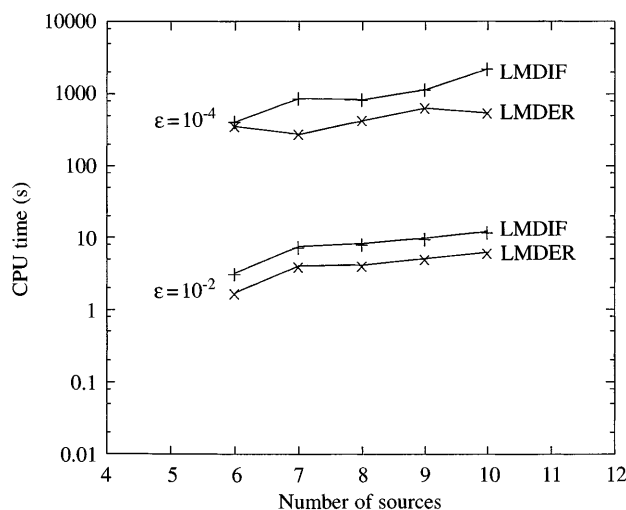


Fig. 4. CPU times required by LMDIF and LMDER for the biharmonic test problem

Table 2. CPU times (in s) required by the least squares minimization routines for the biharmonic test problem

$\epsilon$	$N$	$M$	LMDIF	LMDER	E04UPF Jacobian evaluated internally	E04UPF Jacobian provided by the user
$10^{-1}$	6	72	2.5	1.3	4.9	1.3
	7	84	1.8	1.0	8.4	1.4
	8	96	6.1	3.0	19.5	2.8
	9	108	6.5	3.4	94.8	3.5
	10	120	8.3	4.2	115.3	3.7
$10^{-2}$	6	72	3.2	1.7	51.4	1.5
	7	84	7.5	4.0	69.2	1.5
	8	96	8.2	4.1	146.7	3.3
	9	108	9.8	5.1	343.2	4.6
	10	120	12.1	6.2	467.9	4.5
$10^{-3}$	6	72	27.9	15.4	89.4	9.6
	7	84	53.3	30.2	159.7	21.7
	8	96	78.7	39.2	462.6	26.4
	9	108	125.7	64.4	767.3	53.9
	10	120	120.9	60.0	957.4	62.7
$10^{-4}$	6	72	411.8	352.8	461.4	255.4
	7	84	860.4	274.4	735.6	310.8
	8	96	829.2	427.2	920.7	422.3
	9	108	1153.1	637.2	1541.2	546.4
	10	120	2235.3	544.5	2462.4	601.9

harmonic and biharmonic problems yielding accurate estimates of the leading singular coefficients (Karageorghis 1992b). Compared to other numerical methods which take the leading terms of the singularity into account, the method is easy to implement.

In this study, another modified MFS, in which the unknowns are not restricted only to the coefficients of the leading singular terms but also include the form of the singularity, is developed. This means that the radial and angular dependence of the singularity are considered as unknowns. These new unknowns are naturally incorporated in the nonlinear least squares minimization scheme of the MFS. As mentioned in the introduction, this modification of the MFS is particularly useful when dealing with problems in which the nature of the singularity is unknown.

The objective of this section is to study the accuracy achieved with the above two modified versions of the MFS. All the problems examined were solved with all four subroutines. For comparison purposes with previous work, the results obtained with LMDIF are presented.

The first problem examined is the harmonic problem shown in Fig. 5, known as the Motz problem (Symm 1973):

$$\nabla^2 u = 0 \quad \text{in } \Omega = (-7, 7) \times (-3.5, 3.5), \quad (14)$$

which has a boundary singularity at the point  $O$  where the boundary condition suddenly changes from  $u = 500$  to  $\frac{\partial u}{\partial y} = 0$ . The solution  $u$  in the neighbourhood of the singularity is of the form:

$$u = \sum_{j=1}^{\infty} \alpha_j r^{\left(\frac{2j-1}{2}\right)} \cos\left[\left(\frac{2j-1}{2}\right)\theta\right]. \quad (15)$$

This is considered as a benchmark problem for testing various singular numerical methods. Many special numerical schemes have been proposed for the solution of this problem. Symm (1973) developed a modified boundary integral method using a singularity subtraction technique. Li et al. (1987) employed a boundary approximation method using particular solutions to approximate the boundary conditions as best as possible in a least-square sense. Karageorghis (1992b) employed a modified MFS yielding accurate estimates of the leading singular coefficients. More recently, Georgiou et al. (1996) developed a singular function boundary integral method based on the approximation of the solution by the leading terms of the local solution expansion. The results obtained are in

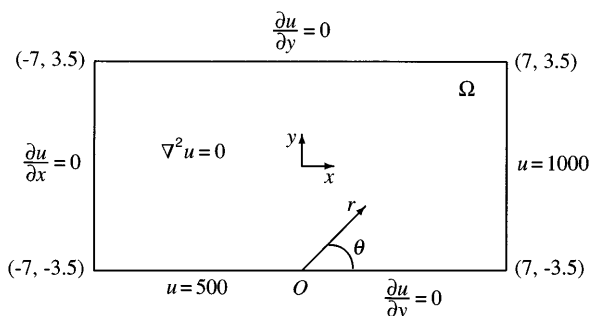


Fig. 5. Geometry and boundary conditions for the Motz problem

close agreement to the exact values obtained by Rosser and Papamichael (1975) using a conformal transformation technique.

In the modified MFS of Karageorghis (1992b), the solution  $u$  consists of two components. The first component approximates the 'singular' part of the solution  $u^s$  and the second approximates its 'regular' part  $u^r$ . As with the MFS,  $u^r$  is approximated by a set of fundamental solutions:

$$\bar{u} = \bar{u}^s + \bar{u}^r = \bar{u}^s + \sum_{j=1}^N c_j \log r_{ij}. \quad (16)$$

In contrast to the above modified MFS, in which the first two terms were included (Karageorghis 1992b), in the new modified version of MFS proposed here,  $\bar{u}^s$  includes only the first singular term. The radial and the angular dependence of the singularity are determined by the unknown parameter  $\beta_1$ :

$$\bar{u}^s = \alpha_1 r^{\beta_1} \cos(\beta_1 \theta), \quad (17)$$

where  $\alpha_1$  is the unknown singular coefficient (the exact value of  $\beta_1$  is 0.50). From Eqs. (16) and (17), we can write

$$\bar{u}(\alpha_1, \beta_1, \mathbf{c}, \mathbf{t}, \mathbf{p}_i) = \alpha_1 r^{\beta_1} \cos(\beta_1 \theta) + \sum_{j=1}^N c_j \log r_{ij}. \quad (18)$$

The problem was solved for various numbers of function evaluations (NFEV) with the sources initially placed outside the domain at different distances  $d$  from the boundary, as before. As with the test problems of the previous section, the accuracy of the approximation improves with NFEV and the number of sources  $N$  (and the corresponding number of boundary points  $M$ ). Because of the nonlinearity of the resulting problem in the new modified method, convergence was achieved only for a restricted range of values of  $d$ . It was observed that the new modified MFS failed to converge for values of  $d$  less than 0.4. In Table 3, comparisons are made between the exact solution near the singularity and the approximations obtained for  $N = 7, M = 66$  and  $NFEV = 4000$  with the following four methods: (a) MFS; (b) Modified MFS with  $\alpha_1$  as the only additional unknown; (c) Modified MFS with  $\alpha_1$  and  $\beta_1$  as additional unknowns; and (d) Modified MFS with  $\alpha_1$  and  $\alpha_2$  as unknowns (Karageorghis 1992b). We observe that the accuracy is improved as we move from (a) to (d). Surprisingly, the solution is more accurate when the form of the leading singular term is considered as unknown, case (c), than when the exact value of  $\beta_1$  is used, case (b). The results of Karageorghis (1992b), however, who considered only the two leading singular coefficients as unknowns, are the most accurate. The calculated values of  $\alpha_1$  and  $\beta_1$  are given in Table 4 for different values of the initial distance of the moving sources from the boundary. These are in good agreement with the exact values of Rosser and Papamichael (1975).

The modified MFS was then applied to the biharmonic problem shown in Fig. 6. This is known as the stick-slip problem and corresponds to the Stokes flow out of a channel of finite thickness and infinite width at infinite surface tension (Richardson 1970). Taking into account

**Table 3.** Calculated solutions of the Motz problem near the singularity ( $0.25 \times 0.25$  grid,  $M = 66, N = 7, \text{NFEV} = 4000$ )

578.95	605.05	631.08	655.27	677.50
547.59	559.30	576.48	598.17	620.75
<b>546.04</b>	<b>557.32</b>	<b>574.20</b>	<b>595.82</b>	<b>618.49</b>
546.31	557.72	574.70	596.31	618.92
546.24	557.64	574.61	596.23	618.85
553.03	590.52	622.50	649.86	673.90
526.33	535.61	555.54	586.07	614.14
<b>524.63</b>	<b>533.17</b>	<b>552.54</b>	<b>583.12</b>	<b>611.44</b>
524.89	533.71	553.30	583.76	611.93
524.81	533.59	553.19	583.67	611.86
530.90	582.26	618.48	647.70	672.73
501.69	502.50	503.46	579.39	611.66
<b>499.97</b>	<b>499.63</b>	<b>496.80</b>	<b>575.80</b>	<b>608.48</b>
500.11	500.18	500.26	576.48	608.96
500.00	500.00	500.00	576.41	608.91

MFS 0  
 Modified MFS, unknowns:  $\alpha_1$   
**Modified MFS, unknowns:  $\alpha_1$  &  $\beta_1$**   
 Modified MFS, unknowns:  $\alpha_1$  &  $\alpha_2$  (Karageorghis 1992b)  


---

 Exact solution (Rosser and Papamichael 1975)

**Table 4.** Calculated values of  $\alpha_1$  and  $\beta_1$  for the Motz problem; the exact values are 151.63 and 0.50, respectively

$N$	$M$	$d$	NFEV	$\alpha_1$	$\beta_1$
7	66	0.4	20000	150.32	0.48
			25000	149.72	0.45
			30000	150.85	0.44
			35000	150.88	0.44
			40000	150.88	0.44
7	66	0.6	20000	150.13	0.47
			25000	150.14	0.47
			30000	150.14	0.47
			35000	150.14	0.47
			40000	150.14	0.47
10	96	0.5	20000	151.64	0.46
			25000	150.92	0.47
			30000	150.51	0.47
			35000	150.43	0.47
			40000	150.39	0.47
10	96	0.6	20000	149.91	0.47
			25000	149.77	0.48
			30000	149.17	0.48
			35000	149.13	0.48
			40000	149.13	0.48

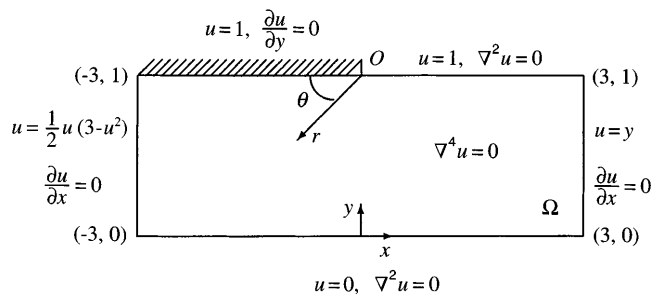
the symmetry of the problem the governing equation in terms of the streamfunction  $u$  is

$$\nabla^4 u = 0 \quad \text{in } \Omega = (-3, 3) \times (0, 1) . \tag{19}$$

The boundary conditions are shown in Fig. 6. The velocity profile is parabolic at the inlet and plug at the exit plane. The problem has a boundary singularity at the point  $O$  where a boundary condition suddenly changes from no-slip,  $\partial u / \partial x = 0$ , to perfect slip,  $\nabla^2 u = 0$ . The analytic nature of the singularity is given by Richardson (1970) as

$$u = 1 + \sum_{j=1}^{\infty} \alpha_j r^{(\beta_j+1)} f_j(\theta, \beta_j) , \tag{20}$$

with two possible sets of solutions for  $f_j(\theta, \beta_j)$ :



**Fig. 6.** Geometry and boundary conditions for the stick-slip problem

$$f_j(\theta, \beta) = \cos(\beta + 1)\theta - \cos(\beta - 1)\theta \quad \text{for } \beta = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots \tag{21}$$

$$f_j(\theta, \beta) = (\beta - 1) \sin(\beta + 1)\theta - (\beta + 1) \sin(\beta - 1)\theta \quad \text{for } \beta = 2, 3, 4, \dots \tag{22}$$

The stick-slip problem was solved analytically by Richardson (1970) using the Wiener-Hopf technique. Kelmanson (1983) employed a direct modified biharmonic boundary integral equation method to solve it. Georgiou et al. (1991) used the Integrated Singular Basis Function Method obtaining good estimates of the leading coefficients. Karageorghis (1992b) obtained accurate estimates of the first two singular coefficients using a modified MFS.

In the present modified MFS for the biharmonic problem, the solution is approximated as follows:

$$\begin{aligned} \bar{u}(\alpha_1, \beta_1, \mathbf{c}, \mathbf{d}, \mathbf{t}, \mathbf{p}_i) &= 1 + \alpha_1 r^{(\beta_1+1)} [\cos(\beta_1 + 1)\theta - \cos(\beta_1 - 1)\theta] \\ &+ \sum_{j=1}^N c_j \log r_{ij} + \sum_{j=1}^N d_j r_{ij}^2 \log r_{ij} , \end{aligned} \tag{23}$$

i.e. only the leading term of the local solution (20) is taken into account and its form is considered unknown. The boundary conditions are modified accordingly.

**Table 5.** Calculated solutions of the stick-slip problem near the singularity ( $0.750 \times 0.125$  grid,  $M = 182, N = 14$ , NFEV = 45000)

		$0$		
1.01706	1.02672	0.95466	0.98268	1.00916
1.00305	0.99198	1.00617	0.99888	0.99820
<b>0.98767</b>	<b>0.98726</b>	<b>0.97934</b>	<b>0.99704</b>	<b>1.00480</b>
0.99988	0.99990	1.00000	1.00020	0.99981
<i>1.0000</i>	<i>1.0000</i>	<i>1.0000</i>	<i>1.0000</i>	<i>1.0000</i>
0.99466	1.00221	0.90386	0.87294	0.88208
0.98088	0.96987	0.96168	0.88767	0.87582
<b>0.96643</b>	<b>0.96506</b>	<b>0.93032</b>	<b>0.88502</b>	<b>0.87958</b>
0.97743	0.97721	0.95539	0.88777	0.87673
<i>0.9778</i>	<i>0.9774</i>	<i>0.9555</i>	<i>0.8877</i>	<i>0.8767</i>
0.92986	0.93388	0.82375	0.75847	0.75590
0.91716	0.90691	0.87627	0.77372	0.75304
<b>0.90521</b>	<b>0.90156</b>	<b>0.84683</b>	<b>0.76959</b>	<b>0.75473</b>
0.91398	0.91300	0.87156	0.77319	0.75332
<i>0.9145</i>	<i>0.9133</i>	<i>0.8716</i>	<i>0.7730</i>	<i>0.7531</i>

MFS  
 Modified MFS, unknowns:  $\alpha_1$   
**Modified MFS, unknowns:  $\alpha_1$  &  $\beta_1$**   
 Modified MFS, unknowns:  $\alpha_1, \alpha_2, \alpha_3$  &  $\alpha_4$  (Karageorghis 1992b)

*Kelmanson (1983)*

The problem was solved for various values of NFEV with the sources initially placed at different distances  $d$  from the boundary. Due to the nonlinearity introduced by the singular term, the new modified MFS converges only for values of  $d$  greater than 3. In Table 5, we tabulate the streamfunction near the singularity obtained for  $N = 14, M = 182$  and NFEV = 45 000 with the following methods: (a) MFS; (b) Modified MFS with  $\alpha_1$  only as an additional unknown; (c) Modified MFS with  $\alpha_1$  and  $\beta_1$  as additional unknowns; and (d) Modified MFS with  $\alpha_1 - \alpha_4$  as additional unknowns (Karageorghis 1992b). The results of Kelmanson (1983) are also given for comparison purposes. It was observed that in case (c) convergence was

slower than in case (b). This is due to the inclusion of the extra nonlinear term in the functional that we minimize. As expected, the solution is more accurate when the nature of the leading singular term is given, case (b), than when  $\beta_1$  is considered as unknown, case (c). The results of Karageorghis (1992b) are in excellent agreement with those of Kelmanson (1983). The calculated values of  $\alpha_1$  and  $\beta_1$  are given in Table 6. These are in good agreement with the exact values.

### 5 Conclusions

A weakness of the MFS is its computational cost which arises from the use of a nonlinear least squares minimization algorithm. In this work, the computational performance of various minimization routines was investigated, in order to improve the efficiency of the method. Two least squares routines from MINPACK, namely LMDER and LMDIF, were first examined. In LMDER, the Jacobian of the system must be provided by the user whereas in LMDIF the Jacobian is evaluated internally by a finite difference scheme. The performance of the two routines on test problems was compared, and it was found that LMDER improves significantly the efficiency of the method. As the user is not required to provide the Jacobian, LMDIF is considerably simpler to code which might be important when solving problems with complicated boundary conditions and/or complex geometries. The performance of the NAG routine E04UPF, which is much more general as it offers many more options, was also examined. One particular option of this routine is that the user may choose whether to supply the Jacobian or not. The results when providing the Jacobian were very similar. In the cases when the Jacobian is evaluated internally, LMDIF is much more efficient than the corresponding version of E04UPF. One important feature of E04UPF, however, is that it can solve constrained minimization problems which can be extremely important when the MFS

**Table 6.** Calculated values of  $\alpha_1$  and  $\beta_1$  for the stick-slip problem; the exact values are 0.69099 and 0.50, respectively

$N$	$M$	$d$	NFEV	$\alpha_1$	$\beta_1$
14	356	9	30000	0.51871	0.45
			40000	0.62042	0.46
			50000	0.66008	0.46
			60000	0.72549	0.47
			70000	0.69019	0.47
28	700	9	30000	0.66673	0.46
			40000	0.57094	0.47
			50000	0.57567	0.47
			60000	0.53798	0.47
			70000	0.54546	0.47
56	1372	7	30000	0.56516	0.48
			40000	0.66575	0.47
			50000	0.66727	0.47
			60000	0.64780	0.47
			70000	0.62114	0.47
70	1708	8	30000	0.54727	0.52
			40000	0.52862	0.48
			50000	0.57662	0.48
			60000	0.62645	0.47
			70000	0.67213	0.47

is used to solve certain classes of problems such as free boundary problems.

A modified version of the MFS for the solution of problems with boundary singularities was also used. The leading singular term is subtracted from the solution and, in addition to the singular coefficient, the form of the leading term can be determined. This modification was achieved with very little extra effort as the unknown singular coefficient and the corresponding power can be included in the nonlinear least squares minimization scheme in a natural way. This is of great importance when the analytic behaviour of the singularity of a given problem is not known *a priori*. The method was applied to two well-known elliptic singular problems. The numerical results indicate that as the number of function evaluations is increased the approximate solution converges to the exact one. This modification of the MFS may be applied to problems involving more complex geometries and boundary conditions.

## References

- Garbow BS, Hillstrom KE, Moré JJ** (1980) MINPACK Project, Argonne National Laboratory
- Georgiou G, Olson L, Schultz W** (1991) The integrated singular basis function method for the stick-slip and the die-swell problems. *Int. J. Numer. Meth. Fluids* 13:1251–1265
- Georgiou G, Olson L, Smyrlis Y** (1996) A singular function boundary integral method for the Laplace equation. *Commun. Numer. Meth. Eng.* 12:127–134
- Guiggiani M** (1995) Hypersingular boundary integral equations have an additional free term. *Comput. Mech.* 16:369–378
- Karageorghis A** (1992a) The method of fundamental solutions for the solution of steady-state free boundary problems. *J. Comput. Phys.* 98:119–128
- Karageorghis A** (1992b) Modified methods of fundamental solutions for harmonic and biharmonic problems with boundary singularities. *Numer. Meth. for Partial Diff. Eqns.* 8:1–19
- Karageorghis A, Fairweather G** (1987) The method of fundamental solutions for the numerical solution of the biharmonic equation. *J. Comput. Phys.* 69:434–459
- Karageorghis A, Fairweather G** (1989) The method of fundamental solutions for the solution of nonlinear plane potential problems. *IMA J. Numer. Anal.* 9:231–242
- Kelmanson MA** (1983) An integral equation method for the solution of singular slow flow problems. *J. Comput. Phys.* 51:139–158
- Li Z-C, Mathon R, Sermer P** (1987) Boundary methods for solving elliptic problems with singularities and interfaces. *SIAM J. Numer. Anal.* 24:487–498
- Mason JC, Parker AP, Smith RNL, Thompson RM** (1984) *Boundary Element Methods for Singularity Problems in Fracture Mechanics*. Royal Military College of Science Report No. 84002 (unpublished)
- Mathon R, Johnston RL** (1977) The approximate solution of elliptic boundary-value problems by fundamental solutions. *SIAM J. Numer. Anal.* 14:638–650
- NAG Ltd** (1991) Numerical Algorithms Group, Mark 15, Wilkinson House, Oxford, UK
- Nagarajan A, Mukherjee S** (1993) A mapping method for numerical evaluation of two-dimensional integrals with  $1/r$  singularity. *Comput. Mech.* 12:19–26
- Olson LG, Georgiou GC, Schultz WW** (1991) An efficient finite element method for treating singularities in Laplace's equation. *J. Comput. Phys.* 96:391–409
- Richardson S** (1970) A 'stick-slip' problem related to the motion of a free jet at low Reynolds numbers. *Proc. Camb. Phil. Soc.* 67:477–489
- Rosser JB, Papamichael N** (1975) A Power Series Solution of a Harmonic Mixed Boundary Value Problem. MRC Technical Summary, Rept. 1405, University of Wisconsin
- Symm GT** (1973) Treatment of Singularities in the Solution of Laplace's Equation by an Integral Equation Method. National Physical Laboratory Report No. NAC 31 (unpublished)