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# Adaptive refinement scheme for the least-squares approach of the method of fundamental solution for three-dimensional harmonic problems

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## Abstract

In this paper we describe how the accuracy of the least-squares approach of the method of fundamental solution can be improved by means of an adaptive refinement scheme. A hierarchical data structure is used for spreading of the source points starting from an initial coarse distribution. The correction indicator used in the refinement procedure is based on the relative influence of the source intensities obtained as parameters in multiple regression analysis. Iterative solution of the linear system of equations is performed at each refinement step. The results of applying the method to test problems from potential theory show that the method gives higher accuracy in the potential and normal derivatives with a reduced number of sources.

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## 1. Introduction

The method of fundamental solution (MFS) is one of the most intuitive approaches to solve numerically linear elliptic partial differential equations. In this type of approach an approximate solution is represented in the form of a linear superposition of source functions (fundamental solutions) located outside the problem domain,  $\Omega$ . As the fundamental solution satisfies the differential equation at any point except at the source point, it follows that this representation exactly satisfies the governing equation and one seeks to satisfy the imposed boundary conditions approximately at a set of boundary points (collocation points). In Ref. [1] a comprehensive review of the MFS is given, in which this approach is related to a regular indirect single layer boundary element approach (indirect-BEM). Some of the most relevant features discussed in Ref. [1] will be addressed in this work.

One of the pioneer works on the MFS was the work by Kupradze and Aleksidze [2] where they prove the completeness of the potentials in  $H(\Omega)$ , the set of harmonics functions in  $\Omega$ . This work was latter expanded upon by Bogomolny [3].

Although the MFS is useful for a large class of problems, the discussion in this paper is restricted to the solution of the three-dimensional (3D) the Laplace equation. In this type of approach, the solution of the Laplace interior problem is approximated by a linear combination of sources located outside the problem domain [4]. The coefficients of the fundamental solutions for given coordinates of the sources are determined in general by solving a system of equations that is obtained imposing the corresponding boundary conditions of the problem. This can be done by means of *direct collocation*, for which a system with a number of linear equations with an equal number unknowns is solved. In this approach, rules of thumb have been proposed in the literature for the positions of the collocation and source points [5]. Alternatively, the boundary conditions can be satisfied *in the least-squares sense* with a number of sources smaller than the number of points where the boundary conditions are specified. This was the approach taken by Bogomolny in Ref. [3] and there is some numerical indication that this approach may be the most efficient [6]. In the present paper the *least-squares* approach is used, focussing our attention on the sequential improvement of the solution by an adaptive distribution of the source points.

The implementation of the MFS appears to be quite straightforward. It is only necessary to specify the source points outside the problem domain and the data or boundary

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points on the contour of the domain then solve the resulting linear system of equations. However, in its numerical application there are several issues that require special attention. Of those some of the most relevant are: location and number of sources and boundary points as well as convergence and stability of the scheme.

Generally, there have been two approaches to choosing the source points, fixed and adaptive. From practical experience and some analytical works, in particular in two-dimension (2D) [7–9], it has been observed that the accuracy of the approximation improves as the sources are moved farther away from  $S$ . When using the fixed approach, it is recommended to distribute uniformly the source points over a large circle enclosing the original problem domain, in  $\mathbb{R}^2$ , or a large sphere, in  $\mathbb{R}^3$  (for more details see Ref. [1]), where the radius of the circle,  $R$ , or the sphere is chosen to be five times the characteristic dimension of the problem domain, when dealing with pure Dirichlet condition, or smaller than five when dealing with Neumann cases. This fixed value of  $R$  is recommended because the system of equations coming from the MFS can become highly ill-conditioned as  $R$  increased [10–12]. However, it has been observed that despite the ill-conditioning, the accuracy of the numerical solution is largely unaffected [3,10,13]. Golberg and Chen [1] reported that in these cases direct solvers, as Gaussian elimination, can be used effectively, even if the resulting condition number of the matrix is very large, by ignoring the message of singular system of the numerical routine.

Traditionally in numerical analysis the stability of the scheme, i.e. the amplification of data errors, is measured by the condition number of the matrix (the ratio between the largest and the smallest singular values of the matrix). Typically ill-conditioning is indicated by very small values of the smallest singular value. It is known that in some cases only the consideration of the condition number will result in an under estimation of the stability. In Ref. [14] it is shown that a full understanding of the numerical stability requires knowledge of the complete singular values (SV) of the matrix and not only its largest and smaller values. In Refs. [11,12] Kitagawa showed that this is the case when using the MFS.

While in a fixed algorithm the number and location of the source points are defined at the beginning of the process, in an adaptive approach these parameters will be considered as part of the solution of the problem. Johnston, Fairweather and Karageorghis [15,16] proposed an adaptive scheme, in which the coefficients of the linear representation of the potential as well as the position the sources, which are given as a fixed number, are chosen by a non-linear least-squares algorithm. This approach is a non-linear optimization problem that only distribute a given fixed number of sources and that can be quite time consuming to solve.

Convergence analysis of the MFS for the solution of the Laplace equation in 2D were considered by Cheng [7], Katsurada and Okamoto [8] and Katsurada [9]. In those

articles it is shown that when the boundary surface  $S$  and the boundary conditions are smooth functions, the MFS converges exponentially to the solution of the partial differential problem. Although not equivalent theoretical analysis are available for the corresponding 3D analogous problems, Golberg and Chen [10] presented an heuristic analysis, in which they suggest that similar convergent behavior could be expected for 3D problems.

In the work on adaptive MFS presented herein we focus on the improvement of the source distribution, and new sources are added by using a correction indicator that is related to sensitivity analysis of the solution. The proposed refinement of the source distribution is based on an approach borrowed from statistical concepts and not on classical re-meshing adaptive procedures used in other numerical techniques.

The basic idea of performing sensitivity analysis of the previous solution to define a possible error estimator that should give information on the global accuracy of the numerical solution is used. However, the correction criterion is expressed in terms of ‘significant parameters’ from multiple linear regression. Regression analysis investigates the relationship between several independent or predictor variables and a dependent variable, which in our case represent the unit intensity fields from the fundamental solutions and the fields at the given boundary collocation points, respectively. The solution is given in terms of *regression coefficients* which are related to the *correlation* of each predictor with the dependent variable, after controlling for all other independent variables. High correlation between such predictors can be reflected as collinearity and ill-conditioning of the least-squares problem. Therefore, the sequential selection of predictors in the refinement procedure must attempt to distribute the contributions of the sources to the reduction of the errors uniformly, and in some sense to minimize the effects of interactions between neighboring sources on the solution of the linear equations. In this paper we follow selection concepts for best subset of predictors in regression for guidance in sequential reduction of the global error starting with a coarse initial distribution of sources.

## 2. The method of fundamental solutions

In this section the MFS is described for interior boundary value problems of the Laplace equation. A domain  $\Omega \in \mathbb{R}^3$  is given, whose boundary  $S$  is a simple closed surface. An unknown harmonic function  $\Phi(P)$  must be found with prescribed boundary values on  $S$ , i.e. the following equations need to be satisfied:

$$\nabla^2 \Phi(P) = 0, \quad P \in \Omega \quad (1)$$

$$\Phi(P) = f(P), \quad P \in S_1. \quad (2)$$

$$\frac{\partial \Phi}{\partial n}(P) = g(P), \quad P \in S_2. \quad (3)$$

where  $S = S_1 \cup S_2$ . Let  $\Phi^*(x, \xi)$  be the fundamental solution of the Laplace equation

$$\Phi^*(P, Q) = \frac{1}{4\pi} \frac{1}{|P - Q|} \quad (4)$$

A direct boundary integral equation method (BEM) gives an integral equation for  $\partial \Phi / \partial n$ , the unknown normal derivative on  $S_1$ , and for the unknown potential  $\Phi$  on  $S_2$ . The integral equation is solved numerically and  $\Phi$  can be evaluated in the interior of  $\Omega$ . The principal advantage of the boundary integral approach is that there is no need to construct a mesh on  $\Omega$ . A main disadvantage is the computational expense to evaluate the required boundary integrals on  $S$ .

Alternative to the direct BEM, the indirect regular BEM approach represents the solution of an interior problem in terms of the single layer potential with unknown density  $\sigma$ :

$$\Phi(P) = \int_{\hat{S}} \Phi^*(P, Q) \sigma(Q) dS \quad (5)$$

where  $\hat{S}$  is the contour of a domain containing  $\bar{\Omega}$ .

Representing the unknown density  $\sigma$  in terms of a complete set of function  $\varphi_j(Q)$  on  $\hat{S}$ , i.e.

$$\sigma(Q) = \sum_{j=1}^n c_j \varphi_j(Q); \quad Q \in \hat{S} \quad (6)$$

the above single layer can be approximated by:

$$\Phi(P) = \sum_{j=1}^n c_j \int_{\hat{S}} \Phi^*(P, Q) \varphi_j(Q) dS \quad (7)$$

In general, the integrals

$$\int_{\hat{S}} \Phi^*(P, Q) \varphi_j(Q) dS \quad 1 \leq j \leq n \quad (8)$$

need to be evaluated numerically, but, since in this approach the collocation points,  $P$ , are always different to the sources points,  $Q$ , where  $P \in \bar{\Omega}$  and  $Q \in \hat{S}$ , the above integrals are non-singular and therefore, can be evaluated by standard quadrature rules,

$$\int_{\hat{S}} \Phi^*(P, Q) \varphi_j(Q) dS \approx \sum_{l=1}^N \omega_l \Phi^*(P, Q_l) \varphi_j(Q_l) \quad (9)$$

And therefore, the above single layer potential can be represented by

$$\hat{\Phi}(P) = \sum_{j=1}^n b_j \Phi^*(P, Q_j) \quad (10)$$

where

$$b_l = \omega_l \sum_{j=1}^n c_j \varphi_j(Q_l) \quad (11)$$

The above superposition of fundamental solutions outside the problem domain, Eq. (10), is known as the MFS. This equation follows naturally from Eq. (5), however, usually it is necessary to add a constant terms in particular in 2D where it is required from completeness purposes.

$$\hat{\Phi}(P) = b_0 + \sum_{j=1}^N b_j \Phi^*(P, Q_j) \quad (12)$$

As can be observed a constant value is always a solution of the Laplace's equation.

From the above analysis, we can say that the MFS is a technique pertaining to the class of boundary elements methods, which is applicable when a fundamental solution is known for the partial differential equation that is desired to solve (for more details see Ref. [1]). Therefore, the MFS is in a way similar to the method of boundary elements, with additional advantages with respect to the simplicity of its formulation and the fact that the distribution of points is practically mesh-free. These advantages make the method an ideal candidate for moving boundary problems [17]. In view of the advantages and applications of the method, in this work we examine a way to improve its accuracy.

As the fundamental solutions satisfy the differential equation,  $\hat{\Phi}(P)$  will automatically be harmonic. A good approximation to  $\Phi(P)$  will then be obtained by imposing the boundary conditions at  $M$  points  $P_i$  on  $S$ . The expression of  $\hat{\Phi}$  or its corresponding normal derivative  $\partial \hat{\Phi} / \partial n$  are then equated to the values given by the boundary conditions. In this way, a system of  $M$  linear equations with  $N$  unknowns  $b_j$  is obtained. Once the system of equations is solved, the potential and its directional derivatives at any point in  $\bar{\Omega}$  can be computed by replacing the intensities  $b_j$  in the expression for the potential  $\hat{\Phi}(P)$  evaluated at the desired point.

After imposing the corresponding boundary conditions, the resulting system of linear equations can be expressed in matrix form as:

$$\mathbf{Xb} = \mathbf{y} \quad (13)$$

where  $\mathbf{X}$  is the matrix of coefficients of the unknown source intensities  $\mathbf{b}$ , i.e. values of  $\Phi^*(P_i, Q_j)$  and  $\partial \Phi^*(P_i, Q_j) / \partial n$ , and  $\mathbf{y}$  is the right-hand-side known vector of potentials and normal derivatives at the boundary points. To obtain the estimate  $b_0$  in the case of Dirichlet conditions a column vector  $\mathbf{x}_0$  with its elements equal to 1 is added to the matrix  $\mathbf{X}$ . For the case of Neumann conditions, the corresponding elements in  $\mathbf{x}_0$  are equal to 0. The direct collocation MFS corresponds to the case where  $M = N$ , whereas, the overdetermined system with  $M > N$ , gives rise to a least-squares MFS.

For the interior Laplace problem with Dirichlet boundary conditions, in the direct collocation method the potentials at the boundary are forced to be exactly satisfied, but errors are present in the computed values for internal points and are easily identified in the normal derivatives at the boundary

points. Errors arise in a reverse fashion when normal derivatives are imposed. In addition, some positions of the sources can give rise to non-physical oscillations in the numerical solution. The error due to the solution of the linear system basically depends on the routine used, and it can be assumed to be negligible with respect to the discretization error, which is caused by the inability of the selected source locations to adequately represent the boundary field. In this context, the selective and local refinement of the discretization arises as a natural and desirable feature in contrast with an initially fixed discretization approach.

It is worth noticing that any given distribution of the boundary points would allow unlimited possible locations of the sources for the same the number of unknowns. The least-squares solution allows flexibility in the error balance over those boundary points by adjusting the intensities or positions of the sources. These possibilities play a central role in the formulation of the proposed refinement procedure. In this paper emphasis is made on the refinement strategy as the specific computation of the error and threshold for refinement can be tailored for a given implementation.

### 3. Formulation of the multiple linear regression problem

A regression model is a formal means of expressing the two essential ingredients of a statistical relation: (1) a tendency of the response variable  $Y$  to vary with the predictor variables in a systematic fashion, and (2) a scattering of points around the curve of statistical relationship. In the proposed approach to solve the present boundary value problem, the solution of the problem is viewed as a parameter estimation scheme where the values of the response variable are the potential fields or their normal derivatives at the given boundary collocation points (boundary conditions), the regression function is linear, and the magnitude of the intensity of the fundamental solutions are the predictors.

We consider a basic regression model where the regression function is linear with  $N + 1$  predictor variables  $\beta_j$ ,  $j = 0, \dots, N$  (model parameters). The response variable  $Y$  is viewed as a random variable, and the model can be stated as follows:

$$Y_i = \beta_0 + \sum_{j=1}^N \beta_j x_{ij} + \varepsilon_i \quad (14)$$

where  $i$  is an index for successive trials or points in a sample,  $i = 1, \dots, M$ , of the random variable  $Y$  corresponding to the response in the  $i$ th trial,  $x_{ij}$  are known constants, namely the  $j$  influence coefficient in the  $i$ th trial, and  $\varepsilon_i$  is a random error term with mean  $E\{\varepsilon_i\} = 0$  and variance  $\sigma^2\{\varepsilon_i\} = \sigma^2$ ,  $\varepsilon_i$  and  $\varepsilon_j$  are uncorrelated so that their covariance is zero for all  $i, j$ ;  $i \neq j$ . From the above,  $Y_i$  is

a random variable with mean

$$E\{Y_i\} = \beta_0 + \sum_{j=1}^N \beta_j x_{ij} \quad (15)$$

and variance  $\sigma^2\{Y_i\} = \sigma^2$ . This model assumes that the probability distributions of  $Y_i$  have the same variance  $\sigma^2$ , regardless of the values of the predictor variables. The errors are assumed to be uncorrelated. Hence, the outcome in any one trial has no effect on the error term for any other trial.

The observational or experimental data to be used for estimating the parameters of the regression function consists of the explanatory term  $x_{ij}$  (influence coefficient) and the corresponding observations, denoted as  $y_i$ . The estimated regression function is

$$\hat{Y} = \sum_{j=1}^N b_j X_j + b_0 \quad (16)$$

where each  $b_j$  is an estimate of the parameter  $\beta_j$ . The above equation can be written in matrix notation as:

$$\hat{Y} = Xb \quad (17)$$

As can be observed our solution of the MFS can be interpreted as a regression analysis to determine the parameters  $b_j$ ,  $j = 0, 1, 2, \dots, N$ , in Eq. (13). In the present application,  $b_0$  accounts for a constant term in the representational formula (12) and  $x_{ij}$  are the matrix coefficients obtained after evaluating the boundary conditions at the  $M$  boundary collocation points.

The method of least-square provide a good estimator of the regression parameters  $b_j$  by minimizing the sum of the squares of the  $M$  residuals. This condition yields to the system of  $N$  linear algebraic equations

$$\mathbf{Ab} = \mathbf{X}^T \mathbf{Xb} = \mathbf{X}^T \mathbf{y} \quad (18)$$

The above equation is called the *normal equation* of the least-squares problem, with solution

$$\mathbf{b} = \mathbf{Cg} \quad (19)$$

where  $\mathbf{C} = \mathbf{A}^{-1}$  and  $\mathbf{g} = \mathbf{X}^T \mathbf{y}$ , with  $N \leq M$ , since there must be more data points than model parameters to be solved for. As can be observed a least-squares solution of the algebraic system of equations arising from the MFS, i.e. Eq. (13), can be interpreted as a linear regression.

Therefore, the point estimators  $b_j$  of the parameters  $\beta_j$  are obtained from the solution of the normal equations corresponding to the minimization of the sum of squares of the residuals, usually denoted by SSE (deviation around fitted regression line).

$$\text{SSE} = F(\mathbf{b}) = \sum_{i=1}^M (y_i - \hat{y}_i)^2 \quad (20)$$

The variance of the error terms  $\varepsilon_i$  needs to be estimated to obtain an indication of the variability of the probability distributions of  $Y$ . An unbiased estimator for the variance  $\sigma^2$

is

$$\text{MSE} = \frac{\text{SSE}}{M - N} \quad (21)$$

The estimate of the mean or expected value of  $Y_i$  is given by the regression analysis in terms of Eqs. (17)–(19) as:

$$\hat{\mathbf{Y}} = \mathbf{H}\mathbf{Y} \quad (22)$$

where  $\mathbf{H}$  is called the *hat matrix*, computed as

$$\mathbf{H} = \mathbf{X}\mathbf{C}\mathbf{X}^T \quad (23)$$

The square  $M \times M$  matrix  $H$  is symmetric and has the special property (called idempotency)

$$\mathbf{H}\mathbf{H} = \mathbf{H} \quad (24)$$

The estimators  $\mathbf{b}$  are thus random variables with an estimated variance–covariance matrix of  $\sigma^2\{\mathbf{b}\} = \sigma^2\mathbf{C}$ , which elements are:

$$\sigma^2\{\mathbf{b}_{ij}\} = \sigma^2\mathbf{c}_{ij} \quad (25)$$

Since  $\sigma^2$  is also estimated from the sample values, we can estimate the variance of the sampling distribution of the parameter estimates by replacing the variance  $\sigma^2$  with its unbiased estimator MSE.

Test for the significance of  $\beta_j$  are usually given in terms of the  $t$  test (selection of predictors), i.e.

$$t_j^* = \left( \frac{b_j}{\sigma^2\{\mathbf{b}_{jj}\}} \right) = \frac{b_j}{\sigma^2\mathbf{c}_{jj}} \quad (26)$$

and the decision rule with  $(1 - \alpha)$  confidence:

$$\begin{aligned} \text{If } |t_j^*| \leq t(1 - \alpha/2; M - N) & \text{ conclude the alternative } \beta_j = 0 \\ \text{Otherwise} & \text{ conclude } \beta_j \neq 0 \end{aligned}$$

It is known that the  $t$  test is a marginal test from the perspective of the general linear test approach [19], in the sense that possible misleading results can be obtained when the predictor variables are highly correlated (for more details about regression analysis see Ref. [20]). In the application of the  $t$  test to our least-squares solution of the MFS the terms  $b_j$  are the estimated intensities of the sources  $j$  and the terms  $c_{jj}$  are the corresponding diagonal terms of the matrix  $\mathbf{A}^{-1}$ .

### 3.1. Alternative selection of predictors

In general in a regression analysis it is desired to know how many independent variables are appropriate to include in the analysis. In computational algebraic it is known that singular value decomposition (SVD) provides what is probably the most accurate way of determining numerically the rank of a matrix such as those resulting from the system of Eq. (13). The rank is determined as the number of non-zero singular values. In practice it will be necessary to discount small singular values, which have arisen due to

computational rounding errors. If any singular value is close to zero, this indicates that there is little error caused though omitting the associated modes. On the other hand, the largest singular values will define those modes, which are more dominant.

Besides, SVD routines produces a solution that is the best approximation in the least-squares sense of over-determined system of equations without dealing with the normal equations. In many cases the normal equations are very close to singular, giving fitted parameters with very large magnitudes in a fragile balance, which cancel out almost precisely when the fitted function is evaluated. SVD is a set of techniques usually recommended against multicollinearity and matrix ill-conditioning problems such as those common in regression analyses. The direct output from SVD gives an indicator of predictor redundancy that is related to the probable uncertainties in the estimates of the parameters. However, for large systems this approach is compositionally expensive.

Recently, Ramachandran [21] used the method of SVD to solve the resulting system of algebraic equations obtained from the use of the MFS for 2D harmonic problems showing extremely accurate results. In the present work, in order to determine which are the most significant sources in a given distribution of sources in the MFS for 3D problems, we will consider criteria of regression analysis, as the one defined by the  $t$  test, instead of looking at the largest SV of the corresponding system, due to the computational cost involved in such estimation. In this sense, the regression equation expresses the best prediction of the dependent variable  $\mathbf{y}$ , given the independent variables  $\mathbf{X}$ . Data will exactly fit the model only asymptotically and there is usually substantial variation of the observed points around the predicted values  $\mathbf{X}\mathbf{b}$ . Beyond the finding of best-fit parameters, we need measures to assess the adequacy of the fit. The smaller the variability of the residual values relative to the overall variability, the better is our prediction.

Besides the  $t$  test, another measure of the ability of the regression to explain the variability of the dependent variable is obtained by performing an analysis of variance (ANOVA). The analysis of variance approach is based on the partitioning of sums of squares and degrees of freedom associated with the response variable  $Y$ . There is a variation in  $y_i$ , which is conventionally measured in terms of the deviations around the mean  $\bar{y}$ . In our MFS the value of  $\bar{y}$  is the mean value of the known potential field for a first kind boundary value problem, or the mean value of the known normal derivative a second kind boundary value problem. In the case of a mixed boundary value problem,  $\bar{y}$  is the mean value of the known potential field and normal derivative at the surface collocation points, both of them considered as a single quantity. In the solution of a mixed boundary value problem the surface potential

and flux are two different physical quantities, however in terms of a regression analysis they are the known observation values of the random variable  $Y$ , i.e. the values of the respond variable.

The measure of total variations or *total sum of squares* denoted by SSTO, is the sum of the squared deviations

$$\text{SSTO} = \sum_{i=1}^M (y_i - \bar{y})^2 \quad (27)$$

When using the predictor variables, the variation reflecting the uncertainty concerning the variable  $Y$  is that of the  $Y_i$  observations around the fitted regression line. The difference between the sums of squares SSTO and SSE is another sum of squares denoted by SSR (deviation of fitted regression value around mean)

$$\text{SSTO} - \text{SSE} = \text{SSR} = \sum_{i=1}^M (\hat{y}_i - \bar{y})^2 \quad (28)$$

The above partition formula of sum of squares follows from the fact that for a linear regression model the cross product

$$\sum_{i=1}^M (\hat{y}_i - \bar{y})(y_i - \hat{y}_i) \quad (29)$$

is identical zero (for more details see Ref. [19]). SSR may be considered a measure of that part of the variability of the  $Y_i$  which is associated with the regression line. The larger SSR is in relation to SSTO, the greater is the effect of the regression relation in accounting for the total variation in the  $y_i$  observations.

For computational purpose it is possible to rewrite the above sums of squares in matrix form as [19]:

$$\text{SSTO} = \mathbf{Y}^T \left( \mathbf{I} - \left( \frac{1}{M} \right) \mathbf{J} \right) \mathbf{Y} = \mathbf{Y}^T (\mathbf{Y} - \bar{\mathbf{Y}}) \quad (30)$$

$$\text{SSE} = \mathbf{Y}^T (\mathbf{I} - \mathbf{H}) \mathbf{Y} = \mathbf{Y}^T (\mathbf{Y} - \hat{\mathbf{Y}}) = \mathbf{Y}^T (\mathbf{Y} - \mathbf{X}\mathbf{b}) \quad (31)$$

$$\text{SSR} = \mathbf{Y}^T \left( \mathbf{H} - \left( \frac{1}{M} \right) \mathbf{J} \right) \mathbf{Y} = \mathbf{Y}^T (\hat{\mathbf{Y}} - \bar{\mathbf{Y}}) \quad (32)$$

where the matrix  $\mathbf{J}$  is a square matrix with all elements equal to 1,  $\mathbf{H}$  is the hat matrix defined by Eq. (23),  $\bar{\mathbf{Y}}$  is a constant vector which elements are  $(1/M)\sum y_i$  and  $\hat{\mathbf{Y}}$  is given by Eq. (17) as  $\mathbf{X}\mathbf{b}$ .

SSTO measures the variation in  $Y_i$ , or the uncertainty in predicting  $Y_i$  when no account of the predictor variables is taken. Similarly, SSE measures the variation in the  $Y_i$  when a regression model utilizing the predictor variables is employed. A natural measure of the effect of the  $x_{ij}$  in reducing the uncertainty in predicting  $Y$  is to express the reduction in variation as a proportion of the total variation

$$R^2 = \frac{\text{SSR}}{\text{SSTO}} = 1 - \frac{\text{SSE}}{\text{SSTO}} = 1 - \frac{\mathbf{Y}^T (\mathbf{Y} - \mathbf{X}\mathbf{b})}{\mathbf{Y}^T (\mathbf{Y} - \bar{\mathbf{Y}})} \quad (33)$$

or

$$\begin{aligned} R^2 &= 1 + \frac{\mathbf{Y}^T \mathbf{X}\mathbf{b}}{\mathbf{Y}^T (\mathbf{Y} - \bar{\mathbf{Y}})} - \frac{\mathbf{Y}^T \mathbf{Y}}{\mathbf{Y}^T (\mathbf{Y} - \bar{\mathbf{Y}})} \\ &= 1 + \frac{\mathbf{b}^T \mathbf{g}}{\mathbf{Y}^T (\mathbf{Y} - \bar{\mathbf{Y}})} - \frac{\mathbf{Y}^T \mathbf{Y}}{\mathbf{Y}^T (\mathbf{Y} - \bar{\mathbf{Y}})} \end{aligned} \quad (34)$$

where the relations  $\mathbf{Y}^T \mathbf{X}\mathbf{b} = \mathbf{b}^T \mathbf{X}^T \mathbf{Y} = \mathbf{b}^T \mathbf{g}$ , according to Eqs. (18) and (19), have been used. The measure  $R^2$  is called the coefficient of multiple determination. This value is immediately interpretable as the fraction of the original variability explained by the regression, and  $1 - R^2$  is the fraction of residual variability. In other words, this is an indicator of how well the model fits the data. Ideally, we would like to explain most if not all of the original variability. Of two models containing different variables, the model with the largest coefficient of determination is preferred.

In this work, we will compare the above two regression analysis criteria for the determination of the most significant sources in the least-squares MFS for 3D harmonic problems, i.e. the  $t$  test and the coefficient of multiple determination  $R^2$ .

#### 4. Adaptive refinement strategy

An adaptive refinement method can be described as a process where the automatic construction of a near-optimal discretization is performed in the course of the computations, according to a correction indicator obtained from previous discretization. An adaptive refinement algorithm for the MFS is made up of a certain number of steps, each of them selectively improving the distribution of sources.

Multiple regression is a seductive technique where the effect of introducing an additional predictor is to reduce the error, thus tempting to capitalize on chance by introducing many predictor variables and expecting that at least a few of them will come out significant. When there is a practically unlimited number of independent variables involved, redundancy may only be manifested after several variables have already been entered into the regression equation. The reason for this is that, rather often, observations do not clearly distinguish between two or more of the basis functions provided. In this sense, our adaptive refinement scheme could be interpreted as a multiple regression, in which the introduction of additional sources is expected to reduce the error of the MFS solution. In the present approach, the problem of source selection is viewed as a parameter estimation scheme where it is desired to select a subset of best unit intensity fields from the fundamental solutions as predictors of the fields at the given boundary collocation points.

At each step  $k$ , some of the  $N_{k-1}$  sources from the previous step need to be selected to be *spread*, so that additional sources are added in their vicinities.

The corresponding  $N_k - N_{k-1}$  columns of basis functions are added to the design matrix  $\mathbf{X}$ , and a new least-squares problem is solved.

#### 4.1. Correction indicators

Approximate numerical solutions obtained by the MFS are sensitive to the selection of collocation points on the boundary and to the selection of source points. As pointed out before, the least-squares solution of the MFS provides a direct way of computing the influence of each parameter based on direct interpretation of the relative *significance* of the sources provided by regression analysis, resulting in a reasonable and inexpensive way of obtaining indicators for refinement.

In any refinement strategy for the MFS, the selection and spreading of sources must find a combination that include as least as possible interactions between highly correlated neighboring sources which may lead to collinearity and ill-conditioning of the least-squares problem. Consequently, care must be exercised to avoid breakdown caused by premature inclusion of predictors. This is accomplished in this work by following selection procedures for best predictor subset in regression analysis to guide the selective refinement with reduction of the global error. In other words, new set of sources will be added without increasing significantly the condition number of the resulting matrix.

According with the  $t$  test and the fact that for a given data  $Y$  the variance  $\sigma$  is constant, a possible criterion to guide the refinement procedure is to select as significant those source intensities whose value (variance of parameters)

$$s_j = \left| \frac{b_j}{c_{jj}} \right| \quad (35)$$

is greater than some prescribed value, i.e. the most significant parameters in the regression analysis [18]. In this way we will be able to refine the sources without increasing substantially the condition number of the resulting matrix. As can be observed, this indicator is not suitable for solution with iterative methods since it is necessary to know the values of the diagonal terms of the inverse matrix  $C$ .

As previously commented the  $t$  test is known to be a marginal test from the perspective of the general linear test approach. Therefore, it will be not surprising that the application of the above criterion does not work all the time, as was observed in our numerical examples. Another alternative to select the new sources can be defined in terms of the variability explained by the regression, i.e. the criterion resulting from the values of  $R^2$ , since the coefficient of determination  $R^2$  is interpreted as a relative measure of the error reduction, as higher  $R^2$  is the model fits better the data. Using this last approach, we can compute a local indicator by selecting the contribution of each source

to explain the total sum of the coefficient of determination. In this way, the sources that contribute more to increase the magnitude of  $R^2$  are the most significant in the solution. Since for a given data file the terms  $\mathbf{Y}^T(\mathbf{Y} - \bar{\mathbf{Y}})$  and  $\mathbf{Y}^T\mathbf{Y}$  in Eq. (34) are constants, it follows that an increase in  $R^2$  obtained by those parameters (sources in our case) that contribute more to produce a larger values of the vector product  $b_j g_j$  in Eq. (34). Therefore, we choose as an alternative criterion to the the  $t$  test one that guarantee an increase of  $R^2$  at every step of the refinement algorithm by chosen as the significant sources those with the higher values of

$$s_j = \frac{b_i \delta_{ij} g_i \delta_{ij}}{\mathbf{Y} \cdot \mathbf{Y}} \quad (36)$$

where for scaling purpose, we have divided the term by the square of  $Y$ . Note that the above equation refers to the individual components whose summation is given in Eq. (34). In our numerical examples we tested the efficiency of the above two criterion for selection of the sources that need to be refined, i.e. those found by using Eq. (35) or (36).

The approach proposed in this work is an extension to 3D problems of our previous work [22] for 2D harmonic problems, in which only the criterion based upon the coefficient of determination  $R^2$  was employed and due to the 2D nature of the problem, the strategy used to spread the sources was simpler.

#### 4.2. Criterion for spreading of sources

A sequentially refined MFS solution will be started on an arbitrarily defined distribution. In principle we need only to define a distribution of the boundary points and the sources sufficient to describe the geometry and boundary conditions of the problem. We assume that the distribution of the boundary points is adequate and we are only concerned with the refinement of the source positions.

The basic idea is that the sensitivity of the error to each specific source intensity will indicate which of them can be split into a local higher number of sources. Starting from the initial coarse distribution of source points on a given surface, the new intensities are added by subdivision of sources in a hierarchical structure. At each step, the correction indicators  $s_j$ , given by Eq. (35) or (36), are computed on the starting distribution to select the areas that must be refined. Various strategies based on the same indicators are possible to obtain an accurate solution in an efficient way. In this work, from the distribution of the values  $s_j$ , the maximum value  $s_{\max}$  and average value  $\bar{s}$  are computed to define a threshold

$$s_c = \alpha \bar{s} + (1 - \alpha) s_{\max} \quad (37)$$

so that all sources with a value  $s_j > s_c$  will be spread.  $\alpha$  is an adjustable refinement parameter, which can vary between 0 and 1. Noticed that with this strategy, when we use  $\alpha = 1$ , we will refine all sources with an indicator larger than

the average value,  $\bar{s}$ , and with  $\alpha = 0$  only refine the source with the larger value of the indicator.

#### 4.3. Geometry of source spreading

As opposed to BEM, MFS is practically grid-free. Tree structures have no preferred geometry and are particularly effective for discretization in the MFS. By partitioning a source distribution into a hierarchy of localized regions, the branched region near the source in question is explored in detail, and the more distant regions are explored more coarsely.

An initial coarse distribution of source points on a surface enclosing the original problem domain is given and a tree structure of nested triangular branching is used for spreading of the sources over such external surface. In what follows we shall introduce the computational molecule associated with the tree construction. Although strictly speaking the distribution does not have a mesh structure, for the purpose of automating the source point generation process, the triangular areas around the sources can be considered as associated cells connect neighboring source points.

In the solution of the least-squares problem at a given refinement stage we want to profit from the reduction in error already achieved with all previous generations of sources. Since we want to use the refinement algorithm to create and modify sequences of nested distributions, the linking of generations and creation of *children* points to be added to the sequence plays an important role in the procedure. In the presented sequence of nested triangular branches, children source points are generated by simple bisection of the arcs connecting the parent source point with the vertices of its associated triangle. In this way, the source distribution is iteratively partitioned into a hierarchy of localized regions. At the next iteration the children of the previous nest becomes the new parents. The construction of a second order tree, i.e. of level two, over a sphere is illustrated in Fig. 1.

Refinement algorithms can be applied in different contexts, for example to be able to develop flexible

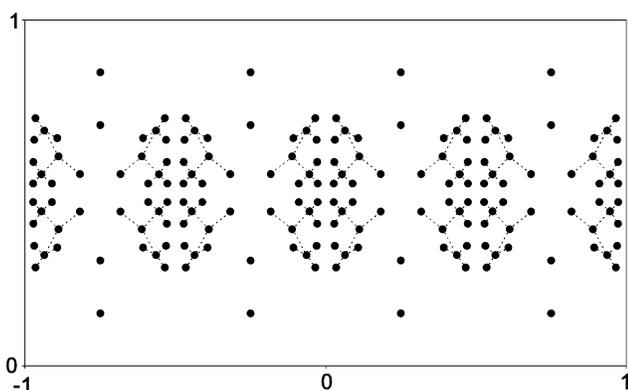


Fig. 1. Tree structure of source refinement on the surface of a sphere.

generators of irregular trees or to locally refine a given tree. In these cases is not necessary to store the complete sequence of divisions. However, some bookkeeping of the sequential branching helps if during further refinement steps it is necessary to eliminate some of the previous branches in order to change sequences of nested branching, as in cases of time dependent problems. Although the advantage of no meshing is surrendered to a certain extent, there is great flexibility and simplicity in the procedure for building the hierarchical tree structure. The molecular structure of the presented spreading algorithm is not intended to be computationally optimal, but its computational burden is small compared to that of the overall operations in the refinement algorithm.

#### 4.4. Termination of refinement

There are many possibilities for the process to come to an end. In an absolute sense, at the last step,  $N_k$  cannot be greater than  $M$ . The refinement can be terminated earlier by consideration of computational limitations or desired accuracy. In the present implementation a maximum number of sources is fixed as  $N_{\max} = M/4$ . However, adequate accuracy is usually obtained before that limit with a near-optimal value of the refinement parameter  $\alpha$ . Failure may be detected otherwise in the solver routine due to ill-conditioning, generally as a result of a bad initial discretization. In this paper emphasis is made on the strategy as the specific computation of the correction indicator and the termination criterion can vary between implementations. The aspect of defining a criterion for the termination of the adaptive process may deserve further study for particular applications.

### 5. Numerical examples

Since the proposed method can be based upon two different criteria borrowed from statistical analysis, its capability to reproduce the potential needs to be tested on different problems. In order to observe the features of the adaptive process, the overall convergence of the numerical solutions obtained with the adaptive scheme are illustrated by computing the relative residual error, which is shown in logarithmic scale in the figures below.

In the examples considered in this section, the adaptive strategy applied on an enclosing surface automatically yields a graded mesh in a relatively short number of steps. In three steps the error obtained is acceptable for practical engineering applications. Further refinement gives increased accuracy, the reduction of error is noticeable in few steps with a relatively small number of sources.

In the present refinement is accomplished by introducing new sources. As a way of comparing efficiency, we used both direct and indirect algorithms to solve the resulting

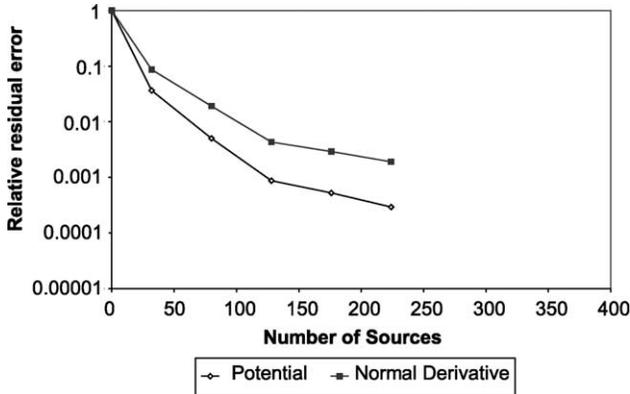


Fig. 2. Error reduction in refinement based on variance of parameters with 2048 imposed potentials on a sphere.

system of algebraic equations at each step of the refinement schemes. When using a direct algorithm to solve the normal equations, the design matrix updated at each refinement step can be partitioned in order to obtain a solution by taking advantage of the one from the previous step. We store the inverse matrix **C** and the cholesky factor of **A** from the previous distribution, so that the procedure to update the vector of parameters and the complete inverse matrix involves full inversion of a relatively small square matrix only. The remaining operations are matrix products which become more computationally expensive as the number of sources increases.

For indirect solution we use GMRES and instead of storing a precomputed square matrix for the normal equations the product needed for each iteration is performed as two matrix-vector products in order to reduce the effect of roundoff error. The required memory for the stored basis vectors grows at each iteration of the refinement procedure but is kept small compared to that required by the whole matrix **X**.

In our numerical experiments, the use of the indirect algorithm was always more efficient than the direct one. Besides, numerical instabilities were encountered when using the direct solver for more than 250 sources in the discretization. In those cases in which both approaches were possible to be used, the corresponding numerical

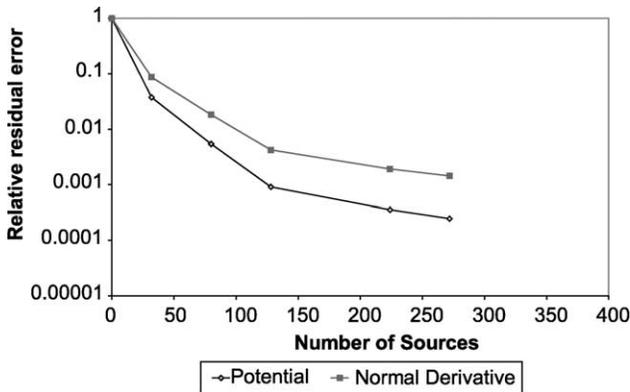


Fig. 3. Error reduction in refinement based on variance of parameters with 2048 imposed normal derivatives on a sphere.

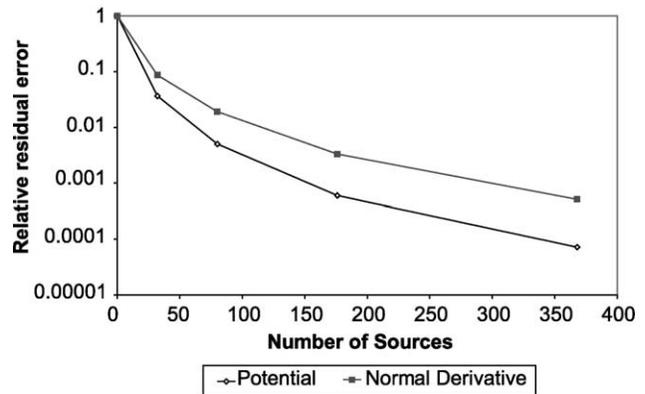


Fig. 4. Error reduction in refinement based on coefficient of determination with 2048 imposed potentials on a sphere.

solutions were found to be identical. The numerical results reported in this section were found with the used of the GMRES solver.

We first consider the problem, which potential is given in spherical coordinates by

$$\Phi = r^2 \sin^2 \theta \cos 2\phi \tag{38}$$

inside a unit radius sphere. Dirichlet boundary conditions are imposed at  $M = 2048$  points uniformly distributed on the surface of the sphere  $r = 1$ . An initial uniform distribution with 32 sources located on a sphere with radius  $a = 2$  is given. In this first example, the refinement indicator,  $s_j$ , is given by Eq. (35), i.e. the indicator based on the variance of parameters. Fig. 2 shows the reduction of the root mean square error in the potential and the normal derivative at the surface in 4 steps.

An additional example with the same potential is considered but imposing the normal derivatives at the same collocation points of the first example, and the value of the potential at the origin is given in order to guarantee uniqueness of solution. Fig. 3 shows the corresponding behavior of the error.

The previous two examples were solved using the alternate indicator given by Eq. (36), i.e. the indicator

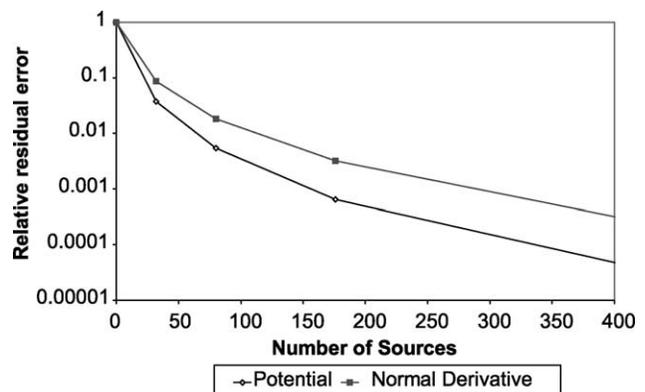


Fig. 5. Error reduction in refinement based on coefficient of determination with 2048 imposed normal derivatives on a sphere.

based on the coefficient of determination, which gives a faster reduction of the error than those obtained with the previous error indicator, i.e. the indicator based on the variance of parameters, as shown on Figs. 4 and 5. In both examples, Dirichlet and Neumann problems, when using the indicator based on the variance of parameters, Eq. (35), it was necessary to keep the number of sub-divisions relatively small at each iteration, i.e. to use a small value of  $\alpha$  corresponding to a slow refinement scheme, in order to guarantee that the resulting algebraic system does not become singular. However, this problem was not observed when using the coefficient of determination, Eq. (36), which always works even for large values of  $\alpha$  corresponding to a fast refinement scheme. The difficulty encountered with the method of the variance of the parameters appears to be consequence of the marginal character of the  $t$  test.

We compare the performance of the iterative and direct solvers with the latter indicator. For all successful runs, i.e. for optimal values of the refining parameter  $\alpha$  and an adequate starting distribution of sources, the results from the iterative solver are indistinguishable from those of the direct solver. However, the iterative solver is faster for larger problems. In addition, when the direct method degenerates due to ill-conditioning the iterative approach was able to produce good results. In general a trial value of the refinement parameter near  $\alpha = 0.6$  can be safely used as an initial approximation.

As a next test using the iterative solver and the coefficient of determination as the more recommended scheme, according to our previous experience, we consider the problem inside of a cylinder which potential given in cylindrical coordinates as:

$$\Phi = I_1(2r)\sin \theta \cos 2z \quad (39)$$

where  $I_1$  is the modified Bessel function of the first kind. This problem is solved in a cylinder with radius 1 and height 2. Potentials are imposed on the circular faces and normal derivatives on the cylinder walls, i.e. a mixed boundary value problem. For this problem the total number of boundary points is  $M = 2568$ . The sources are originally distributed on an ellipsoid with semi-axes  $a_r = 2.2$  and  $a_z = 3.3$ , which encloses the cylinder. Fig. 6 shows an important reduction of the relative residual error in 4 refinement steps.

As a final test using the iterative solver and the coefficient of determination, we consider the steady state heat flow in an infinite hollow circular cylinder, i.e. between two concentric cylindrical surfaces, with constant surface temperature. The analytical solution of this problem is given in cylindrical coordinates as:

$$\Phi = \Phi_1 + (\Phi_2 - \Phi_1) \frac{\ln(r/r_1)}{\ln(r_2/r_1)} \quad (40)$$

where  $\Phi_1$  and  $\Phi_2$  are the temperatures on the inner and outer surfaces with radii  $r_1$  and  $r_2$ , respectively. We deal with this 2D problem as a 3D mixed boundary value problem with

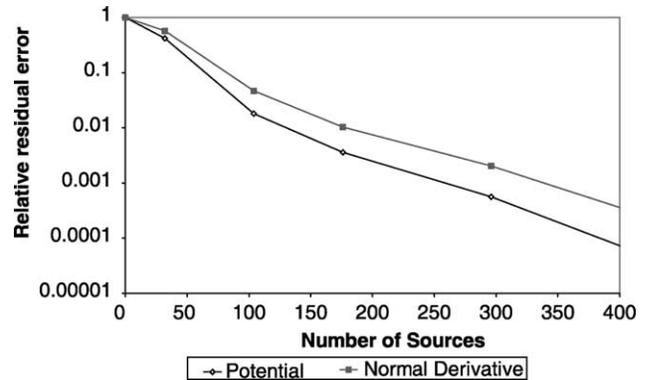


Fig. 6. Error reduction in refinement based on coefficient of determination with 768 potentials and 1800 normal derivatives imposed on a cylinder.

plane covers placed at  $z = \pm h/2$ . This problem is solved with  $\Phi_1 = 1$  at  $r_1 = 1$ ,  $\Phi_2 = 2$  at  $r_2 = 2$  and  $h = 1$ . We impose the corresponding temperatures on the cylindrical surfaces and zero normal derivatives on the plane surfaces. Although consideration of axial symmetry makes this a simple problem, to illustrate its solution in 3D space a uniform fine distribution of boundary points is used. The total number of boundary points is  $M = 3600$ , with 600 of them on the inner cylinder, 1200 on the outer cylinder and 900 on each of the upper and lower plane faces. 120 sources are initially distributed on an toroidal surface generated by an ellipse with semi-axes  $a_r = 1$  and  $a_z = 2$ , with radius of rotation around the  $z$  axis  $r_t = 1.5$ . Fig. 7 shows the results of refinement with  $\alpha = 0.8$ . A sharp decrease of the relative residual error can be noticed in the first refinement step, which rather seems to indicate an excessive number of initial points. This is followed by a slower further reduction to the order of  $10^{-4}$ .

## 6. Conclusions and recommendations

This work introduces an adaptive refinement procedure for the MFS based on concepts from multiple linear regression analysis. The computation of the approximate solution to potential problems through the least-squares

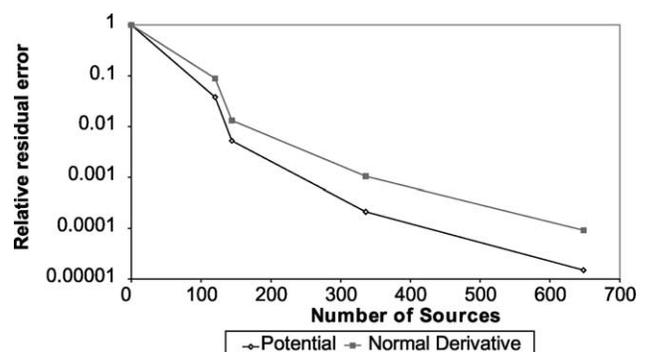


Fig. 7. Error reduction in refinement based on coefficient of determination with 1800 potentials and 1800 normal derivatives imposed on a square ring.

approach provides a notable reduction in the number of source points in relation to those required by the direct collocation scheme. In addition, a more reasonable distribution of the global error in the solution can be achieved. The solution with the iterative solver GMRES makes this refinement scheme a powerful tool for large 3D potential problems.

The numerical experiments carried out in this work (for first, second and mixed boundary value problems) show that the indicator based on the coefficient of determination generally work better than the one base upon the variance of parameters. This technique provides useful information to guide a selective refinement of the source distribution. Reduction of the global error is reached in relatively few steps, even with a very coarse initial starting distribution of sources.

Since the MFS allows great flexibility in the way in which the discretization is carried out, the strategy used in the presented refinement-only implementation for the source spreading can be certainly improved. Simpler and more obvious strategies can be used if it is not necessary to redefine the refinement branches afterwards. However, this redefinition of the branches procedure could be required to manage more complex situations, as is the case of moving boundary problems.

Although the present refinement strategy is based upon the distribution of new sources over a prescribed auxiliary surface enclosing the original problem domain, simulating the effect of an external single layer potential, it is also possible to extend the present idea to the distribution over more than one auxiliary surface by allowing hierarchy trees with branches perpendicular to the original surface and not only tangential to the surface. In this way it is also possible to represented the effect of two or more layer of potentials, i.e. external double or more surface potentials.

In the present refinement strategy based upon the distribution of sources over a prescribed surface, it is clear that the achievable error reduction is strongly dependent on the selection of the surface and the initial distribution of points. Adequate accuracy can be guaranteed provided that the initial distribution of points reflects in some sense the flow pattern and the auxiliary surface is constructed following a compromise between the higher accuracy for farthest distances from the domain and the better matrix condition at shorter distances. Further improvement can be directed towards refining the shape of the auxiliary surface itself.

The proposed error indicator and refinement strategy introduced in this work for harmonic problems could be adapted to other elliptic problems. The approach adopted in this work has potential advantages and more research is needed in this direction for its application to complex practical problems, especially time dependent problems with moving boundaries.

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