A multi-level Method of Fundamental Solutions using quadtree-generated sources

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Abstract

A new strategy to define source points for the Method of Fundamental Solutions is presented based on a quadtree-generated cell system controlled by the boundary of the domain in which the partial differential equation is defined. The quadtree (in 3D, octtree) algorithm results in a cell system, the spatial density of which decreases rapidly when moving away from the boundary. The sources are defined to be the cell centers of the external cells of the quadtree subdivision. This makes it possible to build up a multi-level method, where the 'coarse' sources generate the 'coarse' approximation, while the 'fine' (i.e. the near-boundary) sources provide the 'fine' approximation. On each level, the problem is discretized by using the sources belonging to the actual level only. Thus, the computational cost can be kept under an acceptable limit. Moreover, the problem of severely ill-conditioned linear systems is completely avoided.

Keywords: **Method of Fundamental Solutions, multi-level method, quadtrees**

Introduction

The Method of Fundamental Solutions (MFS, see e.g. [8]) is now a popular computational method for solving elliptic partial differential equations due to its simplicity and meshfree character and also to the fact that it is a boundary-only technique i.e. no discretization is needed inside the domain.

In its original form, the approximate solution is defined as a linear combination of the fundamental solution shifted to some external points (*source points*). Thus, the approximate solution exactly satisfies the partial differential equation to be solved. The a priori unknown coefficients of the linear combination are calculated by enforcing the boundary conditions at some *boundary collocation points*.

For instance, consider the example of the simplest 2D Laplace equation:

$$\Delta u = 0 \qquad (1)$$

defined in a bounded 2D domain Ω. Suppose that Equation (1) is equipped with pure Dirichlet boundary condition:

$$u|_{\Gamma} = u_0 \,, \qquad (2)$$

where $\Gamma := \partial\Omega$, the boundary of the domain Ω. The approximate solution defined by the MFS has the form:

$$u(x) \sim \sum_{j=1}^{N} \alpha_j \, \Phi(x - \tilde{x}_j) \,, \tag{3}$$

where Φ denotes the fundamental solution of the Laplacian (apart from a multiplicative constant):

$$\Phi(x) \ = \log||x|| \tag{4}$$

and $\tilde{x}_1$, $\tilde{x}_2$, …, $\tilde{x}_N$ are predefined external source points. Here $||.||$ denotes the 2D Euclidean norm. The coefficients α_1, α_2, …, α_N can be calculated by requiring the boundary conditions. In case of Dirichlet boundary condition, this results in the following linear system of equations:

$$\sum_{j=1}^{N} \alpha_j \, \Phi\left(x_k - \tilde{x}_j\right) = u_k \coloneqq u_0(x_k) \qquad\qquad (k = 1,2, \dots, M), \tag{5}$$

where $x_1, x_2, \dots, x_M$ are predefined boundary collocation points.

The numbers of sources and the boundary collocation points need not be equal. If $N \neq M$, Equation (5) should be solved in a generalized sense using e. g. the least squares approach. For the sake of simplicity, however, in a lot of practical cases, the numbers N and M are defined to be equal, that is, Equation (5) has a square matrix. Unfortunately, though the MFS has excellent accuracy in general (see [10]), in a number of cases, the discretized linear system is severely ill-conditioned, especially when the sources are located far from the boundary. On the other hand, if they are too close to the boundary, numerical singularities appear in the approximate solution.

Another problem of the Method of Fundamental Solutions is the proper definition of the locations of sources (preferably in an automated way). In [1], [4], the sources are located along a sufficiently large circle; however, this leads to extremely ill-conditioned linear systems. In [12], the initial set of points is thinned by several strategies. See also [3], where the original boundary is transformed to the boundary of a somewhat larger domain along which the source points are located.

A popular technique is to allow the source and boundary collocation points to coincide. Thus, the problem of the proper definition of sources is automatically circumvented. However, in this approach, some singular terms generally appear, and the main problem is how to evaluate these singular terms properly or how to avoid the singularity. To treat this difficulty, a lot of special methods have been developed. The boundary knot method [2] utilizes general nonsingular solutions instead of the traditional fundamental solutions: thus, the problem of singularity is avoided, but the problem of severely ill-conditioned character of the discretized system remains the case. The situation is similar, when fundamental solutions concentrated to straight lines instead of points are used, see [6]. Using the traditional fundamental solutions, the evaluation of singular terms can be performed by special tools (regularization and desingularization techniques, see e.g. [7], [9], [11], [13]).

In this paper, we return to the traditional form of the MFS. However, the sources are generated in a completely automatic way using the well-known quadtree/octtree subdivision technique (see e.g. [5]). This algorithm produces a cell system; the individual cells belong to different levels of subdivision. The cell system exhibits automatic local refinements in the vicinity of the boundary. Taking the centers of the outer cells as source points, we obtain a point set, the spatial density of which decreases rapidly when moving away from the boundary. This makes it possible to build up a multi-level discretization in a natural way. The method avoids also the problem of solving severely ill-conditioned systems of equations and has a relative low computational complexity as well.

A two-level technique

As a model problem, consider the 2D Dirichlet problem (1) - (2). Suppose that the boundary collocation points $x_1, x_2, \dots, x_M$ are given. Let $\tilde{x}_1^F, \tilde{x}_2^F, \dots, \tilde{x}_N^F$ be external source points at a distance δ from the boundary (more or less equally spaced), they will be considered 'fine level' sources. Moreover, let $\tilde{x}_1^C, \tilde{x}_2^C, \dots, \tilde{x}_{N/2}^C$ be additional ('coarse level') sources at a distance 2δ from the boundary (N is supposed to be an even number). Define the approximate solution of (1) - (2) as follows:

$$u(x) \sim \sum_{j=1}^{N} \alpha_j^F \, \Phi\left(x - \tilde{x}_j^F\right) + \sum_{j=1}^{N} \alpha_j^C \, \Phi\left(x - \tilde{x}_j^C\right) \qquad (6)$$

Enforcing the boundary condition in the boundary collocation points, we have:

$$\sum_{j=1}^{N} \alpha_j^F \, \Phi\left(x_k - \tilde{x}_j^F\right) + \sum_{j=1}^{N} \alpha_j^C \, \Phi\left(x_k - \tilde{x}_j^C\right) = u_k \qquad (k = 1,2,\dots,M) \qquad (7)$$

In a more compact form:

$$A^F \boldsymbol{\alpha}^F + A^C \boldsymbol{\alpha}^C = \boldsymbol{u} \qquad (8)$$

where A^F is an M-by-N and A^C is an M-by-$N/2$ matrix with entries:

$$A_{kj}^F = \Phi\left(x_k - \tilde{x}_j^F\right), \quad A_{kj}^C = \Phi\left(x_k - \tilde{x}_j^C\right) \qquad (9)$$

The direct solution of Equation (8) is not recommended, since Equation (8) is even more ill-conditioned than the single-level equation

$$A^F \boldsymbol{\alpha}^F = \boldsymbol{u}$$

Instead, it can (and should) be solved in an iterative way (in the sense of least squares) by splitting it into a coarse-level and a fine-level subproblem:

$$A^C \boldsymbol{\alpha}^C = \boldsymbol{u} - A^F \boldsymbol{\alpha}^F \qquad (10)$$

$$A^F \boldsymbol{\alpha}^F = \boldsymbol{u} - A^C \boldsymbol{\alpha}^C \qquad (11)$$

The above equations are to be solved in the sense of least squares, i.e. by solving the corresponding Gaussian normal equations:

$$(A^C)^* A^C \boldsymbol{\alpha}^C = (A^C)^* (\boldsymbol{u} - A^F \boldsymbol{\alpha}^F) \qquad (12)$$

$$(A^F)^* A^F \boldsymbol{\alpha}^F = (A^F)^* (\boldsymbol{u} - A^C \boldsymbol{\alpha}^C) \qquad (13)$$

The main idea of the method is that if the coarse subproblem is already solved, then, in order to solve the fine level subproblem, it is sufficient to apply some steps of the familiar (conjugate) gradient method, which significantly reduces the computational complexity.

Remark: Without going into deep details, the idea behind the method is as follows. The solution of the coarse level subproblem (nearly) eliminates the low-frequency error components from the approximate solution. Thus, the fine level operator maps the subspace of the high-frequency components into itself. It can be shown that the fine level operator restricted to the high-frequency subspace is uniformly well-conditioned (independently of the fineness of the discretization). Thus, though the (conjugate) gradient method converges slowly, if the corresponding operator is not well-conditioned, the high-frequency error components are damped much more efficiently.

By introducing additional sources on even coarser levels, the method can be extended to a multi-level technique in a straightforward way. At the coarsest level, the corresponding subproblem should be solved exactly. In practice, it is often sufficient to apply several (conjugate) gradient iterations at the coarsest level as well.

Automatic generation of source locations using quadtrees

To build up a multi-level method outlined above, several *groups* of sources are needed. The greater the distance from the boundary, the lower the spatial density of the sources is. The quadtree algorithm produces point sets with exactly the same property. Recall that the quadtree subdivision is a systematic, recursively defined subdivision of an initial square controlled by a finite set of points (controlling points). A subsquare is divided into four congruent subsquares (cells), if the number of controlling points contained in the actual subsquare exceeds a predefined minimal value, provided that the level of subdivision remains under a predefined maximal level. This results in automatic local refinements in the vicinity of the controlling points. By additional subdivisions, it can be assured that the ratio of the neighboring cell sizes is at most 2, i.e. no abrupt changes in cell sizes occur. Note that in 3D, the procedure is similar: here an initial cube is divided recursively into eight congruent subcubes (octtree algorithm). Note also that the obtained cell system is suitable for defining simple finite volume schemes as well (see e.g. [5]), however, here it is used to define source point locations only.

In the presented multi-level technique, the quadtree subdivision is controlled by the boundary of the domain of the original partial differential equation, more precisely, by the predefined boundary collocation points. Having created the quadtree cell system, the source points are defined to be the centers of the external cells. The cell centers belonging to low levels of subdivision are considered 'coarse level' sources, while the (near-boundary) cell centers belonging to high levels of subdivision are regarded as "fine level' sources.

Numerical examples

The above outline method is demonstrated through two simple examples.

Example 1. Let Ω be a circle centered at the midpoint of the unit square with radius 0.3. Consider the test solution of the Laplace equation

$$u(x, y) = e^{4\pi x} \cdot \sin 4\pi y, \tag{14}$$

where the more familiar notations *x, y* are used for the space variables. The Laplace equation (1) is supplied with Dirichlet boundary condition consistent with the above test solution. Figure 1 shows the quadtree cell system controlled by the boundary Γ of the domain and the source point locations as well. The maximal subdivision level was 8, i.e. the smallest cell size was 1/256. Table 1 shows the relative L_2-errors of the above outlined two-level method for different numbers of sources calculated on the boundary of the domain. Here L_{coarse} and L_{fine} are the quadtree subdivision levels of the coarse and fine sources, respectively, while

N_{coarse} and N_{fine} denote the numbers of sources at the coarse (resp. fine) level. The number of boundary collocation points was always $= 476$.

The results demonstrate that the accuracy is acceptable. Note, however, that the numerical complexity is much less than that of the traditional direct method.

Table 1. Two-level MFS, relative boundary L_2-errors. Domain: circle

L_{coarse}/L_{fine} N_{coarse}/N_{fine}	3/4 12/88	4/5 88/104	5/6 104/216	6/7 216/376
Relative L_2-error (%)	0.16591	0.04687	0.01604	0.02571

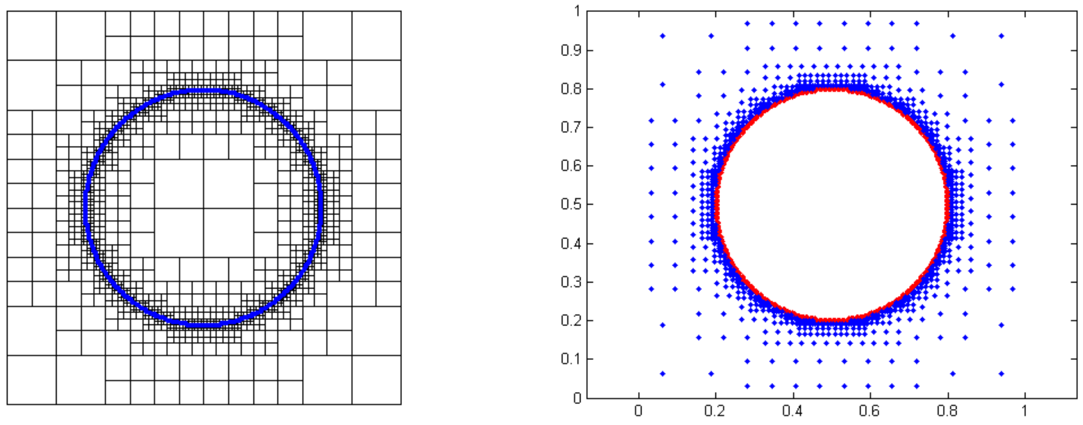

Figure 1. A quadtree cell system generated by a circle and the external source points

Example 2. Let Ω be an amoeba-shaped domain contained in the unit square. Figure 2 shows the quadtree cell system controlled by the boundary Γ of the domain and the source point locations as well. The maximal subdivision level was again 8. The test solution (14) was the same as in Example 1. The number of boundary collocation points was always $M = 236$. Table 2 shows the relative L_2-errors of the above outlined two-level method calculated on the boundary of the domain. L_{coarse} and L_{fine} are the quadtree subdivision levels of the coarse and fine sources, respectively. N_{coarse} and N_{fine} denote the numbers of sources at the coarse (resp. fine) level. Due to the more complicated geometry, the accuracy is now somewhat less than in Example 1, but it is still acceptable.

Table 2. Two-level MFS, relative boundary L_2-errors. Amoeba-shaped domain

L_{coarse}/L_{fine} N_{coarse}/N_{fine}	3/4 19/70	4/5 70/122	5/6 122/227	6/7 227/480
Relative L_2-error (%)	1.3801	0.12707	0.10469	0.06078

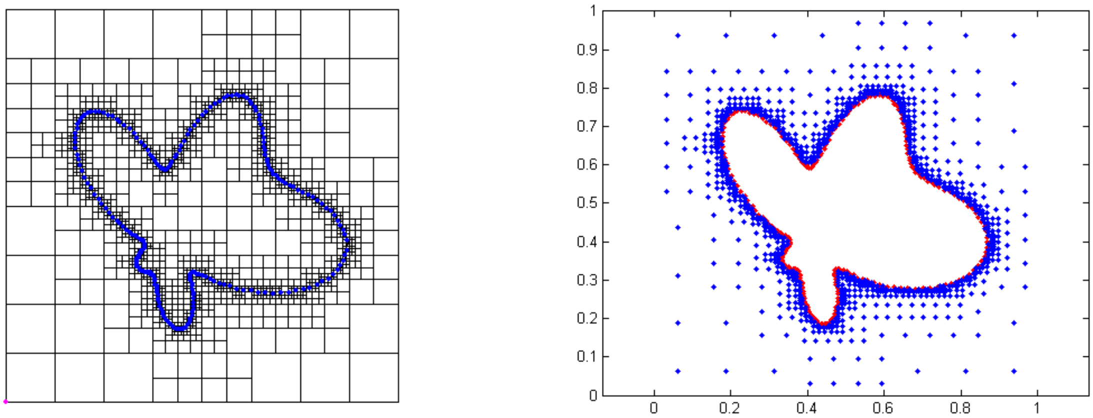

Figure 2. A quadtree cell system generated by an amoeba-like curve and the external source points

Summary and conclusions

The traditional Method of Fundamental Solutions has been revisited. The sources are defined in a completely automatic way using the quadtree/octtree subdivision algorithm. This algorithm generates sources, the spatial density of which is greater in the vicinity of the boundary and becomes low far away from the boundary. These groups of sources result is multi-level MFS-based approximations. As a smoothing procedure the classical (conjugate) gradient method was used. The number of boundary collocation points was always greater than that of the sources at any level, so that the MFS-equations were solved in the sense of least squares, i.e. the Gaussian normal equations were taken into account. The accuracy of the method has been proved acceptable. At the same time, the computational complexity of the method is much less than that of a traditional direct solver. Moreover, the problem of the severely ill-conditioned algebraic system is also avoided.

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References

[1] Alves, C. J. S., Chen, C. S. and Šarler, B., The method of fundamental solutions for solving Poisson problems. *Int. Series on Advances in Boundary Elements. (Proceedings of the 24th International Conference*

on the Boundary Element Method incorporating Meshless Solution Seminar. Sintra, Portugal, 2002, C.A.Brebbia A.Tadeu, V.Popov, Eds. Vol. 13. WitPress, Southampton, Boston, 67–76.

[2] Chen, W., Shen, L. J., Shen, Z. J. and Yuan, G. W. (2005) Boundary Knot Method for Poisson Equations. *Engineering Analysis with Boundary Elements* **29**, 756–760.

[3] Chen, C. S., Karageorghis, A. and Li, Y. (2016) On choosing the location of the sources in the MFS. *Numerical Algorithms* **72**, 107–130.

[4] Fam, G. S. A. and Rashed, Y. F., A Study on the Source Points Locations in the Method of Fundamental Solutions. *Int. Series on Advances in Boundary Elements. (Proceedings of the 24th International Conference on the Boundary Element Method incorporating Meshless Solution Seminar*. Sintra, Portugal, 2002, C.A.Brebbia A.Tadeu, V.Popov, Eds. Vol. 13. WitPress, Southampton, Boston, 297–312.

[5] Gáspár, C. (2004) A Meshless Polyharmonic-type Boundary Interpolation Method for Solving Boundary Integral Equations. *Eng. Anal. with Boundary Elements,* **28**, 1207–1216.

[6] Gáspár, C. (2013) Some Variants of the Method of Fundamental Solutions: Regularization Using Radial and Nearly Radial Basis Functions. *Central European Journal of Mathematics* 11/8, 1429–1440.

[7] Gáspár, C. (2015) A Regularized Multi-level Technique for Solving Potential Problems by the Method of Fundamental Solutions. *Engineering Analysis with Boundary Elements* **57**, 66–71.

[8] Golberg, M. A. (1995) The Method of Fundamental Solutions for Poisson's Equation. *Engineering Analysis with Boundary Elements* **16**, 205–213.

[9] Gu Y., Chen W. and Zhang J. (2012) Investigation on Near-boundary Solutions by Singular Boundary Method. *Engineering Analysis with Boundary Elements* **36**, 1173–1182.

[10] Li, X. (2005) On convergence of the method of fundamental solutions for solving the Dirichlet problem of Poisson's equation. *Advances in Computational Mathematics* **23**, 265–277.

[11] Šarler, B., A Modified Method of Fundamental Solutions for Potential Flow Problems. *The Method of Fundamental Solutions - A Meshless Method.* C.S.Chen, A.Karageorghis, Y.S.Smyrlis Eds. Dynamic Publishers, Inc., Atlanta, USA, 2008, 299–321.

[12] Schaback, R., Adaptive Numerical Solution of MFS Systems. *The Method of Fundamental Solutions - A Meshless Method.* C.S.Chen, A.Karageorghis, Y.S.Smyrlis Eds. Dynamic Publishers, Inc., Atlanta, USA, 2008, 1–27.

[13] Young, D. L., Chen, K. H. and Lee, C.W. (2005) Novel Meshless Method for Solving the Potential Problems with Arbitrary Domain. *Journal of Computational Physics* **209**, 290–321.