

Enrichment Techniques and the Method of Fundamental Solutions

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Abstract

It is well known that the method of fundamental solutions (MFS) provides excellent numerical results while solving boundary value problems for linear elliptic differential equations on smooth boundaries and smooth data. However, despite the theoretical density results, when the solution is not smooth the performance of the MFS might be compromised by discontinuities on the boundary conditions or by the nonsmoothness of the boundary. Moreover, even with some boundary regular data, we may have poor approximations generated by classical choices for the artificial source points, for instance on a circle. In this work we discuss the long standing issue of collocating the source points in the MFS, and propose a method mixing local – global features of the MFS approach, that we will call *glocal*. This choice for the location of the source points is adapted not only to the geometry but also to the boundary problem data. This technique can be used together with standard enrichment, but it can also be seen as some type of enrichment since the justification for the sources position is based on the local approximation. This *glocal* approach to the MFS, together with basis enrichment (using particular solutions), keeps advantages of Trefftz methods and avoids larger systems, worse conditioned.

1 Introduction

The Method of Fundamental Solutions (MFS) is a simple but powerful technique that has been used to obtain highly accurate numerical approximations for boundary value problems in PDEs, using remarkably simple codes and small computational effort. It has been introduced in the 1960's (cf. [10]) and used as an alternative numerical method to the boundary integral methods in several elliptic homogeneous problems, eg. [5], [11] and [6]. For an account of initial developments and applications, see [7]. The application of the MFS can be justified by density results that have been established for simply connected domains with regular boundary (e.g. [6], [3]); its generalization to multiply connected domains is straightforward.

One of the main drawbacks of the MFS as an alternative to BEM is exactly the question where to place the artificial boundary, or more generally where to put the source-points. In many cases good results will be obtained “almost” *no matter where these points are placed*, whereas in some other situations “almost” *all choices lead to poor approximations*. It is usually said that exponential convergence occurs for the MFS, when the source points are placed on a circle with increasing radius, but this is only verified in some optimal situations – usually meaning analytical boundary data. Many times, the MFS arrives to a good result (under the possibilities for machine precision under ill-conditioned systems), but increasing blindly the number of points on the artificial boundary does not provide much better results. One possibility to overcome these difficulties with the MFS is to consider enrichment, meaning adding new basis functions – that are also particular solutions, to keep the Trefftz feature of the method. While considering enrichment, some a priori knowledge is needed, or one can try to use solutions available from other methods (such as BEM or even FEM) to adjust some local *difficulty* on the data (discontinuities, singularities...) or some difficulty on the geometry (corners, cracks). This technique has been explored in [4] for crack problems. Another possibility, that should not exclude the previous one, is to consider appropriate choice for the location of the source points, instead of placing them in some pre-chosen artificial boundary. In this work we will propose a *glocal* method – using first a local MFS to find the positions of the source points, and then use those calculated source points to solve the global MFS system.

2 Basis functions in the MFS

2.1 Enrichment, completeness and accuracy

In the usual framework of the method of fundamental solutions, given a fundamental solution Φ the approximation on a point $x \in \Gamma$ is made using basis functions that are point-sources $\Phi(x - y)$ where y denotes source points placed on an artificial boundary Σ . Using m artificial points, the approximation of the boundary function g is then given by

$$g(x) \approx a_1 \Phi(x - y_1) + \dots + a_m \Phi(x - y_m) \quad (1)$$

The position of the source points y_1, \dots, y_m defines the quality of the approximation. If the artificial curve is predefined then we are limited in the approximation possibilities.

Consider a trivial example, with data g produced by a single point-source. Let $g(x) = \Phi(x - z)$ with z exterior but close to the boundary. Then, in one hand there is a near-singularity on the boundary data, but in the other hand, the correct choice of a single source point z is enough to produce a correct solution. This correct choice is not possible if we pre-chose an artificial boundary set Σ that does not include z .

This simple example allows to conclude that if we limit the possibilities of point-sources y_k to be on a certain prescribed artificial curve Σ then we may skip a simple solution.

From the previous remarks, we conclude that a good choice for the position of the artificial curve strongly depends on the boundary data to be considered. For some a boundary function g_1 a certain artificial curve Σ_1 is better than Σ_2 that might be a better choice to other boundary function g_2 .

Therefore instead of using blindly (1) as an MFS approximation we should consider an enrichment that simply consists in adding appropriate basis functions, ψ_1, \dots, ψ_M when an inspection of the boundary problem suggests the need of these new functions

$$g(x) \approx a_1 \Phi(x - y_1) + \dots + a_m \Phi(x - y_m) + b_1 \psi_1(x) + \dots + b_M \psi_M(x). \quad (2)$$

We can not specify these new functions, since they strongly depend on the type of problem that is being addressed! For instance, while considering the MFS for the 2D Laplace problem it is well known that constants are needed, and therefore at least $\psi_1(x)=1$ should be used as additional basis function. In other circumstances, for instance while considering domains with corners, specific particular solutions should be used.

We distinguish two different situations where enrichment for the MFS is needed:

1. Completeness – some special functions are needed to ensure that, in the limit, the basis is enough to approximate the boundary data, in the appropriate norms.
2. Accuracy – although approximation might be possible with the standard MFS, it is probably better to include some special functions to enhance the accuracy of the approximation, right from the start.

Moreover, the standard use of the MFS approximation leads to usual numerical problems, similar to the ones occurring in other global approximation processes. For instance, like in the Fourier series approximation, an effect, similar to the Gibbs effect, will occur while trying to approximate discontinuous data functions. It is also clear that exact interpolation of the boundary data will lead to an effect similar to the Runge problem in standard polynomial interpolation, and therefore it is better to consider a least-squares approach.

2.2 Choosing source-points

Choosing an appropriate artificial curve Σ to place the source points is the usual choice in the MFS since it has been proven to lead to completeness results (some extra basis functions might be needed, as it happens for the 2D Laplace problem). It is clear that this is far from being a restriction.

Usually an external circle is used for Σ , following [6] or [8], but any other external curve enclosing the domain will work, as it has been proved, and early used in [5]. Moreover, we can just use arbitrary or even random points outside the domain to produce good results – this can be included as a particular case of an external curve, since for a finite number of source-points we can produce a curve Σ that includes these arbitrary points.

The question is not just to know whether the MFS works or not with a certain number of arbitrary source points, the question is to know where to add more source-points to obtain a better result.

First, we remark that arbitrary choices for source-points might lead to impossible approximations.

- (i) For instance, if the fundamental solution has a radial feature, meaning $\Phi(x) = \phi(|x|)$, then if we just consider the source points y_1, \dots, y_m on a line L , it is clear that the approximation will have a symmetry property along that line. If the line cuts the boundary this means that only boundary data with that symmetry property can be approximated using these source-points. Therefore some unsymmetrical boundary data can not be approximated.
- (ii) If we choose the source points on a circle C with radius R , and again the fundamental solution has a radial feature, being null for some value R , meaning $\Phi(x) = \phi(|x|) = \phi(R) = 0$, then the approximation value in the center is null. Therefore, solutions not null at that center point can not be approximated. This is what happens with the 2D Laplace fundamental solution because $\log(1)=0$, giving impossible approximations for some circles Σ , when the solution is not null at that center (or if we do not add an extra constant basis function).

From these considerations we learn that an arbitrary choice for the location of the source-points might lead to poor results. Several works on this subject have been produced over the years, from the most common simple choice of an external circle, or an expansion of the boundary, to nonlinear least square choices of source-points, see [7] for an account of these works. However these choices face several problems. They usually lead to a very good approximation for regular domains and regular data, but they face difficulties in non smooth cases. In these situations, it is not clear where to add source-points to improve the good results. The usual picture is that we get a good approximation, but we can not go further easily. The MFS is a global approximation that when it fits better some part of the boundary it compromises the approximation in some other part.

In this work, in the next paragraph, we propose a strategy that consists in a mixture of global and local approximation.

2.3 *Glocal* strategy for the choice of source-points

We will use the current word *glocal* to adopt a concept for the choice of source points:

- first we look for source points that produce a fairly good local approximation of the data;
- then, using those source points, we produce a global approximation.

More precisely, we start by choosing the collocation points x_1, \dots, x_n on the boundary Γ .

From these points we produce a partition $\{x_1, \dots, x_{n_1}\}, \dots, \{x_{n_{k+1}}, \dots, x_n\}$. From each subset of this partition we define possible source-points $\{y_1, \dots, y_{m_1}\}, \dots, \{y_{m_{k+1}}, \dots, y_m\}$, such that, for instance:

- the location of the source-points $\{y_1, \dots, y_{m_1}\}$ is the one that produces an approximation $\varphi(x) = a_1 \Phi(x - y_1) + \dots + a_{m_1} \Phi(x - y_{m_1})$, that fits better to the Dirichlet data $\{g(x_1), \dots, g(x_{n_1})\}$.

One practical possibility is to consider a partition with a small number of collocation points in each subset (for instance, 5 or 6 points), and to consider a smaller number of source-points (for instance, 2 or 3). These 2 or 3 source-points are then chosen to better fit the data values of g on the 5 or 6 collocation points. While the collocation points are fixed, the source-points might be taken along the external normal, in such a way that its distance to boundary is defined to be the point of minimum for the residual. See Figure 1.

The counterpart of this procedure is that to find the minimum, the residual must be evaluated by solving a 2×2 or 3×3 linear system. The minimum can be found using a nonlinear minimization scheme, or to avoid constrained minimization techniques, it can also be approximated just by testing with a fixed step along the external normal. The later possibility is usually good enough, since we are not really interested in finding a good local fitting... we are just interested in some local fitting with the goal of obtaining source points suited for the global approximation. This strategy is quite similar to enrichment. In some sense each one of these small sets of source points is particularly adapted to fit some part of the boundary data. In that sense, the whole acts like a new basis function, added to deal with specific local boundary data. On the other hand, they are just source-points that will be used to produce the final global approximation.

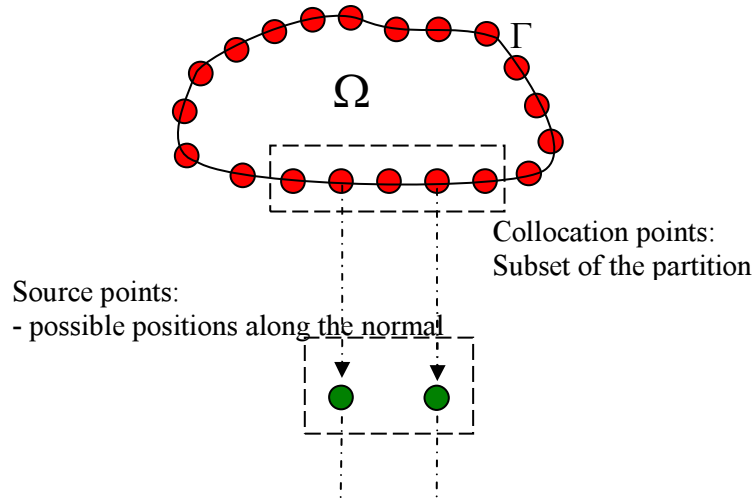


Figure 1: From the collocation points on the boundary Γ (in red) in the *global* construction we define the source points (in green) to be in a position along the external normal direction. This position is defined to be the one that fits better the given data on the boundary.

2.4 Solving the linear system with Tikhonov regularization

In the following, due to the ill posedness of the linear system, we will use Tikhonov regularization. Being \mathbf{S} the $n \times m$ collocation matrix and \mathbf{g} the $n \times 1$ vector defined by $g_i = g(x_i)$, to fit the overdetermined system of equations, when $n > m$, we take a Tikhonov parameter $\alpha > 0$ very small (we will consider $\alpha = 10^{-7}$) and we solve the linear system

$$(\alpha \mathbf{I} + \mathbf{S}^T \mathbf{S}) \mathbf{a} = \mathbf{S}^T \mathbf{g} \quad (3)$$

and the solution vector \mathbf{a} gives the coefficients for the approximation (1) (or (2) when enrichment is considered). Although the solution \mathbf{a} and the coefficients will be highly affected by the choice of the parameter α , the approximation given by the sum in (1) or (2) will be about the same if small α are considered. To confirm the quality of the approximation a higher number of test points $N > n$ is to be considered on Γ . This quality can be then tested with an average absolute or relative error on those points that should not be the same used as collocation points. It should also be noticed that taking $n=m$ and then solving directly $\mathbf{S}\mathbf{a} = \mathbf{g}$ may lead to good results, when the data and the boundary are simple and regular, but this interpolation procedure may also easily lead to highly noisy results due to the ill conditioning.

3 Laplace equation as a model problem

In Figure 2 we consider a non-smooth boundary $\Gamma = \Gamma_1 \cup \Gamma_2$ (in red) defined by the two parts:
 Γ_1 that consists in a segment path with points $\{(0.2,0);(0.4,0.2);(0.2,0.4);(-0.2,0.4);(-0.4,0);(-0.6,0)\}$;
 Γ_2 that it is simply an half ellipse with major axes 0.4 and 0.8, centered in $(-0.2,0)$;
 and (in green) an artificial boundary $\Sigma = B(0,1)$, ie. given by the unit circle centered in the origin.

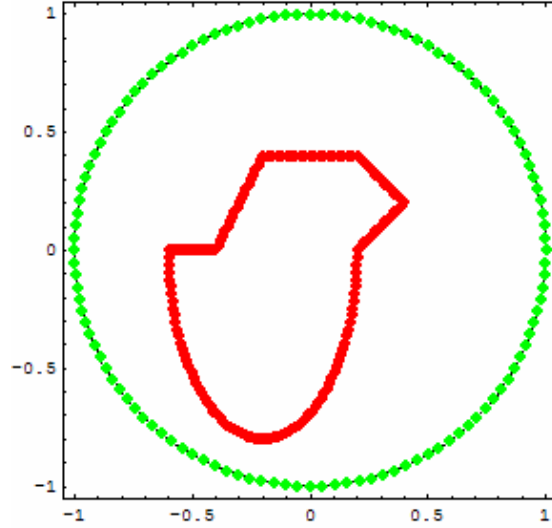


Figure 2: A non-smooth boundary Γ (in red) and the artificial source-points in the boundary Σ (in green);

Being Ω the domain such $\Gamma = \partial \Omega$ the model problem consists in solving the Laplace boundary problem:

$$\Delta u = 0, \quad \text{in } \Omega; \quad (3a)$$

$$u = g, \quad \text{on } \Gamma = \partial \Omega. \quad (3b)$$

We will present some tests using with different data functions g .

3.1 Example with known solution

Source points on a circle. In a first test, let $g(x) = 1 + x_1^2 - x_2^2$. In Figure 3 we plot the function g (in black) and the approximation \hat{u}_A (in red) obtained by the simple MFS using 120 source-points on Σ and 360 collocation points on Γ .

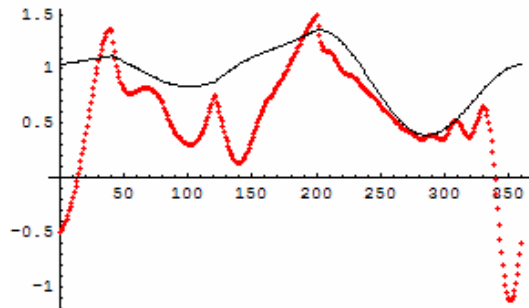


Figure 3: Simple MFS approximation (in red) and the exact data g (in black), along 360 points on Γ . The lack of the constant function leads to an impossible approximation.

Given this data g on the boundary it is clear that the extension of g is also the exact solution in Ω . Therefore the approximation \hat{u}_A can not be good, because the source-points located in the unit circle Σ are at constant distance = 1 from the origin, and therefore $\hat{u}_A(0)=0$ no matter what number of source points are being used on the unit circle. On the other hand the true solution is $u(0)=g(0)=1$.

Recall that the fundamental solution for the 2D Laplacian is $\Phi(x) = \log(|x|)/(2\pi)$.

As it is well known this huge approximation error can be overcome just by adding constants, ie. enriching the approximation with $\psi(x)=1$ as a new basis function. Then, the results dramatically change, and from 100% relative errors we drop to relative errors below 0.0000001% as plotted in Figure 4.

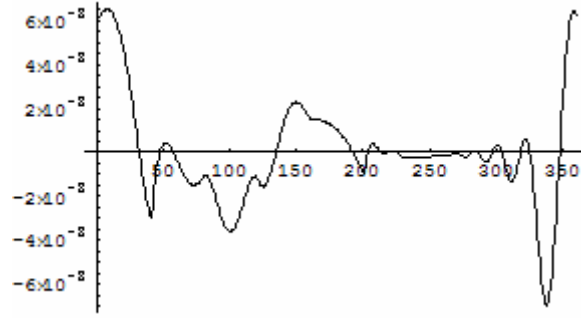


Figure 4: Error of MFS approximation now enriched with $\psi(x)=1$.

This simple example and the theoretical density result suggest that adding a constant function is always necessary to obtain good results. However, we can also see that for a different circle say $\Sigma = B(0, \rho)$ with $\rho \neq 1$ that this problem would not occur, and about the same level of precision can be obtained.

Source points given by a *glocal* construction. It is interesting to see what happens by using the *glocal* construction presented above, without enrichment. Taking again the same 180 collocation points partitioned into subsets of 5 points, and each of them associated to 2 source points, this leads to an approximation with 72 source points distributed as presented in Figure 5.

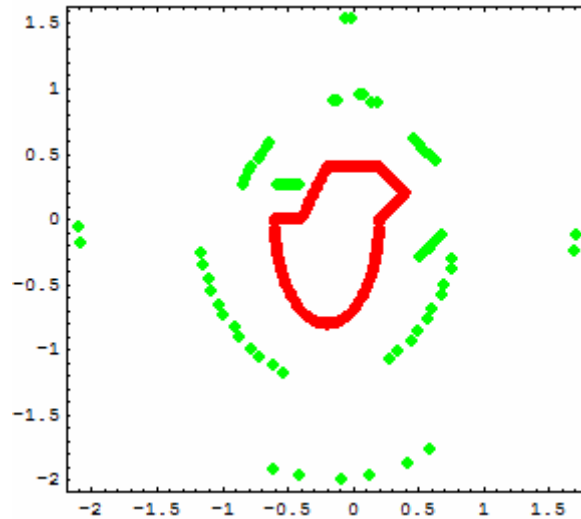


Figure 5: A *glocal* distribution of MFS source points (in green).

For presentation purposes, some upper limitation for the distance of the source points was considered. We can see in Figure 5 that the best local position varies not only with the boundary but also with the data function g . The implementation was not expensive since only 2×2 systems had to be solved. However the

amount of systems to be solved might be high – we considered 70 positions for each of the 36 positions. The number of operations is reasonable when related to the operations needed to solve a whole large system, thus this extra pre-computation can be considered quite acceptable.

3.2 Example with regular data

We consider a different example, $g(x) = 1/4 + x_1 |x|^2$, and now the exact solution is not available – note that although g presents a singularity at $x=0$, inside the domain, the function g is regular on Γ .

We make the same tests for the MFS with 360 collocation points: (i) using the classical circle with 120 source points and adding the constant functions; (ii) using a *glocal* choice also with 120 source points generated from a partition into subsets of 6 points associated to 2 source points. The approximation results for both cases are presented in Figure 6, where the thin black curve stands for the values of g on those 360 points, and the red dots for the approximations obtained in (i) and (ii).

The *glocal* distribution (ii), presented in Figure 7, led to a result 10 times better (average error) than the one obtained with the standard MFS (i). Note that constant functions were not added in (ii), while worst results would be obtained in (i) if constant functions were to be suppressed.

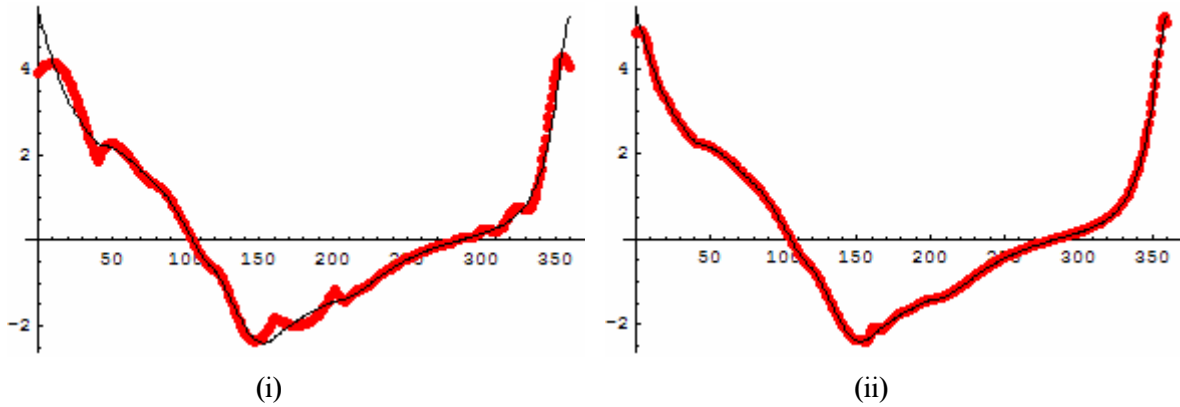


Figure 6: Comparison of the MFS approximations: in (i) with the classical distribution of source points on a circle; in (ii) with a *glocal* distribution, as presented in Figure 7.

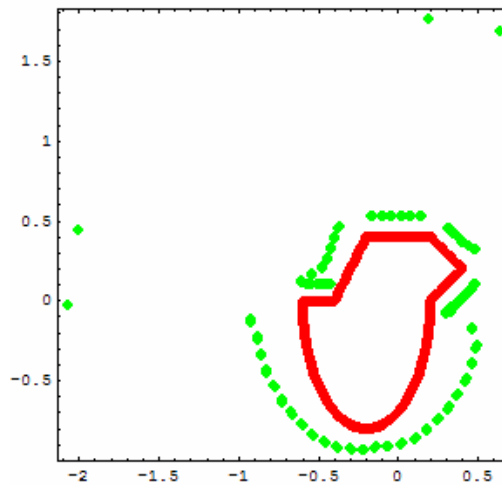


Figure 7: Source points (green) used in (ii) with a *glocal* distribution.

The results presented in the previous example show that a good choice of the source points has a considerable influence, even when the performance of the classical MFS is already acceptable.

3.3 Example with discontinuous data

In the previous examples we considered regular data. We now consider an example with discontinuous data, more precisely $g(x) = -0.4$ if $x_2 = 0.4$, and $g(x) = 1 - x_2$ otherwise.

In this situation to deal with the discontinuity we enrich the basis with an appropriate particular solution, we considered $\psi_2(x) = \arctan((0.2 - x_1)/(x_2 - 0.4^+)) - \arctan((-0.2 - x_1)/(x_2 - 0.4^+))$. This function plotted in Figure 8a) can be seen as a *cracklet* (see [2]) and is not defined for $x_2 = 0.4$, the notation 0.4^+ means that we consider the interior trace, which is a particular solution of the Laplace equation, adapted to the crack segment $[-0.2, 0.2] \times \{0.4\} \subseteq \Gamma_1$ (where the discontinuity occurs, since $x_2 = 0.4$).

In Figure 8a) we plotted the new function ψ_2 in 560 collocation points on Γ and from these collocation points, given the data function g , we obtained the source points (in green) plotted in Figure 8b) for the *glocal* distribution with a partition

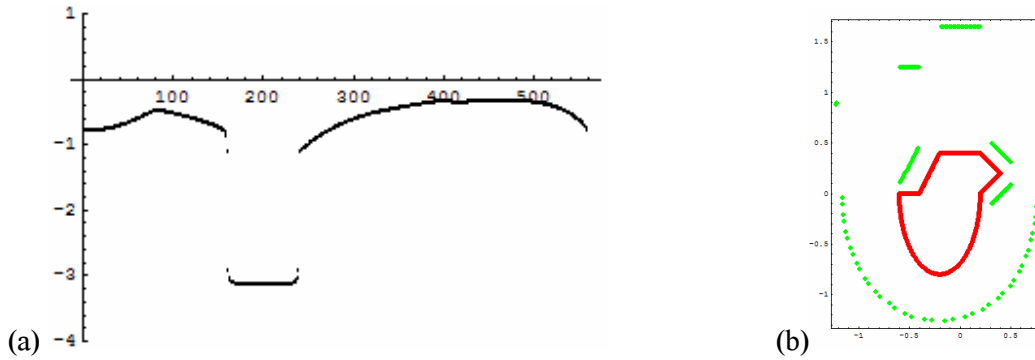


Figure 8: (a) Plot of the enrichment function ψ_2 ; (b) *glocal* distribution of source points.

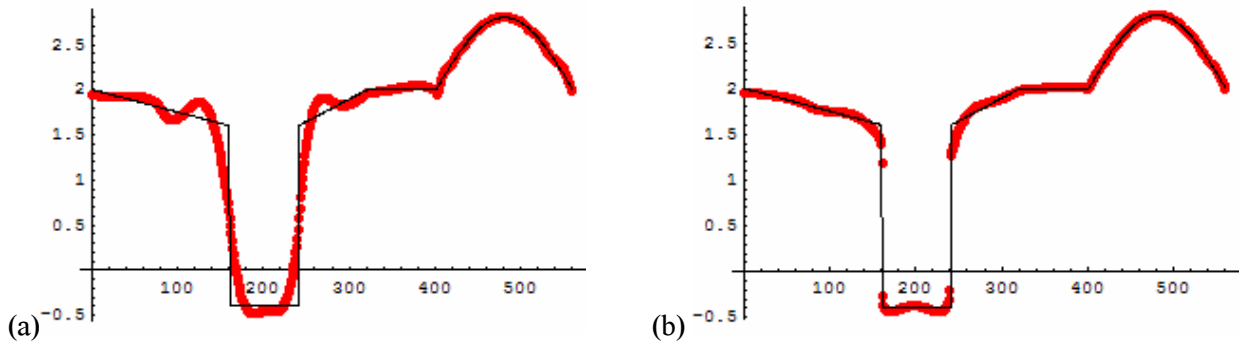


Figure 9: MFS results for the classical distribution: (a) standard; (b) adding ψ_2 to the basis.

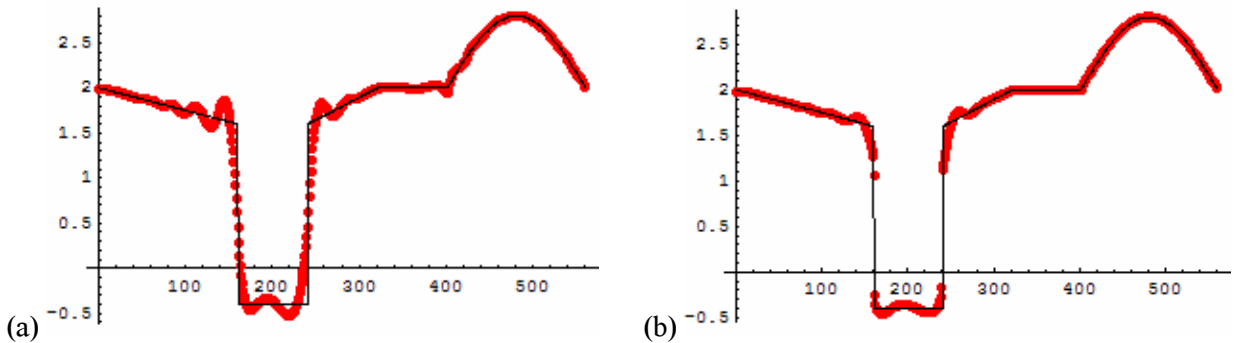


Figure 10: MFS results for a *glocal* distribution: (a) no enrichment; (b) adding ψ_2 to the basis.

In Figures 9 and 10 we present the results for the MFS using a classical source points distribution on the circle and for the *glocal* distribution (respectively). In both cases there were 560 collocation points and 140 source points. In Figure 9 the MFS results for the classical distribution are presented in

- (a) – adding constants, meaning an extra basis function $\psi_1=1$;
- (b) – adding $\psi_1=1$, and the new basis function ψ_2 .

By direct observation we see that adding just one extra appropriate function to the basis led to a considerable improvement of the approximation: in (a) the average relative error was about 8% and in (b) it decreased to about 2%.

The same situation can be seen in Figure 10 for the *glocal* distribution. Note that, unlike the previous case, the constant function $\psi_1=1$ was not added. The approximation in Figure 10a) with an average error about 4% is better than the one obtained in Figure 9a), but it is clear that adding the appropriate function ψ_2 allowed to decrease further this error, and Figure 10b) gives a better approximation, similar to Figure 9b).

Therefore, we conclude that although the *glocal* distribution gives better results than the classical one, this results are mainly improved by adding an appropriate new function to the basis. In this case a simulation just by source points is not able to follow the abrupt slope in the data, and a phenomena like the Gibbs effect tends to occur. Therefore in these situations an enrichment by appropriate particular solutions is needed. In this example we just considered a single one, but this enrichment can lead to even better results by using more similar particular solutions. In the next paragraph we briefly address this question.

3.4 Enrichment with particular solutions adapted to corners or cracks

As presented in [4] an enrichment of the MFS approximation can be made using particular solutions adapted to cracks. This is of course also true with domains that present other type of non regular geometry, like domains with corners.

In the Laplace case, writing the 2D Laplace operator in (r, θ) polar coordinates, $\Delta = \partial_r^2 + r^{-1} \partial_r + r^{-2} \partial_\theta^2$, and by separation of variables we get for $u(x) = v(r) w(\theta)$, the following possibilities for particular solutions:

$$v(r) = r^\mu, w(\theta) = \alpha \cos(\mu \theta) + \beta \sin(\mu \theta) \quad (5)$$

with coefficients α, β, μ are to be determined. Demanding that $u=0$ when $\theta=0$ and when $\theta=\Theta$, which corresponds to a corner defined by these angles, then we obtain first $\alpha=0$ and second $\sin(\mu \Theta) = 0$.

This means $\mu \Theta = k \pi$ for integer k , and this gives $\mu = k \pi / \Theta$.

Thus, particular solutions adapted to a corner are of the form $u(r, \theta) = r^{k \pi / \Theta} \sin(k \theta \pi / \Theta)$.

In the case of cracks, we may then consider $\Theta=2\pi$ and $u(r, \theta) = r^{k/2} \sin(k \theta / 2)$ verifies the null Dirichlet condition on the crack.

3.5 Example with an exterior corner solution

If the previous results obtained for Laplace problems are quite acceptable for the classical MFS distribution of sources points (plus adding constants), we now consider an example where this is not so. We consider a particular solution generated by an artificial corner outside the domain. More precisely, following the previous notations, we considered a function g produced by a corner with $\Theta = 3\pi/2$ with $k=-1$. The function $g(r, \theta) = r^{-2} \sin(-2\theta)$ is singular, but with polar coordinates centered in the exterior point $(-0.2, 0.5)$ the singularities are exterior and it is a particular solution in the whole domain Ω .

A simple inspection of the graph of g (see Figure 11a or 12a) shows that, beside a high slope on the boundary points near to $(-0.2, 0.4)$, this function is analytic through the boundary, and therefore no problems could be anticipated, unless we knew.

In Figures 11 and 12 we plot the results obtained by the application of the classical setting for the MFS (Figure 11) and by using the same *glocal* distribution as used in paragraph 3.3 (Figure 12). For this different data g the *glocal* distribution calculated the source points plotted in Figure 13.

In Figures 11a) and 12a) we see that the boundary approximation (in red) using the *glocal* distribution clearly follows the data (with an average error about 0.2%) while the classical approximation failed to follow the data properly. In Figures 11b) and 12b) we plotted the relative error on an inner circle centered in the origin with radius 0.15. The classical MFS presented relative errors up to 25%, while the proposed *glocal* distribution gave excellent results, smaller than 0.04%. This was done without any enrichment, in both cases.

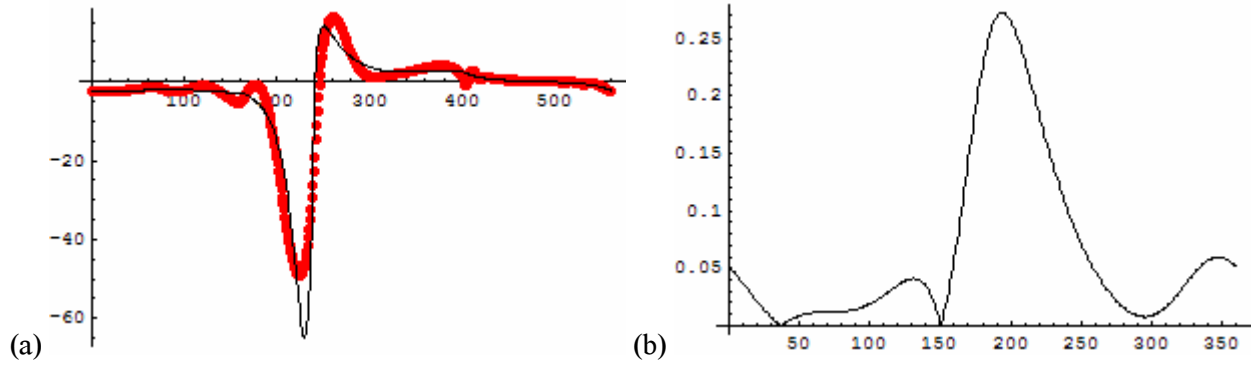


Figure 11: MFS results - classical distribution: (a) on the boundary; (b) relative error on an interior circle.

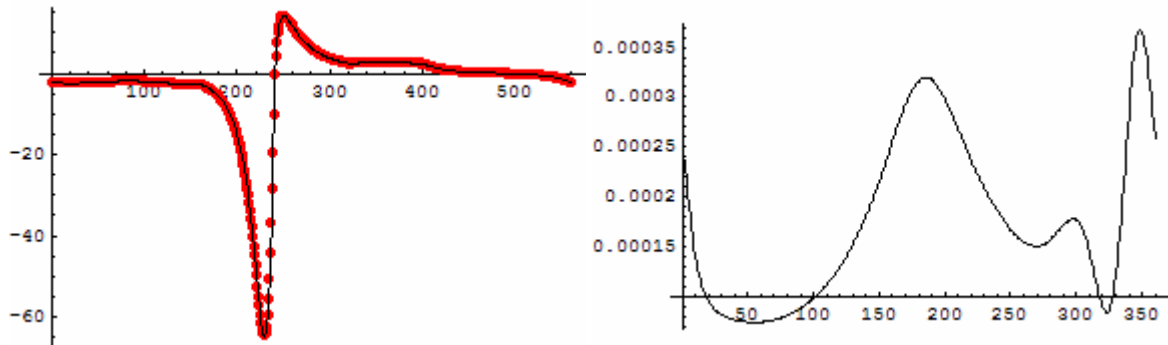


Figure 12: MFS results - *glocal* distribution: (a) on the boundary; (b) relative error on an interior circle.

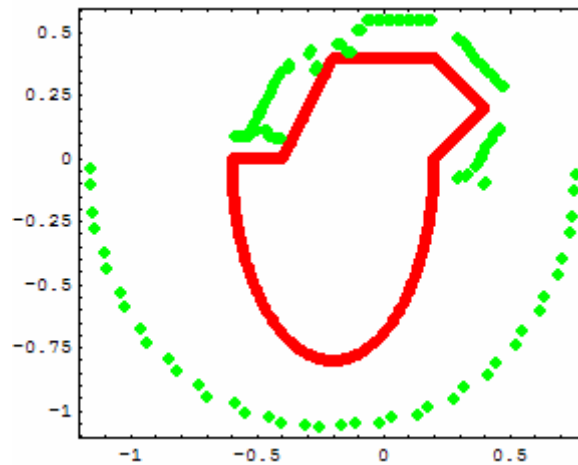


Figure 13: Source points (in green) for the *glocal* distribution cited in Figure 12.

4 Conclusions, current and future work

In this work we presented a method to choose the source points in the MFS, called *glocal*, that gives an automatic procedure to choose the source points, adapted to the geometry of the boundary and to the particularities of the boundary function to be fitted. This method proved to be better while compared to classical choices, such as the classical choice of an external circle, when approximation difficulties occur with regular boundary data. For small systems and simple regular data this choice is usually not needed, and it requires a small pre-computation. When the data is not regular, this *glocal* technique might not be sufficient and enrichment with known particular solutions should be considered, keeping the Trefftz meshless feature of the MFS.

It should be noticed that in some cases, it is not clear what type of enrichment should be considered, and in those cases, adding basis functions just by adding, will increase the ill conditioning without giving a real improvement for the approximation. In these situations it may also be considered a pre-computation with other known methods (BEM, or even FEM or FDM). These methods allow to obtain an approximation of particular solutions that fit locally some irregular part of the boundary geometry or of the boundary data. These calculated approximations can then be used for an enrichment of the basis, together with the MFS or with other Trefftz method.

The techniques here presented for the Laplace equation have been already applied to other PDEs, namely the Helmholtz equation. In those preliminary tests the improvement of the results with a *glocal* choice revealed to be even a better option, in particular while facing geometrical difficulties. An extension of this *glocal* method to other PDEs, even vectorial, is straightforward, since it does not depend on the fundamental solution. Some minor restriction should be considered for some geometry of the domains, since highly non-convex domains will present not only lower but also small upper bounds for the location along the normal direction. A similar restriction happens for multiply connected domains, because the source points must be inscribed inside the inner cavities. Although the *glocal* concept here introduced is easily understood, the particular way to implement it – for instance using a discrete number of positions along the normal direction – is just one of the many possibilities.

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