Improved calculation of higher order partial derivatives in the DRM

B. Natalini\textsuperscript{1} & V. Popov\textsuperscript{2}
\textsuperscript{1}Facultad de Ingeniería, Universidad Nacional del Nordeste, Argentina
\textsuperscript{2}Wessex Institute of Technology, UK

Abstract

A new way of representing partial derivatives (PDs) in the DRM is proposed. This formulation can be implemented only for corner nodes where two boundary elements join under angle different from \(\pi\). The new formulation reduces the order of the PDs of the DRM approximation function by one in respect to the order of the approximated PDs. In this way the introduction of the singularities at the nodes due to differentiation of the DRM approximation function can be avoided. A number of non-linear case studies are shown where different DRM approximations are used for first and second order partial derivatives using four different radial basis functions and four different formulations for partial derivatives. In all cases where second order derivatives were involved the new formulation was the only one that performed satisfactorily.

1 Introduction

Dual Reciprocity Method (DRM) is considered to be one of the most effective techniques to transform domain integrals appearing in BEM formulations into boundary integrals. Introduced by Nardini & Brebbia [1] in the early 80’s, the number of applications of the DRM in the BEM literature grew steadily during the last decade. Partridge \textit{et al.} [2] compiled the early development of the method up to 1990. This book, which mainly uses \(1 + r\) as DRM approximation function, describes the computational implementation of the method in a variety of cases. Later, Golberg and Chen [3], among others introduced the theory of the radial basis functions (RBFs) in the DRM, of which \(1 + r\) is a particular case, in the context of the DRM, providing in this way a solid mathematical foundation for the procedure.
DRM approximates a particular solution of the PDE by means of a RBF in order to apply the Method of Particular Solutions (MPS). This makes the accuracy of the DRM strongly dependent on the function used in the approximation. A variety of functions can be used as an interpolation function. Early work [2] has shown good performances in a variety of cases with simple expansions, like for example $1 + r$. In the classical approach, the partial derivatives are approximated by means of partial derivatives of the interpolation function used. Zhu and Zhang [4] have shown that when performing partial derivatives of the $1 + r$ interpolation function the procedure introduces singularities, as a result of which large numerical errors are produced. Zhu and Zhang and Chen [5] avoided these artificially created singularities by constructing a transformation, which leads to improved numerical results. Natalini and Popov [6] proposed an alternative way to represent PDs (the new formulation) as a function of the normal derivatives in corner nodes, where two boundary elements join under angle different from $\pi$. Therefore this formulation can be applied for problems with large number of subdomains as a result of the problem requirements or where a large number of subdomains are used as a way of implementing the DRM, i.e. Dual Reciprocity Method – Multy Domain (DRM-MD) [7], [8]. It can also be used for single domain meshes where the boundaries are not smooth and there are a large number of boundary elements that join under an angle different from $\pi$. When $1 + r$ is used, it has been shown that the new formulation improves the accuracy of the first PDs by at least one order of magnitude in respect to the classical DRM representation of PDs.

Something analogous happens in 2D problems when second order partial derivatives are represented using the DRM approximation and the augmented thin plate splines (ATPS) [9]. The second order derivative of the 2D-ATPS is singular at $r = 0$, which leads again to singularities in the classical way of representing second order partial derivatives.

2 The radial basis functions used in this work

Let us consider the non-homogeneous Laplace equation defined in the domain $\Omega$ which is enclosed by the contour $\Gamma$

$$
\nabla^2 u(x) = b(x, u(x), \frac{\partial u(x)}{\partial x_i}, \frac{\partial^2 u(x)}{\partial x_i \partial x_j})
$$

(1)

where $u(x)$ is a scalar field (potential function), $b(x)$ is the non-homogeneous term and $x$ is a position vector in the domain with components $x_i$.

In this work three different radial basis functions are tested in the DRM approximation (for more details on the DRM see Partridge et al. [2]). The first one is thin plate splines (ATPS). This function is a linear combination of thin plate splines and linear functions, which for 2D problems are two-dimensional analogues of one-dimensional cubic splines. Using ATPS, $b(y)$ can be expanded as
where
\[ P(y) = ax_1 + bx_2 + c \] (3)
and \( \alpha_k \) are unknown coefficients.

Hardy [10] introduced another class of RBF, the multi quadric (MQ)
\[ f(r) = \left( r^2 + c^2 \right)^{1/2} \] (4)
where \( c \) is a free parameter referred to as a shape parameter. Franke [11], in a Landmark study, tested 29 methods for fitting two-dimensional data. Hardy’s MQ performed the best followed by the thin plate splines. An important constraint to using MQ in practical applications is that the shape parameter \( c \) needs to be chosen conveniently, and how to do this is still matter of research.

The third one is \( 1 + r^3 \) but only for representing the second order PDs, following the idea of Partridge et al. [2]

### 3 Treatment of partial derivatives in the DRM

An algorithm is established to express partial derivatives in the vector \( b \) in (3) as functions of either \( u \) or the normal derivatives \( g \).

In the classical approach the starting point is to express the potential at a point \( x \) in terms of the approximation function \( f \), in a similar way as it was done for \( b \) in (2)
\[ u(x) \equiv \sum_{k=1}^{J+1} f(x, z_k) \beta \] (5)
or expressed in matrix form
\[ u = F \beta \] (6)
where \( \beta \) are unknown coefficients and \( \beta \neq \alpha \).

Differentiation of equation (6) produces
\[ \frac{\partial u}{\partial x_i} = \frac{\partial F}{\partial x_i} \beta \] (7)
After re-writing (6) as \( \beta = F^{-1} u \), equation (7) becomes
\[ \frac{\partial u}{\partial x_i} = \frac{\partial F}{\partial x_i} F^{-1} u \] (8)
Second order partial derivatives can be expressed in two ways. The first one is obtained by differentiating twice (6)
\[ \frac{\partial^2 u}{\partial x_i \partial x_j} = \frac{\partial^2 F}{\partial x_i \partial x_j} F^{-1} u \] (9)
The second one uses the DRM approximation for representing the first order partial derivatives, as was previously used for representing \( b \) in (2) and \( u \) in (6)
Differentiating (10)
\[ \frac{\partial^2 u}{\partial x_i \partial x_j} = \frac{\partial F}{\partial x_i} \frac{\partial u}{\partial x_j} \] (11)
and replacing \( \gamma \) from (10) yields
\[ \frac{\partial^2 u}{\partial x_i \partial x_j} = \frac{\partial F}{\partial x_i} F^{-1} \frac{\partial u}{\partial x_j} \] (12)
Finally, expressing \( \frac{\partial u}{\partial x_i} \) through (8) produces the final expression
\[ \frac{\partial^2 u}{\partial x_i \partial x_j} = \frac{\partial F}{\partial x_i} F^{-1} \left( \frac{\partial F}{\partial x_j} F^{-1} u \right) \] (13)
As the diagonal elements of the \( \frac{\partial^2 F}{\partial x_i \partial x_i} \) matrix are undefined when \( f \) is ATPS in 2D, (9) introduces singularities. The DRM-MD offers the option of expressing the partial derivatives through the normal derivatives \( q \). To introduce this algorithm let us consider a corner node on the boundary of a subdomain as shown in Figure 1.

![Figure 1: A corner node on the boundary.](image)

In a single subdomain, at every corner node there will be three variables, some of which can be given as the boundary condition: the potential \( u \), the normal derivative before the node \( q^b \), and the normal derivative after the node \( q^a \). The normal derivatives can be represented as a scalar product of the gradient \( \nabla u_i \) and the outward unitary vector normal to the boundary
\[ q^b_i = \nabla u_i \cdot n^b_i \] (14)
and
\[ q^a_i = \nabla u_i \cdot n^a_i \] (15)
Eqns (16) and (17) can be re-written as
These two equations form a linear system that yields

\[
\frac{\partial u_i}{\partial x_{1i}} = u_{i,1}(q^b_i, q^a_i) = \left(q^b_i n^a_1 i - q^a_i n^b_2 i\right) J_i \tag{18}
\]

and

\[
\frac{\partial u_i}{\partial x_{2i}} = u_{i,2}(q^b_i, q^a_i) = \left(q^a_i n^b_1 i - q^b_i n^a_1 i\right) J_i \tag{19}
\]

where

\[
J_i = n^b_1 i n^b_2 i - n^a_1 i n^a_2 i \tag{20}
\]

In order to produce the second order partial derivatives, a similar scheme to (12) is applied in (18) and (19) yielding

\[
\frac{\partial^2 u}{\partial x_i \partial x_j} = \frac{\partial F}{\partial x_i} F^{-1}\begin{pmatrix} u_{i,j}(q) \end{pmatrix}, \quad (j = 1, 2) \tag{21}
\]

The formulations given by (18), (19) and (21) reduces the order of the PDs of the approximation function by one, in respect to the formulation given by (8) and (9). This algorithm can be implemented in the corner nodes only and therefore for the DRM nodes, which are located in the interior of the domain, the classical approach must be applied. This scheme can be applied to 3D problems in a similar way. It is evident that this approach offers substantial benefits when the proportion of corner nodes is high, typically, in the DRM-MD meshes.

4 Numerical examples

In order to test the representation of the second order PDs using the new scheme, the non-linear advection-diffusion equation is considered. A set of 6 DRM-MD codes to solve 2-D advection-diffusion problems of a compressible fluid in porous media were compared. These codes solve the equation

\[
D \nabla^2 u + K \nabla \cdot (u \nabla u) + p = 0 \tag{22}
\]

Where \(D\) is the coefficient of diffusion, \(p\) represents the source or the sink term and \(K\) represents the permeability of the porous media.

Before introducing the features of the codes let us expand the second term in (22)

\[
D \nabla^2 u + K (\nabla u) \cdot \nabla u + Ku \nabla^2 u + p = 0 \tag{23}
\]

The governing equation can be re-written in terms of the Laplacian operator in two different ways

\[
\nabla^2 u = \frac{1}{D + Ku} \left\{ -K (\nabla u) \cdot \nabla u - p \right\} \tag{24}
\]

or
In order to apply the DRM to these equations, an iterative procedure, which requires an a priori known value of $u$, in notation $\tilde{u}$, is used. Therefore the DRM can be applied on the following equations

$$\nabla^2 u = \frac{1}{D} \left\{ K(\nabla u) \cdot \nabla u - Ku\nabla^2 u - p \right\}$$ (25)

Equation (27) gives opportunity to test the accuracy of the second order PDs when represented using the new scheme.

The features of the codes used are shown below:

**Code A:** solves (26) using the formulation (8) for representing the first order PDs and ATPS as interpolation function.

**Code B:** solves (27) using the formulation (8) for representing the first order PDs and the formulation (21) for representing the second order PDs and ATPS as interpolation function.

**Code C:** solves (27) using the formulation (8) for representing the first order PDs, the formulation (13) for representing the second order PDs and ATPS as interpolation function.

**Code D:** solves (27) using the formulation (8) for representing the first order PDs, the formulation (9) for representing the second order PDs and ATPS as interpolation function.

**Code E:** solves (27) using the formulation (8) for representing the first order PDs, the formulation (9) for representing the second order PDs and MQ as interpolation function.

**Code F:** solves (27) using the formulation (8) for representing the first order PDs and the formulation (9) for representing the second order PDs. Two different interpolation functions are used: $1+R^3$ for representing the second order PDs, following the idea of Partridge et al. [2], and ATPS for the remaining part.

These codes were applied to a 1-D multi-layer problems with boundary conditions $q(x=0) = (\partial u/\partial n)_{x=0} = 0$ and $u(x=L) = U_L$. The analytical solution of this problem is given in [12]. The domain was a rectangle of length $L = 12$ in the $x$ direction and width $W = 6$ in the $y$ direction. In order to produce equivalent 1-D results from the 2-D codes, the following boundary conditions were used

$$q(0,y) = 0 \text{ and } u(L,y) = U_L$$
$$q(x,W/2) = q(x,-W/2) = 0$$

(28)

The initial value of the vector $\tilde{u}$ was set equal to zero for those nodes were the potential was not defined as boundary condition. All the examples used a mesh of $6 \times 12$ subregions (6 subdivisions in the $y$ direction and 12 subdivisions in the $x$ direction) without interior DRM nodes. The subdomains were rectangular and linear elements were used within each subdomain. The domain considered had three layers of different properties except for the Case 4 that had two layers. Details of the four cases analysed are shown in Table 1. The relative errors for
the potentials and normal derivatives for the Cases 1 to 4 are presented in Figures 2 to 5, respectively. The results show the improvement of formulation (21) in respect to both, formulation (9) and formulation (13) as a way of representing second order partial derivatives. Code A did not deal with the second order PDs as they were incorporated in the Laplacian on the left-hand-side of (26). Therefore, Code B was the only one that included a DRM representation of the second order PDs and converged in all four cases. Codes A and B produce errors of the same order of magnitude indicating that the new DRM representation of the second order PDs did not produce errors of higher order of magnitude than the rest of the code.

Table 1: Description of the properties of the media and fluid used in the four cases studied.

<table>
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<tr>
<th>Layer 1</th>
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<th>Case2</th>
<th>Case3</th>
<th>Case4</th>
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<td>100</td>
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<tr>
<td>$p$</td>
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<td>0.5</td>
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</tr>
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</table>

It was expected that Code D, which uses formulation (9) and ATPS, would perform poorly because the second order derivative of the 2D-ATPS is singular at $r = 0$. However, even for codes E and F, which use MQ and $1+R^2$ respectively and consequently are not affected by singularities, the performance was not satisfactory considering the lack of convergence in cases 2 and 3 for code E and in all cases for code F.

5 Conclusions

A new way of representing second order partial derivatives (PDs) in the DRM is proposed. This formulation can be implemented only for corner nodes where two boundary elements join under angle different from $\pi$. Therefore this formulation can be applied for problems with large number of subdomains as a result of the problem requirements or where a large number of subdomains are used as a way of implementing the DRM, i.e. DRM-MD. It can also be used for single domain meshes where the boundaries are not smooth and there are a large number of boundary elements that join under an angle different from $\pi$. It is expected that the accuracy of the approach would deteriorate as the angle approaches $\pi$.  

Figure 2: Error distribution for the: (a) potential and (b) normal derivative for the Case 1. Code F did not converge. Errors for the normal derivative for codes C and D were 14% and 260%, respectively.

Figure 3: Error distribution for the: (a) potential and (b) normal derivative for the Case 2. Codes C, D, E and F did not converge.
Figure 4: Error distribution for the: (a) potential and (b) normal derivative for the Case 3. Codes C, D, E and F did not converge.

Figure 5: Error distribution for the: (a) potential and (b) normal derivative for the Case 4. Codes C, D and F did not converge.
The new formulation reduces the order of the PDs of the DRM approximation function by one in respect to the order of the original PDs that are approximated. In this way the introduction of singularities at the nodes due to the PDs of the DRM approximation function can be avoided.

A number of non-linear 2D case studies are shown where different DRM approximations are used for first and second order partial derivatives using four different radial basis functions. In all cases where second order derivatives were involved the new formulation was the only one that performed satisfactorily.

References


