Performance of spatial derivatives using interpolation with radial basis functions

Desempenho de derivados espaciais utilizando interpolação com funções de base radial

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Carlos Friedrich Loeffler
PhD. in Mechanical Engineering Post-Graduate Program from the Universidade Federal do Espírito Santo (UFES) - Campus Goiabeiras, Vitória
Institution: Universidade Federal do Espírito Santo (UFES) - Campus Goiabeiras, Vitória
Address: Av. Fernando Ferrari, 514, Goiabeiras, Vitória - ES, CEP: 29075-910
E-mail: loefflercarlos@gmail.com

Luciano de Oliveira Castro Lara
PhD. in Mechanical Engineering Post-Graduate Program from the Universidade Federal do Espírito Santo (UFES) - Campus Goiabeiras, Vitória
Institution: Universidade Federal do Espírito Santo (UFES) - Campus Goiabeiras, Vitória
Address: Av. Fernando Ferrari, 514, Goiabeiras, Vitória - ES, CEP: 29075-910
E-mail: castrolara@hotmail.com

Fernando Ramos Ourique
Master in Mechanical Engineering Post-Graduate Program from the Universidade Federal do Espírito Santo (UFES) - Campus Goiabeiras, Vitória
Institution: Universidade Federal do Espírito Santo (UFES) - Campus Goiabeiras, Vitória
Address: Av. Fernando Ferrari, 514, Goiabeiras, Vitória - ES, CEP: 29075-910
E-mail: fernando.orique@gmail.com

ABSTRACT
Initially applied in the context of the Boundary Element Method as an auxiliary tool, interpolating the domain core and allowing its transformation into boundary integrals, the radial basis functions have expanded their field of application. They are currently widely used as a solution technique for partial differential equations, generating the meshless formulations of the Finite Element Method. These functions also have recently become an important numerical resource as a more straightforward solver for spatial derivatives calculation. Of course, precision is lost compared to the performance as a direct interpolation tool. Still, even so, it can be advantageous because of the complexity of procedures related to the analytical derivation of primary variables and other more classical techniques. This work evaluates a series of characteristics of the derivation procedure, such as the
influence of the dimensions of the problem on the results. In this work, the initial results for the research are performed through the cubic radial function, following the guidelines of the previous works. This function has no arbitrary parameter in its structures, which is a great advantage.

**Keywords:** boundary element method, radial basis functions, interpolation techniques.

**RESUMO**
Inicialmente aplicadas no contexto do Método do Elemento de Limite como uma ferramenta auxiliar, interpolando o núcleo do domínio e permitindo sua transformação em integrais de limites, as funções de base radial expandiram seu campo de aplicação. Eles são atualmente amplamente utilizados como uma técnica de solução para equações diferenciais parciais, gerando as formulações sem malhas do Método dos Elementos Finitos. Estas funções também se tornaram recentemente um recurso numérico importante como um solucionador mais direto para o cálculo de derivadas espaciais. É claro que a precisão é perdida em comparação com o desempenho como uma ferramenta de interpolação direta. Ainda assim, ainda assim, pode ser vantajoso por causa da complexidade de procedimentos relacionados à derivação analítica de variáveis primárias e outras técnicas mais clássicas. Esse trabalho avalia uma série de características do procedimento de derivação, como a influência das dimensões do problema nos resultados. Neste trabalho, os resultados iniciais para a pesquisa são realizados através da função radial cúbica, seguindo as diretrizes dos trabalhos anteriores. Essa função não tem nenhum parâmetro arbitrário em suas estruturas, o que é uma grande vantagem.

**Palavras-chave:** método do elemento de limite, funções de base radial, técnicas de interpolação.

**1 INTRODUCTION**

In engineering, the limitations of analytical solutions for solving problems are well known. Such restrictions cause an enormous advantage for the approximate methods, which bring solutions with agility, high precision, and generality. Thus, more and more approximate methods are used, especially for solving two-dimensional and three-dimensional complex problems.

It is known that physical problems are mainly represented by differential, ordinary or partial equations. There are cases governed by algebraic equations; however, they are much simpler and less numerous. However, the solution of the models given by differential equations is done numerically, in an approximate way, by converting them into algebraic equations. This is done through the discretization process [1], which it can be understood as the transformation of differential
mathematical models into algebraic mathematical models. In this context, the following methods can be mentioned: the Boundary Element Method (BEM), the Finite Element Method (FEM), the Finite Difference Method (FDM), and the Finite Volume Method (FVM) [1, 2].

However, within these are a group of problems or even steps in their solution, which require approximations related to the interpolation and extrapolation of data and the description of derivatives. In this context, the first and most classic solution methodologies involve polynomial approximation.

Despite its elegance and precision, classical polynomial interpolation has mathematical restrictions when applied in two dimensions. Not all of them can be listed here. Still, it should be noted. First, the fundamental theorem of algebra that guarantees the factorization of polynomials in one dimension does not apply in two or more dimensions; that is, most of the polynomials are irreducible in the real field [3]. Second, the powers of $x$ or $y$ do not necessarily constitute a sequence of linearly independent polynomials. Thus, polynomials in two variables cannot reconstruct unique functions based on sample values taken from arbitrary positions [3].

On the other hand, the interpolations using radial basis functions are very attractive due to their generality, use of positive real numbers, matrix symmetry, and ease of implementation, among other advantages.

2 INTERPOLATION USING RADIAL BASIS FUNCTIONS

In engineering and applied science, it is usually desired to know solutions from sample data defined by observation or experimental procedures. This is done in a certain number of circumscribed regions to determine, with satisfactory precision, the behavior in the full extension of a domain. In a practical application, in most cases, there is no condition to reconstruct an exact solution. A soil analysis kilometers away deep, for example, only provides test results valid locally.

The process of finding intermediate values in this domain based on sample data is called interpolation. In this case, the approximate function built from the sample data must reproduce precisely the solution obtained at the points used for its construction, commonly called base points.

For example, according to Chapra and Canale [4], Newton's polynomial method is one of the most popular interpolation methods, making it a great
example of an approximate method; however, according to the same authors, specific numerical methods converge faster than others, thus requiring refined initial information or more complex programming than methods with slower convergence. Therefore, there is a constant search for more precise, agile, and less computational methods.

Problems in which a valid approximation is required, based on sparse data, but which needs to be implemented involving two or more variables in two- or three-dimensional domains, are increasingly common. In these cases, there are great operational difficulties and imperative mathematical restrictions to the classical methods. The generalization of one-dimensional procedures may, therefore, not be feasible. The numerical procedure based on the concept of finite difference has been the most commonly used resource in these cases, with a significant advantage over global polynomial approximations; however, treating irregular domains and certain boundary conditions can make the procedure equally prohibitive in these cases. The main alternative in these cases, and which is treated in this study, is the use of using radial basis functions for interpolation, which reproduces unknown functions from known data. For the development of the methodology for interpolation, one must have known data in N dimensions, found in ξ locations that belong to Rₙ. In short, we have F (ξ) ∈ R.

The authorship of the first proposition of using radial functions as an interpolation tool is unclear. Buhmann [5] highlights the works of Cheney [6], Davis [7], Duchon [8], and Powell [9]. On the other hand, authors widely cited in the study of radial functions, such as Wendland [10] and Fasshauer [11], already approach such functions as a tool to numerically discretize and solve partial differential equations. In this sense, the literature is unanimous in recognizing the work of Kansa [12], published in 1990, who developed the first numerical method based on radial basis functions for solving differential equations. It’s called Kansa’s method and was used to solve Poisson’s elliptic equation and the linear diffusion-advection equation.

Returning to the issue of using radial basis functions (RBF) as an approximation tool, it is worth noting that it is possible to use the same idea of radial functions to perform regressions or adjustments. According to Epperson [3], an important field of study in approximation problems is the fitting of curves given
experimental data. It is assumed that the data obtained experimentally have errors and, therefore, must be adjusted. Curve fitting consists of a family of mathematical techniques that seek to find behavior patterns in a data set. The objective is to study the physical phenomenon in the form of a trend where, according to Seiffert, Chiquetti, and Avila [13], among the curve fitting and regression categories, there is the interpolation category, when you have sparse data with good precision and reliability, which corroborates the use of radial basis functions also for this application, however, this text deals only with the interpolation procedure.

3 DEFINITION AND PROPERTIES OF RADIAL BASIS FUNCTIONS

According to Fasshauer [11], a given function $F: \mathbb{R}^S \rightarrow \mathbb{R}$ is named radial since there is a linear transformation, comprised of a unique argument $F: [0, \infty) \rightarrow \mathbb{R}$ such that:

$$F(X; \xi) = F(r) \quad \text{onde}, \quad r = \|X\| \quad (1)$$

Thus, as explained above, the value of $F$ is constant for any point that is at the same fixed distance from the origin. So $F$ is radially symmetric about the center. An extensive set of radial basis functions has been used, among which the most common examples are:

<table>
<thead>
<tr>
<th>RBF's</th>
<th>$F(X)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thin Plate</td>
<td>$r^2 \ln(r)$</td>
</tr>
<tr>
<td>Multiquadric</td>
<td>$(r^2 + c^2)^k$</td>
</tr>
<tr>
<td>Gaussian</td>
<td>$e^{r^2}$</td>
</tr>
<tr>
<td>Cubic Radial</td>
<td>$r^3$</td>
</tr>
</tbody>
</table>

It is considered as a definition of the approximation by radial basis functions to the sequence:

$$(x) \approx \sum_{\xi=1}^{n} \alpha^{\xi}F^{\xi}(r) \quad (2)$$

Therefore, using indexical notation, where the dummy indices add up, one has:
\( (x) \approx \alpha_i F_i(\xi; X) \) \hspace{1cm} (3)

The approximation by radial functions is a sequence; thus, each of the radial functions with the same base point but different field points generates linearly independent equations, forming a basis in the functional space in a finite space. \( N \) is the maximum number of known points, \( r \) is the Euclidean distance between \( X \) and \( \xi \), \( F_i(\xi; r) \) are the radial basis interpolating functions and \( \alpha_i \) are unknown influence coefficients, which are determined by imposing:

\[
S(X_i) = f(x_i), i = 1, 2, 3 ... N
\] \hspace{1cm} (4)

It appears that the combination of equations results in a system of linear equations that would be properly presented in its matrix form, such as:

\[
\begin{pmatrix}
\text{s}(x_1) \\
\vdots \\
\text{s}(x_N)
\end{pmatrix}
= 
\begin{pmatrix}
F(\xi_1) & \cdots & F(\xi_N; x_N) \\
\vdots & \ddots & \vdots \\
F(\xi_N; x_1) & \cdots & F(\xi_N; x_N)
\end{pmatrix}
\begin{pmatrix}
\alpha_1 \\
\vdots \\
\alpha_N
\end{pmatrix}
\] \hspace{1cm} (5)

In summary, the above equation becomes:

\[
F\alpha = s
\] \hspace{1cm} (6)

In Eq. (6), \( F \) is a square symmetric matrix, called the interpolation matrix, and \( \alpha \) and \( s \) are column matrices.

It is considered that the solution will exist and be unique if and only if the interpolation matrix is non-singular, that is if its determinant is different from zero. It is known that for a matrix to have this characteristic, function \( F_i(\xi; X) \) must be defined as positive, which contributes to the use of radial basis functions, as there are several functions defined as positive.

4 COMPACT RADIAL BASIS FUNCTIONS

With the growing desire to obtain a solution with less error and a reduction in computational cost, classical numerical methods such as the FEM continue developing. Especially in three-dimensional problems, the FEM suffers from problems of high computational cost if mesh restructuring techniques (adaptive
methods) need to be employed because the finite elements are connected through compatibility between nodes. Any change in densifying the mesh or redefining it implies a significant computational effort. In this sense, proposing techniques in which the concept of connectivity was abolished began to occupy a vast research effort. Radial compact support functions were necessarily employed to eliminate interconnectivity between numerous discretization points. Thus, domains of influence are delimited, where only a reduced set of nodes interact with each other, as shown in Figure 1.

![Figure 1: Scheme for compact radial basis functions.](image)

Compact support radial functions differ from the previously mentioned ones because from a particular value of the radius, the function is zero. The objective of these functions is to make that not all the base points interact with the field points, generating sparse matrices with a better conditioning level. Thus, they meet the proposal to eliminate connectivity and form a banding in typical FEM matrices.

It is well known that from the already mentioned work by Kansa [12], compact support radial basis functions can be efficiently used to solve partial differential equations, which is done according to FEM standards in so-called meshless formulations. However, in this study, although compact radial support functions can be used for the purposes of this study, only full support functions are used. Furthermore, it should also be noted that its use is not directed to the solution of partial differential equations but to approximating spatial derivatives of the field of variables.

5 CALCULUS OF DERIVATIVES USING RADIAL BASIS FUNCTIONS

It is worth noting that RBFs were pioneered in engineering with the work of Nardini and Brebbia [14] to solve domain integrals related to the inertial force in elastodynamic problems. The method used was called Dual Reciprocity and was
developed for several scalar field problems by Loeffler and Mansur [15, 16]. These authors defined the importance of interpolating internal points, additional resources such as subregions, and the adequate treatment of body forces, which had not yet been studied in the literature. Later, in 1991, the book by Partridge et al. [17] was released, complementing the research begun in 1990 [18] where is making a synthesis on Dual Reciprocity and extending its application to diffusive-advective problems, which highlights the use of radial functions to describe spatial derivatives. The aforementioned book also presents several classes of radial functions, initially explored in Loeffler's doctoral thesis [19] but which had not yet been widely tested. Two articles by Patridge [20, 21] extensively explore the behavior of the various classes of radial functions in the Boundary Element Method.

In the mentioned applications, dealing with the Boundary Element Method and in certain situations using the Finite Element Method, the use of RBF is made as an auxiliary resource. In both methods, it is strategic to calculate spatial derivatives through the derivative of approximations generated with radial basis functions. Naturally, there is a loss of precision related to interpolation in these cases; even so, its use may be advantageous due to the complexity of specific procedures related to the analytical derivation of the model's primal variables.

In the case of the Boundary Element Method, diffusive-advective problems modeled by the Dual Reciprocity formulation need to be properly complemented with the approximate calculation of the spatial derivatives through an interpolation procedure with radial functions. In other cases, the calculation of spatial derivatives on the boundary through the hypersingular formulation of the BEM demands continuity of shape functions in the connection of elements, which is quite laborious. Using derivatives through radial functions is also an interesting tactic in this case. The determination of products at the centroid of finite volumes can also be done by radial basis functions, as undertaken by Queiroz et al. [22]. Recently, a study related to Electromagnetism solved by the Finite Element Method used this tactic to represent derivatives [23].

Having already considered the discretization of the domain and with \( u(X) \) being the vector of the primal variables, one has:
\[ \mathbf{u}(X) = \mathbf{F}(X^j; X) \alpha \] (7)

Thus:

\[ \mathbf{u}_i(X) = \mathbf{F}_i(X^j; X) \alpha \] (8)

Considering that:

\[ \alpha = \mathbf{F}^{-1} \mathbf{u} \] (9)

Substituing the value of \( \alpha \) in Eq. (9), one has:

\[ \mathbf{u}_i(X) = \mathbf{F}_i(X^j; X) \mathbf{F}^{-1} \mathbf{u} \] (10)

There is a loss of precision in this procedure. However, it is necessary to evaluate it correctly, testing a series of problems, and different functions and examining the influence of the dimensions of the problem in the results. Many functions have an arbitrary parameter in their structure, like the Gaussian function. In this work, the initial results for dues are obtained through the cubic radial function, following the guidelines of Massaro’s work [24]:

\[ F(X; \xi) = r^3 \] (11)

5 EXAMPLES
5.1 METHODOLOGY

Despite the importance of the presented technique with the BEM, the procedure can be applied with any numerical method. Thus, in the examples shown here, any scalar field is established, and the derivatives are calculated using the typical definition:

\[ u_i(X) = \frac{\partial u}{\partial x_i} \] (12)

Normal derivatives and tangential derivatives on the boundary also be
calculated, that is:

\[ u_n(X) = \frac{\partial u}{\partial x_i} \frac{\partial x_i}{\partial n} \]  

\[ u_t(X) = \frac{\partial u}{\partial x_i} \frac{\partial x_i}{\partial t} \]  

As can be seen from Figure 2 there is an important local relationship between \( s \) and \( q \):

![Figure 2: Normal and tangential vectors on the boundary.](image)

Whereas:

\[ q = \frac{\partial u}{\partial x_1} \frac{\partial x_1}{\partial s} + \frac{\partial u}{\partial x_2} \frac{\partial x_2}{\partial s} = u_{x_1}s_1 + u_{x_2}s_2 = u_t s_i \]  

It can be written that, at each point on the boundary, one has:

\[
\begin{bmatrix}
\frac{\partial u}{\partial x_1} \\
\frac{\partial u}{\partial x_2}
\end{bmatrix}
= \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}
\begin{bmatrix}
\frac{\partial u}{\partial r} \\
\frac{\partial u}{\partial n}
\end{bmatrix}
\]  

The local transformation matrix \( R \) is orthogonal, so: \( R^T = R^{-1} \), like this:

\[
\begin{bmatrix}
\frac{\partial u}{\partial n} \\
\frac{\partial u}{\partial r}
\end{bmatrix}
= \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix}
\begin{bmatrix}
\frac{\partial u}{\partial x_1} \\
\frac{\partial u}{\partial x_2}
\end{bmatrix}
\]  

Then:
\[ u_m = [Tm][F_{x_1} u_1 + F_{x_2} u_2]F^{-1}u = Nu \]  
\[ u_s = [F_{x_1} s_1 + F_{x_2} s_2]F^{-1}u = Su \]  

A computational program was elaborated, using the FORTRAN programming language, considering the previously presented mathematical formulation for the two-dimensional cases, in order to meet the objective of the study in question. Therefore, the developed algorithm assists in the reading of two-dimensional data prescribed for the construction of an approximate function and knowledge of the alpha coefficients. In addition, it enables the knowledge of the derivatives, calculated from the approximate function found.

In the two examples solved here, a square domain of unitary sides is solved, where 36, 84, 164 and 320 interpolating points (base points) were imposed on the boundary and 49, 81, 255 and 576 internal points to carry out future comparisons of results mesh comparisons. Figure 3 shows a schematic discretization of the domain. Equidistant base points within the domain are proposed for comparative tests with the analytical functions and with the result of approximate functions using the cubic radial function.

Figure 3: Schematic arrangement of boundary and internal interpolation points.

Graphs shown hereinafter were prepared for the visual interpretation of the data obtained, comparing the information from the derivatives of the analytical functions and those obtained from the derivatives of the radial function. The average percentage error is given on the ordinate of each graph, calculated in poles located on the boundary or then internally. On the abscissa axis is the number of interpolation points located on the boundary. Color lines identify the boundary mesh with a given number of the internal interpolation points. It is evident
that the number of internal interpolation points is fundamental to achieve more accurate results.

5.2 FIRST EXAMPLE

In this first example the following two-dimensional function was chosen:

\[ f(x; y) = e^{x/x_0} + e^{y/y_0} \]  \hspace{1cm} (20)

Concerning equation (20), \( x_0 \) is the maximum distance in \( x \) and \( y_0 \) is the maximum distance in \( y \). Boundary results for tangential and normal derivatives using cubic radial basis function are given in figures 4 and 5.

Figure 4: Tangential derivatives calculated on the boundary.

Figure 5: Normal derivatives calculated on the boundary.
It must be highlighted the convergence of the method for both values of derivatives calculated on the boundary. It is noticed that there are no disturbances in the graph of the percentage error and the number of functional nodes, reinforcing the relative robustness of the proposed model. Although the error values are not insignificant, it is noted that they tend to be minimal values as the number of the interpolation nodes increases on the boundary and as well internally. Thus, through mesh refinement, it is possible to improve the accuracy of the analysis and satisfactorily approach the analytical result.

However, the normal derivative values are much less accurate, as expected, because of the difficulty of predicting the function's behavior internally. In contrast, tangential derivative values are meaningfully more accurate, since they depend mainly on the adjacent lateral interpolation points.

Analyses of derivatives are also carried out in the X1 and X2 directions at the internal poles. Due to the diagonal symmetry, the results of X1 and X2 are equal and both are shown in figure 8. The error levels, surprisingly, were much lower than those obtained on the boundary. A likely reason for this is the lower density of points around the boundary poles, while the inner points are surrounded by other points. Calculated values at the innermost interpolation points have better accuracy.

Figure 6: Errors in derivatives for directions X1 or X2, calculated internally.

The following analysis focuses on the ability of the radial basis functions to calculate the spatial derivatives without being affected by the domain dimension. Thus, to identify whether the domain size affects the convergence and quality of
the results, the square edges are magnified ten times. It should be noted that the function values are dimensionless; it should be noted that if this were not done, the radial functions would have to deal simultaneously with small and large values, due to the exponential behavior. This imposes an enormous loss of numerical precision.

These new large dimensions did not change the results, which are not shown for sake of space. Thus, the same weightings carried out for the unit side domain also apply in this new configuration, reinforcing the robustness and adequacy of the cubic function in the use in the calculation of derivatives. However, if a rectangular domain is taken (as shown in figure 7), the major proximity of two edges changes the results. These new error curves for tangential and normal derivatives are presented in figures 8 and 9.

Figure 7: Schematic arrangement of boundary and internal interpolation points in a rectangular domain.

Figure 8: Errors in derivatives in tangential direction on the boundary for a rectangular domain.
Again, the tangential derivative was highlighted, presenting an error of around 0.1%. The normal derivatives just have acceptable results, approximately 1.9%. However, its results are better than those obtained with the test considering the 1x1 grid. This may be explained since the horizontal boundaries are now closer, facilitating the interpolation of internal values from boundary points.

Regarding internal results, values for X1 and X2 directions are now different, as shown by Figures 10 and 11. Internal errors are lesser than previously presented boundary errors. In general, as can be verified, errors in the rectangular domain are inferior that the square domain.
5.3 SECOND EXAMPLE

In this second example, a trigonometric two-dimensional function was chosen:

\[ f(x; y) = \sin(mx) \cdot \sen(my) \]  

(21)

The parameter m has the purpose of verifying the behavior of the method as the argument of the trigonometric function is varied, which acts similarly to an excitation frequency, increasing the accentuation of the curve.

Initially, the figures 12 and 13 present the error curves for tangential and normal derivatives to m=1.
Figure 13: Errors in normal derivatives on the boundary.

The tangential derivative again presented an excellent performance compared to the other results, one of the method's highlights. It did not require many interpolation points for a satisfactory result; in addition, considering the denser analyzed mesh, the error was 0.009%. Although less accurate, in this case, the normal derivative, converged very well, obtaining errors smaller than 0.02%.

Errors inside follow the pattern of the previous example and will not be displayed. The interest in this example turns to the expansion of the control parameter $m$, which imposes a more accentuated behavior of the sinusoidal function. This directly impacts the method's accuracy, as seen in the following curves.

Now, $m=\pi$ is assumed, and the errors are calculated for the normal and tangential derivatives only, shown in figures 14 and 15.
For the tangential derivative, it can be seen that the errors continue to reduce with the refinement of the meshes, but the precision is lower. Denser meshes are needed for the error to reach the levels reached with $m=1$. A different behavior occurs with normal derivatives, whose errors stabilize without converging to the analytical value. The error is small for finer meshes but is not close to zero. The same pattern occurs with the directional derivatives on the inside but with smaller errors than the values obtained for the normal derivative on the boundary.

Figures 16 and 17 are the last graphics, where are shown the errors for the tangential and normal derivatives on the boundary with parameter $m=3\pi$. Now, just the tangential derivative error values decline significantly with mesh density. The behavior of the normal derivative on the boundary is similar to the previous
one, but the errors are greater. The same pattern was observed in the directional derivatives in the interior, with slightly smaller errors, but the quality was just reasonable.

Figure 16: Errors in tangential derivatives on the boundary.

![Tangential errors in boundary interpolation points](image)

Figure 17: Errors in normal derivatives on the boundary.

![Normal errors in boundary interpolation points](image)

Results for larger values of the m parameter will not be shown here, but the error values in calculating the normal derivative on the boundary and directional derivatives on the interior become very large, even for finer meshes, which makes their application inadequate in these cases. Only the tangential derivative shows an acceptable level of errors.
7 CONCLUSIONS

This research aimed to evaluate the ability of radial functions to calculate directional derivatives. Other radial functions were tested previously, but the cubic radial function performed the best. Although it is within the scope of this research to expand the examination of other radial functions and the solution of other scalar fields, it can already be concluded that the performance of the cubic radial function is entirely satisfactory. Considering the examples examined, there was convergence in the accuracy of the results. However, the error is not insignificant in some instances, depending on the complexity of the function's derivative to be approximated. However, in many cases of interest, this error reduces depending on the number of functional nodes and internal points used in each approximation process of the imposed scalar field.

It was also noted that the directional derivatives calculated at the internal nodes presented a superior approximation to the directional derivatives calculated on the boundary due to the lower density of points around them. The results of the normal derivative on the boundary were just passable. This is justified because its value depends very little on adjacent values on the boundary and strongly on the density of internal values.

However, the most important conclusion refers to the high precision of the results obtained for the tangential derivative. This calculation proved to be the most effective, as opposed to the calculation of the normal derivative, which was barely tolerable. This fact is the most important since it is possible to use radial basis functions in the interpolation to calculate this type of derivative, which is essential in several practical applications. Unfortunately, such a derivative could only be calculated with good precision using the hyper singular formulation of the Boundary Element Method, which is much more complicated since it imposes the analytical derivation of fundamental solutions and special treatment for high-order singularities.

These satisfactory preliminary results indicate that the research must be deepened, aiming to calculate derivatives of more intricate functions and perform three-dimensional analysis, which can be helpful in several applications besides the Boundary Elements Method.
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