Computational Mechanics 28 (2002) 129–136 © Springer-Verlag 2002
DOI 10.1007/s00466-001-0276-9

Application of a simulated annealing algorithm in the optimal placement of the source points in the method of the fundamental solutions

A. P. Cisilino, B. Sensale

Abstract The placement of source points constitutes a key issue for the method of the fundamental solutions. In particular, for problems with singularities of any kind the determination of the optimal placement of source points becomes relevant, as no linear combination of arbitrarily located source points can guarantee a reasonable approximation to the solution. This paper investigates the use of a "Simulated Annealing" algorithm in the optimal placement of source points in singular problems. The algorithm is essentially an iterative random search with adaptive moves along the coordinate directions. It permits uphill moves under the control of a probabilistic criterion, thus tending to avoid the first local minima encountered. The proposed methodology is employed with a variety of test problems. Results are compared to those of an analytical optimisation routine and their relatively merits and disadvantages discussed. Simulated annealing is shown to be an attractive option for the optimisation of singular problems, with a high rate of success, and able to solve problems for which analytical optimisation routines fail.

1 Introduction

The method of fundamental solutions (MFS) is attributed to Kupradze in a paper published in Russian in 1964. The method has recently reappeared in the literature and solutions of an extraordinary accuracy have been reported using relatively few data points. The MFS has found extensive application in computing solutions to a broad range of problems such as potential problems, acoustics, elastostatics and biharmonic problems (Fairweather and Karageorghis, 1998).

The MFS can be viewed as either an indirect boundary element method or a modified Trefftz method. The basic idea is to approximate the solution by a linear combination of fundamental solutions with sources located outside the problem domain (Fairweather and Karageorghis, 1998; Bogomolny, 1985; Kita and Kamiya, 1995). The coefficients of the linear combination are determined so that the approximate solution satisfies the problem boundary conditions as accurately as possible. Advantages of the method are its relatively easy implementation and its adaptivity since it can easily incorporate difficult boundary conditions.

In the MFS, the locations of the sources are either preassigned or determined along with the coefficients of the linear combination. Simpler MFS approaches involve fixed (preassigned) singularities with the solution being determined by linear least squares or by collocating boundary conditions at boundary points. Most papers in the engineering literature use the version of the MFS with fixed sources but this not always guarantees that, the computed solution converges to the exact solution as the number of source points increases. This is the case of problems with singularities of any kind, as no linear combination can assure a reasonable approximation to the solution since the computed solution will be analytic everywhere except at the sources.

The MFS with moving sources has been considered by several authors (Fairweather and Karageorghis, 1998). Most of the approaches use nonlinear analytical optimisation algorithms to determine the position of the sources. It has been reported that the initial placement of the sources is extremely important in the convergence of these algorithms, as they converge to the first local minima encountered.

In the present work the use of a simulated annealing (SA) algorithm is investigated for optimising the placement of source points for potential problems possessing singular behaviours. SA is based essentially on iterative random search with adaptive moves in such a way that transitions out of local minima are possible. It does not ensure the finding of a global minimum, but it is able to discriminate between "gross behaviour" of the function and finer "wrinkles". Results are presented for a number of test problems and compared to those of analytical optimisation routines. Its relative merits and disadvantages are discussed.

Received 18 July 2001

A. P. Cisilino (✉)
División Soldadura y Fractomecánica – INTEMA,
Facultad de Ingeniería,
Universidad Nacional de Mar del Plata – CONICET,
Av. Juan B. Justo 4302-(7600) Mar del Plata, Argentina
e-mail: cisilino@fi.mdp.edu.ar

B. Sensale
Instituto de Estructuras y Transporte,
Facultad de Ingeniería, Universidad de la República,
J. Herrera y Reissig 665 – 11300 Montevideo, Uruguay

This work was financed by grant PIC 12-04586 of Agencia Nacional de Promoción Científica de la República Argentina and CSIC from Uruguay. Authors wish to thank Prof. A. Karageorghis from University of Cyprus for his helpful suggestions on the manuscript and for kindly providing much of the reference material used in this work.

2
The MFS formulation for Laplace's equation with mixed boundary conditions

Consider a two-dimensional potential problem in a bounded region. The governing equation and the boundary conditions are given by

$$\nabla^2 u = 0 \quad \text{in } \Omega \tag{1}$$

and

$$u_i = \bar{u}_i \quad \text{on } \Gamma_1$$

$$\frac{\partial u}{\partial n} = \bar{q} \quad \text{on } \Gamma_2 \tag{2}$$

where ∇^2 denotes the Laplace operator; u and q are the potential and its derivative in the normal direction (flux), respectively; Ω, Γ_1 and Γ_2 denote the object domain, its potential- and flux-specified boundaries, respectively; n denotes the unit outward normal vector on the boundary and ($^-$) the prescribed value on the boundary.

In the MFS, N sources, the coordinates of which are to be optimised, are placed outside the domain Ω, and M fixed points are chosen along the boundary Γ for collocation. Let $Q_j = (q_{jx}, q_{jy})$ denote the position of source j, and $P_j = (p_{jx}, p_{jy})$ be the position of the boundary collocation point i. Then, the solution at an arbitrary boundary point P is represented by the linear combination of the singular fundamental solutions u^* to Eq. (1) as follows:

$$\begin{aligned} u(P_i) \cong \tilde{u}(a, P_i, Q) &= a_1 u^*(P_i, Q_1) + a_2 u^*(P_i, Q_2) + \cdots \\ &\quad + a_k u^*(P_i, Q_k) + \cdots + a_N u^*(P_i, Q_N) \\ &= \mathbf{a}^{\mathrm{T}} \mathbf{u}^*(P_i, Q) \end{aligned} \tag{3}$$

where $\mathbf{a} = \{a_1, a_2, \ldots, a_\lambda, \ldots, a_N\}^{\mathrm{T}}$ denotes the vector of the coefficients of the linear combination.

The fundamental solution of the two-dimensional Laplace problem in a bounded domain, u^*, is given by

$$u^*(P, Q) = \frac{1}{2\pi} \log\left(\frac{1}{r(P, Q)}\right) \tag{4}$$

where $r(P, Q)$ is the distance between the points P and Q.

Differentiating Eq. (3) in the normal direction, the approximate solution for the flux is obtained

$$q(P_i) \cong \tilde{q}(a, P_i, Q) = \frac{\partial \tilde{u}(a, P_i, Q)}{\partial n} = \mathbf{a}^{\mathrm{T}} \mathbf{q}^*(P_i, Q) \tag{5}$$

Following Karageorghis and Fairweather (1987) the coefficients a_j and the locations of the sources Q are chosen so that the boundary conditions are satisfied in a least-square sense, namely by minimizing the functional

$$F(a, Q) = \sum_{i=1}^{M_1} |\bar{u}_i - u|^2 \sum_{i=M_1+1}^{M_1+M_2} |\bar{q}_i - q|^2 \tag{6}$$

where M_1 and M_2 are the numbers of the boundary collocation points placed on Γ_1 and Γ_2, respectively.

3
Optimal placement of source points

The determination of the optimal choice of collocation points and sources has been addressed by several authors in the case of the Dirichlet problem for the Laplace's equation in the plane with analytic boundary data. Bogomoly (1985) showed that for this kind of problems, if sources are chosen on a surface more or less equidistant to the boundary Γ, the greater the distance from the sources to Γ the better the approximation is to be expected. This conclusion contradicts the fact that the conditioning of the corresponding discrete problem deteriorates as the distance between the sources and the boundary Γ increases. However, it is observed that this often does not affect the quality of the numerical solution, although the resulting system can be highly ill-conditioned.

There is unfortunately no guarantee that the computed solution will always converge in the case of problems with singularities of any kind. Suppose for example we wish to solve Laplace's equation in a circular domain, subject to the Dirichlet boundary condition

$$u(P) = \log \frac{1}{R_0} \tag{7}$$

where R_0 is the distance from P on the boundary to a point X_0 as shown in Fig. 1, and let us suppose that sources are distributed around the contour Γ'. Accordingly, the exact solution of the problem is $u(P) = \log(1/R_0)$ throughout the domain. It is easy to see that it is impossible to obtain by any linear combination of sources on Γ' a function that is infinite at X_0, whatever large the number of sources. Convergence could be achieved if Γ' were taken closer to Γ than X_0, or if a source were placed at X_0, but for practical problems the location of singularities in the approximation to the solution are not known in advance.

In the MFS with moving sources not only the coefficients of the linear combination but also the best locations of the sources are determined through the minimization of the cost function (6). This leads to a nonlinear least squares problem that is solved using available software. Early applications made use of the Harwell subroutine VA07AD (Hopper, 1973) which incorporates features from the Newton–Raphson, steepest descent and Marquart methods. In Karageorghis and Fairweather (1987), the MINPACK (Gargow et al., 1980) routine LMDIF, which is a

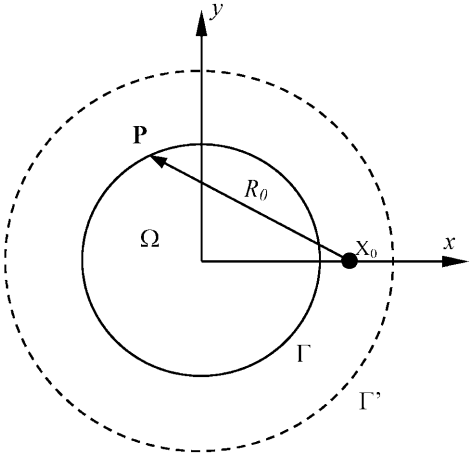

Fig. 1. Boundary value problem for Laplace's equation in circular domain with a singularity near the boundary

modified version of the Levenberg–Marquardt algorithm, is found to be more efficient than VA07AD. The performance of the routines LMDIF and LMDER from MINPACK and the routine E04UPF from NAG was investigated by Poullikkas et al. (1998). The routine LMDER is identical to LMDIF with the exception that the user has to provide the Jacobian. As expected E04UPF leads to substantial savings in both storage and cost. The routine E04UPF uses a sequential quadratic programming, and offers a variety of features, for example the use of constrained optimisation which can be extremely useful for certain MFS applications.

The initial placement of the source points can be extremely important in the convergence of the algorithms quoted above as pointed out by Fairweather and Karageorghis (1998). If the cost function has ridges and plateaus these algorithms stop at the first minimum encountered, and cannot be used easily for finding the global one.

4
Simulated annealing algorithm

Simulated annealing's roots are in thermodynamics, where one studies a system's thermal energy. A description of the cooling of molten metal motivates this algorithm. After slow cooling (annealing), the metal arrives at a low energy state. Inherent random fluctuations in energy allow the annealing system to escape local energy minima to achieve a global minimum. But if cooled very quickly (or 'quenched'), it might not escape local energy minima and when fully cooled it may contain more energy than annealed metal. SA attempts to minimize some analogue of energy – in a manner similar to annealing – to find the global minimum. As reported by Goffe et al. (1994), SA has been used successfully in computer and circuit design, pollution control, neural networks, reconstruction of polycrystalline structures, image processing and econometrics. The routine employed in this work is due to Goffe et al. (1994) and it is available from Netlib. The routine is an extension of the continuous SA global optimisation algorithm described in Corana et al. (1987).

The essential starting parameters to minimize the cost function $f(X)$ are T_0, the initial "temperature"; X, the starting vector of parameters; and V, the step length of X. It is worth to note that the value of the "temperature" T_0 has no physical meaning, and that this denomination follows from the analogy of the SA algorithm with the cooling process in which it is inspired. Note that X and V are both vectors of length n, the number of parameters of the model. A function evaluation is made at the starting point X and its value f is recorded. Next, a new X, X', is chosen by varying element j of X,

$$x'_j = x_j + w \cdot v_j \tag{8}$$

where w is a uniformly distributed random number from $[-1, 1]$ and v_j is the element j of V. The function value f' is computed. If f' is lower than f, X' is accepted, X is set to X', and the algorithm moves downhill. If f' is lower than f, it and X are recorded since this is the best current value of the optimum.

If f' is greater than or equal to f, the Metropolis criterion decides on acceptance (thermodynamics motivates this criterion). The value

$$p = \mathrm{e}^{(f'-f)/T} \tag{9}$$

is computed and compared to p', a uniformly distributed number from [0, 1]. If p is greater than p', the new point is accepted, X is updated with X', and the algorithm moves uphill. Otherwise, X' is rejected. Two factors decrease the probability of an uphill move: lower temperatures and larger differences in the function's value. Also, note that the decision on uphill moves contains a random element.

After N_S cycles through all elements of X (all such 'N' parameters are set by the user), the step length V is adjusted so that 50% of all moves are accepted. The goal here is to sample the function widely. If a greater percentage of points is accepted for x_j, then the relevant element of V is enlarged. For a given temperature, this increases the number of rejections and decreases the percentage of acceptances. After N_T iterations through the above loops, the temperature, T, is reduced. The new temperature is given by

$$T' = s_T \cdot T \tag{10}$$

where s_T is between [0, 1]. A lower temperature makes a given uphill move less likely, so that the number of rejections increases and the step lengths decrease. In addition, the first point tried at the new temperature is the current optimum. The small the steps and starting at the current optimum focuses attention on the most promising area.

The algorithm ends by comparing the last N_ε values of the smallest function values from the end of each temperature reduction with the most recent one and the optimum function value. If all these differences are less than a prescribed ε, the algorithm terminates. This criterion helps ensure that the global minimum is reached.

5
Implementation

When applying the SA algorithm described above in the optimisation of the source point locations in two-dimensional MFS problems, the vector of parameters, X, is given by the $n = 2N$ coordinates of the sources, Q_j. At the same time expression (6) constitutes the cost function $f(X)$, which in order to make it independent of the number of boundary collocation points, M, can be rewritten as

$$f(a, X) = \frac{\sqrt{\sum_{i=1}^{M_1} |\bar{u}_i - u|^2 + \sum_{i=M_1+1}^{M_1+M_2} |\bar{q}_i - q|^2}}{M} \tag{11}$$

where the vector of coefficients a is computed for a given X through the solution of the system of linear equations resulting after collocation of Eq. (3) on the M_1 boundary points on Γ_1, and Eq. (5) on the M_2 boundary points on Γ_2. Note that usually, this will result in systems of equations for which the number of rows is not equal to the number of columns. For the solution of these systems, a singular value decomposition algorithm is employed (Press et al., 1992).

With the exception of the initial temperature, T_0, the temperature reduction parameter, s_T, and the number of iterations, N_T, all other parameters were set as suggested by Corana et al. (1987). Thus, the number of cycles $N_S = 20$, and the number of final function values used for termination $N_\varepsilon = 4$. On the other hand, values suggested by Corana et al. (1987) for $N_T = \max(100, 5N)$, and $s_T = 0.85$ were found to be too conservative according to Goffe et al. (1994), and so were left open to experimentation in the examples.

The selection of the initial temperature, T_0, is an important consideration. If the initial temperature is too low, the step length, V, will be too small and the area containing the optimum may be missed. If too high, then the step length is too large and an excessively large area is searched. The methodology suggested by Goffe et al. (1994) was employed to find T_0. This makes use of a preliminary program run in which the temperature is set to very high value (say 10^7) and the temperature reduction parameter, $s_T = 0.1$. Rather than finding the minimum, the goal is to quickly find the temperature at which the step length vector adjusts to the search area.

6
Examples

The previous sections demonstrated that SA has promise for optimising the placement of sources in the MFS. To see if this promise holds, SA is employed in this section for optimising the placement of source points for several problems possessing singularities, and results compared to those obtained using the subroutine LMDIF.

LMDIF terminates when either a user-specified tolerance is achieved or the algorithm estimates that the relative error between X and the solution is at most the value of the given tolerance. Additionally LMDIF terminates when a user-specified maximum number of iterations is reached. This number was set to (200N + 1). The tendency of the sources to move to the interior of the domain Ω is overcome as in Karageorghis and Fairweather (1987) by an internal check of the position of the sources during the iterative process. If a source is found inside Ω, it is repositioned at the exterior of the domain.

6.1
Laplace's equation in a circular domain with singularities near the boundary

The first example considered consists in the Dirichlet problem of Laplace's equation in a circular domain already introduced in Sect. 3 (see Fig. 1). The radius of the domain was $R = 1$, and 18 collocation points were placed on its boundary ($M = 18$). In the first case, a singularity was placed at (2, 0), and the position of just one source ($N = 1$) was optimised using the SA algorithm. The initial temperature was $T_0 = 0.1$, with the temperature reduction parameter, $s_T = 0.1$. The number of iterations, $N_T = 1$, 5 and 10 were explored. Initial placement of the source point was randomly selected on a 20×20 square area centred around the model domain.The termination tolerance was arbitrarily chosen $\varepsilon = 10^{-6}$.

Table 1 shows the results using the SA algorithm together with those obtained by LMDIF. For all cases, results correspond to the average value after ten runs. As can be seen both routines had a hundred per cent success in placing the source point coincident with the position of the singularity. However LMDIF, did it at a fraction of the computer cost of the SA algorithm.

A more challenging problem is considered next, in which two singularities were placed at (−2, 0) and (2, 0). Accordingly, the positions of two source points were optimised. Table 2 shows the results obtained using various combinations of s_T and N_T values. The percentage of success was higher than 80% for the values explored. A 100% success was achieved for all s_T values after increasing N_T. In contrast, LMDIF had only an 8% success. (Note that LMDIF results correspond in this case to the average of 100 runs).

6.2
Stationary heat conduction problem in a hollow cylinder

This example consists in the stationary heat conduction problem for a hollow cylinder with constant fixed temperatures u_1 and u_2 for the interior and exterior walls respectively (see Fig. 2a). Symmetry conditions allow only one quarter of the problem to be considered by imposing appropriate boundary conditions. These are given in Fig. 2b, together with the locations of the 17 boundary collocation points employed (double collocation points were placed at corners). The exact solution of the problem is given by

Table 1. Results for Laplace's equation in circular domain with one singularity near the boundary

N_T	$s_T = 0.10$	
	Success	FCN eval
1	10/10	633
5	10/10	1961
10	10/10	3921

LMDIF Success: 10/10 FCN evaluations: 38

Table 2. Results for Laplace's equation in circular domain with two singularities near the boundary

N_T	$s_T = 0.10$		$s_T = 0.25$		$s_T = 0.50$	
	Success	FCN eval	Success	FCN eval	Success	FCN eval
1	9/10	1876	9/10	2045	8/10	2301
5	8/10	3951	9/10	5001	10/10	9121
10	10/10	8001	10/10	10961	10/10	18081

LMDIF Success: 8/100 Average number of function evaluations: 50

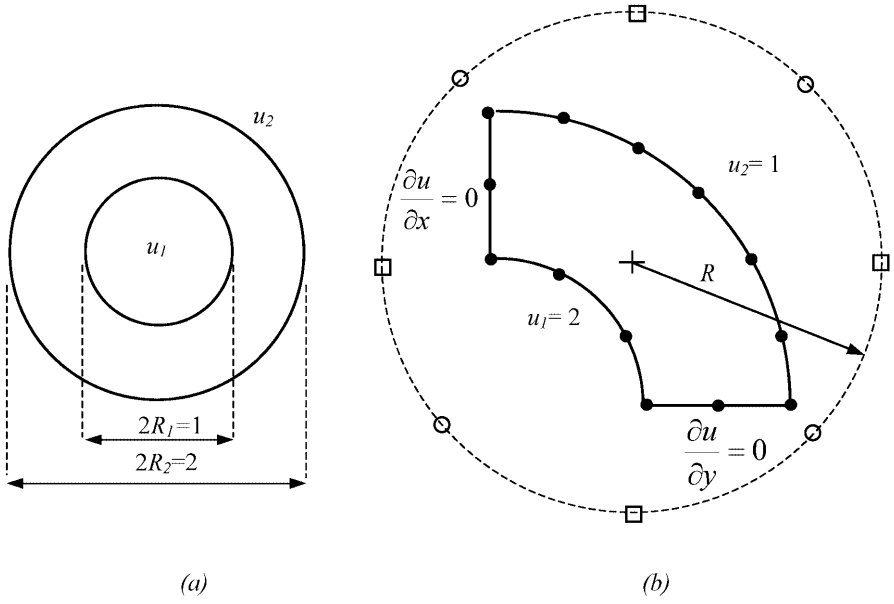

Fig. 2. Stationary heat conduction problem in a hollow cylinder: **a** problem geometry, **b** model details

$$u = u_1 - \frac{\ln(r/R_1)}{\ln(R_2/R_1)}(u_1 - u_2) \tag{12}$$

which consists of a constant and singular term, the last one of the form $\log(1/r)$.

Numerical results are given in Table 3 using source point numbers $N = 4$ and 8, for different combinations of s_T and N_T values. As in the previous example the search area for the source positions was adopted as a 20×20 square area, with their initial placements randomly selected. Ten runs were performed in each case. Termination tolerance was set to $\varepsilon = 10^{-6}$ and initial temperature $T_0 = 0.5$. Successful runs were considered as those for which residuals on the boundary conditions (as given in Eq. 11) resulted lower than 10^{-5}. Percentage of success was at least of 70%, and with the exception of the case $s_T = 0.50$, no much difference can be observed between the results obtained with 4 and 8 source points.

Source points for LMDIF were uniformly distributed around the domain, on circular surfaces centred at the centroid (see Fig. 2b). For the case $N = 4$, two angular arrays were addressed. They are indicated with hollow circles (○) and squares (□) in Fig. 2b. Forty runs were performed for both $N = 4$ and 8, in which sources were initially placed on circumferences with normalized radius ranging $0.74 < R/R_1 < 2.1$. As shown in Table 3, a strong dependency in the performance of LMDIF with the initial placement of source points was encountered for $N = 4$. For the case given by the (□) only one of the 40 runs was successful ($R/R_1 = 1.06$), while 34 of 40 runs ended successfully with the initial disposition as indicated by (○). The ratio of success with $N = 8$ was 50%.

It is worth noting that for all cases successful runs were found to be able to place one of the sources at the centre of the cylinder, a position coincident with the singularity in the exact solution (see Eq. (12)).

6.3
Torsion problem in a circular sector

The torsion problem of the circular sector given by $\Omega = \{(x-1)^2 + y^2 < 1\} \backslash \{x^2 + y^2 < 1\}$ (see Fig. 3) is analysed in this example. Under the Saint Venant's model the stress function u is governed by

$$\nabla^2 u = 4 \tag{13}$$

with the Dirichlet boundary condition $u = 0$ along the boundary Γ. The exact solution

$$u = \frac{\lfloor (x-1)^2 + y^2 - 1 \rfloor (x^2 + y^2 - 1)}{x^2 + y^2} \tag{14}$$

has a strong singularity of the form $1/r$ at (0, 0).

When solving the Poisson equation given in (13) using the MFS, the formulation given in Sect. 2 needs to be

Table 3. Results for the stationary heat conduction problem in a hollow cylinder

N	N_T	$s_T = 0.10$		$s_T = 0.25$		$s_T = 0.50$	
		Success	FCN eval	Success	FCN eval	Success	FCN eval
4	5	7/10	12230	8/10	12801	8/10	21601
	10	9/10	18312	10/10	27841	9/10	41423
8	5	7/10	16641	9/10	22757	10/10	39041
	10	10/10	32961	10/10	47041	10/10	79041

LMDIF $N = 4$ (□) Success: 1/40 Number of function evaluations: 1020
(○) Success: 34/40 Number of function evaluations: 269
$N = 8$ Success: 20/40 Number of function evaluations: 722

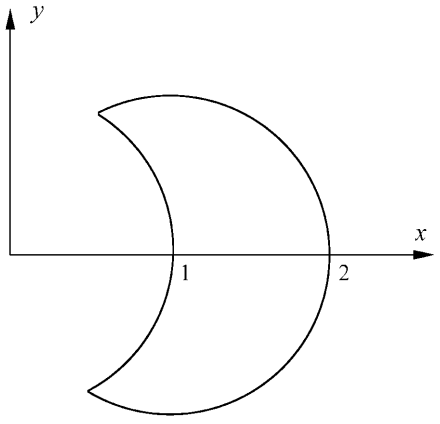

Fig. 3. Torsion problem in a circular sector

changed in order to handle the inhomogeneous term. This can be simply done by using the method of the particular solution. If a particular solution u^p is available such that

$$\nabla^2 u^p = 4 \ , \tag{15}$$

the field u can be written as

$$u = \hat{u} + u^p \tag{16}$$

where $\hat{u}$ satisfies Eq. (1) with boundary conditions given by

$$\hat{u}(P_i) = \bar{u}(P_i) - u^p(P_i) \ . \tag{17}$$

In this way, the problem given by Eq. (13) was solved for $\hat{u}$ by using the procedures outlined in the previous sections, and considering the particular solution $u^p = x^2 + y^2$.

Table 4 shows the obtained results using 34 boundary collocation points and $T_0 = 0.5$. Each result corresponds to the average of 10 model runs. In this case an important improvement in accuracy results from the increase of the number of sources from 4 to 8. At the same time, and as was observed in the other examples, increments in N_T show to have a more marked influence on the results than increments in the value of s_T. Figure 4 illustrates a typical distribution of sources after optimisation. Note that more than one source end up very close to the position of the singularity.

On the other hand, results obtained using LMDIF were very poor. Reported results correspond to the best obtained from 40 model runs, for which following the previous example source points were initially distributed around the domain, on circular surfaces centred at (1, 0).

6.4
The Motz problem

The previous examples were devoted to solve problems with singularities outside their boundaries. Solutions for these problems were found though the optimisation of the source point positions. Note that for problems exhibiting boundary singularities the referred solution scheme is not applicable, as the optimum solution would involve the placement of the source points on the boundary, what it is not compatible with the MFS formulation. Hence, to tackle these problems a new MFS is introduced which incorporates the coefficient and strength of the singularity as unknowns.

This last example examines the ability of the SA algorithm to solve the so-called Motz problem (see Fig. 5) which has a singularity at the point O where the boundary conditions suddenly changes from $u = 0.5$ to $\partial u/\partial n = 0$. This is considered as a benchmark problem for testing various singular numerical methods.

The solution in the neighbourhood of the singularity is of the form

$$u = \sum_{j=1}^{\infty} \alpha_j r^{(2j-1/2)} \cos[(\frac{2j-1}{2})\theta] \ . \tag{18}$$

In this example a modified version of the MFS due to Karageorghis (1992), is employed in which the unknowns are not restricted only to the coefficients of the approximation but also the form of the singularity. In it, the solution u consists of two components: the first component approximates the 'singular' part of the solution, u^s, and the second one approximates its 'regular' part, u^r. As in the standard MFS u^r is approximated by a set of fundamental solutions, while u^s includes only the first singular term with angular dependence of the singularity determined by the unknown parameter β. Then, from Eqs. (3) and (18) results

$$u(P_i) = u^r + u^s = \sum_{j=1}^{n} a_j u^*(P_i, Q_j) + \alpha \cdot r^{\beta} \cos(\beta\theta) \tag{19}$$

The problem was solved for two different number of sources ($N = 4$ and 8) and collocation points ($M = 17$, 41

Table 4. Results for the torsion problem in a circular sector

N	N_T	$s_T = 0.10$		$s_T = 0.25$		$s_T = 0.50$	
		Residual	FCN eval	Residual	FCN eval	Residual	FCN eval
4	1	$0.57{\cdot}10^{-3}$	11203	$0.71{\cdot}10^{-3}$	8177	$0.56{\cdot}10^{-4}$	5761
	5	$0.26{\cdot}10^{-4}$	12081	$0.37{\cdot}10^{-4}$	16241	$0.11{\cdot}10^{-4}$	21440
	10	$0.32{\cdot}10^{-4}$	19841	$0.25{\cdot}10^{-4}$	28641	$0.21{\cdot}10^{-4}$	41281
8	1	$0.13{\cdot}10^{-5}$	5548	$0.12{\cdot}10^{-5}$	5441	$0.42{\cdot}10^{-6}$	7894
	5	$0.22{\cdot}10^{-6}$	17441	$0.16{\cdot}10^{-6}$	23681	$0.11{\cdot}10^{-6}$	39521
	10	$0.15{\cdot}10^{-6}$	34561	$0.43{\cdot}10^{-7}$	47361	$0.53{\cdot}10^{-7}$	79361

LMDIF (Best results)
$N = 4$ Residual $0.11{\cdot}10^{-1}$ Number of function evaluations: 37
$N = 8$ Residual $0.15{\cdot}10^{-2}$ Number of function evaluations: 2376

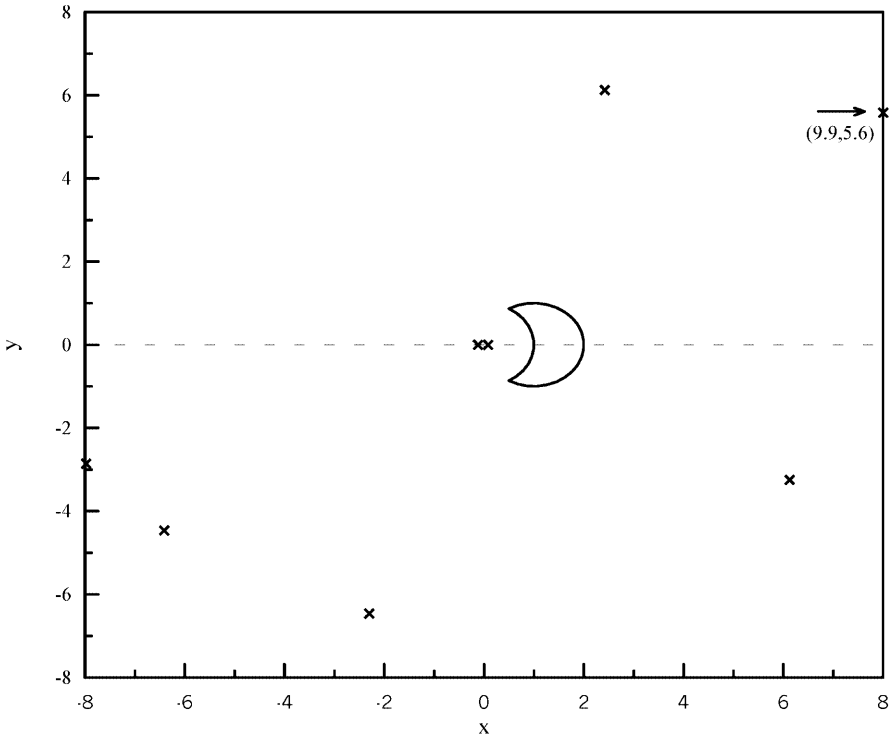

Fig. 4. Typical distribution of the sources after optimisation

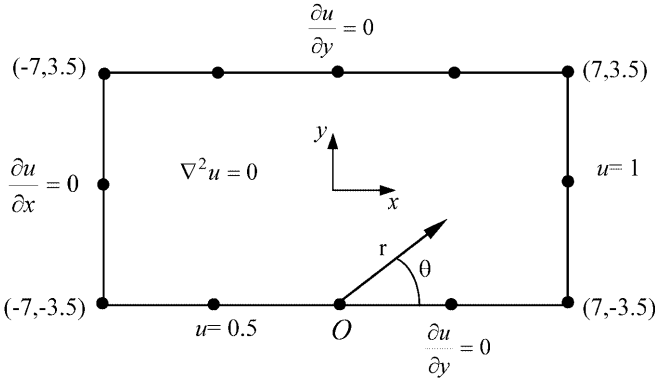

Fig. 5. Geometry and boundary conditions for the Motz problem

and 65), with the sources initially placed at random in a 100×100 square around the model domain. The parameter β was incorporated into the optimisation process within the range $[-10, 10]$. The parameters for the SA algorithm were chosen as $T_0 = 0.001$, $s_T = 0.5$, $N_T = 5$. In Table 5, comparison is made between the computed and the exact values of α and β. Each of the computed values correspond to an average of 20 runs. Karageorghis and Fairweather (1987) studied this problem using LMDIF obtaining very similar results at almost the same computing cost. However, for LMDIF convergence was achieved only for restricted initial positions of the sources.

An interesting fact of the SA algorithm when applied to the Motz problem is that the angular dependency β as well as the coefficient of the singularity α are determined early during the optimisation process (see Fig. 6). This suggests that for the sake of reducing computing time, stopping criteria can be relaxed for analyses focused on the determination of α and β only.

Table 5. Calculated values of α and β for the Motz problem; the exact values are 0.5 and 0.1516 respectively

	$M = 17$		$M = 41$		$M = 65$	
	$N = 4$	$N = 8$	$N = 4$	$N = 8$	$N = 4$	$N = 8$
α	0.452	0.461	0.471	0.487	0.472	0.490
β	0.1443	0.1452	0.1480	0.1523	0.1492	0.1609
FCN eval	26659	43490	28790	48734	33206	52611

7 Conclusions

The application of a SA algorithm was investigated in this work to optimise the position of source points in the solution of singular problems with the MFS. SA algorithm resulted easy to integrate into the point collocation MFS formulation, and it was applied to the solution of well-known singular problems for both Laplace's and Poisson's equations.

The proposed methodology demonstrated a high rate of success, being able to solve problems for which analytical optimisation routines fail. Very good results were obtained using a small number of sources and relatively low temperature reduction parameters ($s_T = 0.1$). At the same time the number of iterations per cycle (N_T) showed to have in most cases a marked influence on the results.

SA was also employed with a modified version of the MFS, in which the optimisation parameters are not restricted only to position of the sources but also the form of the singularity. In addition to the very good results for the complete solution of the problem, SA showed an excellent performance in capturing the singularity exponent very early during the optimisation process. This is found as a powerful feature to explore when it is

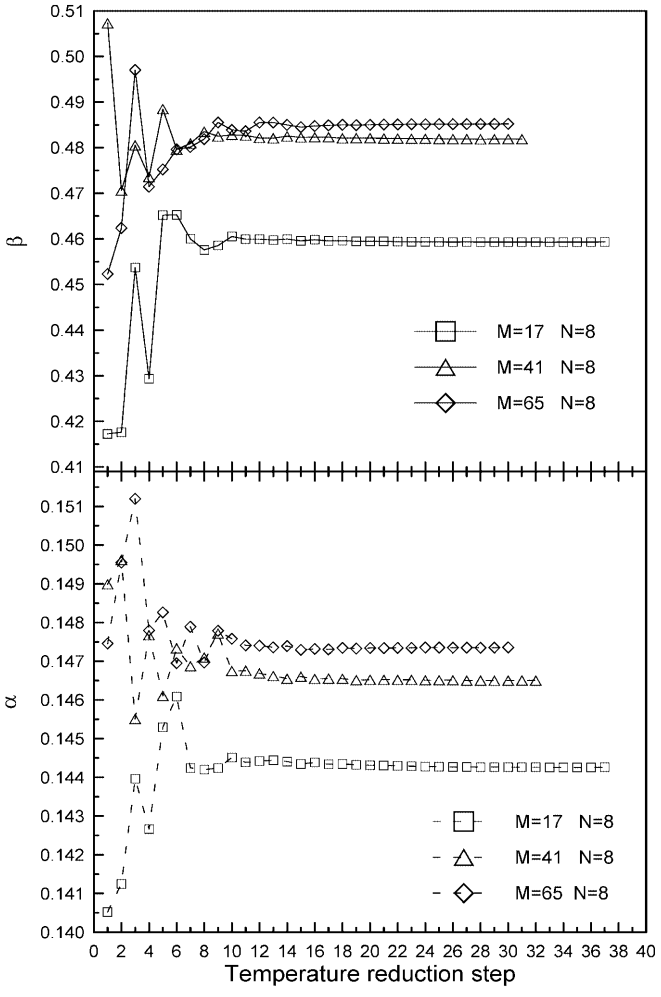

Fig. 6. Evolution of the optimum α and β parameter values with temperature reduction

intended to study the behaviour of problems for which singularities are not known a priori.

The sole drawback of simulated annealing is the required computational power, but this problem is disappearing or has disappeared with the continuous improvements in computer power. At the same time, the combined use of SA and analytical optimisation routines can be seen as an interesting option to explore. SA could be employed in the early stages of the optimisation process to discriminate "gross behaviour" of the function, after which a much faster analytical optimisation algorithm could be used to deal with the fine optimisation. In this way, the benefits of both methodologies are exploited.

References

Beer G, Watson JO (1992) Introduction to Finite and Boundary Element Methods for Engineers. John Wiley & Sons, Chichester, England

Bogomolny A (1985) Fundamental solutions methods for elliptic boundary value problems. SIAM J. Numer. Anal. 22(4): 644–669

Corana A, Marchesi M, Martini C, Ridella S (1987) Minimizing multimodal functions of continuous variables with the simulated annealing algorithm. ACM Trans. Mathematical Software 13: 262–280

Fairweather G, Karageorghis A (1998) The method of fundamental solutions for elliptic boundary value problems. Adv. Comput. Mathematics 9: 69–95

Gargow BS, Hillstron KE, Moré JJ (1980) MINPACK Project. Argonne National Laboratory, USA

Goffe WL, Ferrier GD, Rogers J (1994) Global optimization of statistical functions with simulated annealing. J. Econometrics 60: 65–99

Hopper MJ (1973) Harwell Subroutine Library Catalogue. Theoretical Physics Division, AERE, Harwell, UK

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 (1992) Modified methods of fundamental solutions for harmonic and biharmonic problems with boundary singularities. Numer. Meth. Partial Differ. Equa. 8: 1–19

Kita E, Kamiya N (1995) Trefftz method: an overview. Adv. Eng. Software 24: 3–12

Netlib Repository. www.netlib.org

Numerical Algorithms Group Library. NAG(UK) Ltd., Oxford, UK

Poullikkas A, Karageorgis A, Georgiou G (1998) Methods of fundamental solutions for harmonic and biharmonic boundary value problems. Comput. Mech. 21: 416–423

Press WH, Teukolsky SA, Vetteling WT, Flannery BP (1992) Numerical Recipes in Fortran. Cambridge University Press, England